It is with great pleasure that we welcome you to the 64th Electronic Materials Conference (EMC 2022) at The Ohio State University. We expect this Conference to follow in EMC’s long tradition of offering premier research on the preparation, characterization and use of electronic materials. Below, we have outlined highlights we believe will be of interest to you.

Conference Chair
Lisa Porter
Carnegie Mellon University

Program Chair
Daniel Wasserman
The University of Texas at Austin

CONFERENCE HIGHLIGHTS

The 64th EMC Program
Features over 300 oral/poster presentations and 36 technical sessions focused on Electronic Materials Science and Technology; Energy Storage and Conversion Materials; Nanoscale Science and Technology; Organic Materials, Thin Films and Devices; Oxide Semiconductors and Dielectrics; and Wide Bandgap Semiconductors.

EMC Awards Ceremony & Plenary Session
The 64th EMC kicks off Wednesday morning with the Awards Ceremony & Plenary Session. First, the 2021 Best Student Presentation Award winners and the 2021 NIST Uncertainty Analysis Student Award winner will be announced and honored. The Plenary Lecture follows, where Susan Trolier-McKinstry of The Pennsylvania State University will give her presentation, New Materials for Three-Dimensional Ferroelectric Microelectronics.

Welcome Reception/Poster Session
Join us for a Welcome Reception on Wednesday evening from 6:00 pm – 8:00 pm in the Performance Hall located in the Ohio Union. During this time, poster authors will be available for in-depth discussions at the Poster Session, also located in the Performance Hall in the Ohio Union. Both of these events are great for meeting with longtime colleagues, making new connections and sharing information. Light snacks and refreshments will be served.

Exhibit
Be sure to visit the EMC exhibitors Wednesday and Thursday in the Performance Hall located on the first floor of the Ohio Union. Learn more about the latest products and services in the rapidly evolving world of electronic materials. See page 18 for exhibit hours.

Conference Dinner Reception
Don’t miss this year’s Conference Dinner Reception, Thursday evening from 6:00 pm – 8:30 pm, in the Archie M. Griffin East Ballroom of the Ohio Union. Full Conference registration includes one Dinner Reception ticket. You can purchase additional Dinner Reception tickets at the EMC Registration Desk for $90 per person, subject to availability.

Save the Date
The 65th Electronic Materials Conference (EMC 2023) will be June 28 – 30, 2023, at the University of California, Santa Barbara. Mark your calendar today!

EMC is being coordinated with the Device Research Conference (DRC 2022), held at the Ohio Union from June 26 – 29. Badges will be accepted for admittance to both Conferences on Wednesday, June 26.

DRC attendees who wish to attend EMC sessions must sign the EMC Code of Conduct prior to admittance.

EMC respectfully requests that attendees wear masks while in the technical session rooms.

The 64th EMC has been managed by

SPECIAL THANKS!

CONFERENCE SUPPORT

ACS APPLIED ELECTRONIC MATERIALS
https://pubs.acs.org/journal/aaembp

NSF www.nsf.gov

THE OHIO STATE UNIVERSITY
INSTITUTE FOR MATERIALS RESEARCH
www.imr.osu.edu

UMC UNITED MINERAL & CHEMICAL CORP.
www.umccorp.com

TMS FOUNDATION
www.tms.org/foundation

NIST www.nist.gov

TABLE OF CONTENTS

Committees..................................................2
Maps............................................................4
EMC Awards Ceremony & Plenary Session....5
Daily Schedule of Events..............................6
Travel Resources..........................................6
Program At-A-Glance.................................7
Poster Session...........................................10
Exhibit......................................................18
Wednesday Oral Presentations..................20
Poster Presentations.................................59
Thursday Oral Presentations......................77
Friday Oral Presentations............................122
EMC Index..................................................144

WELCOME TO THE CONFERENCE!
COMMITTEES

Executive Committee

Chair
Lisa Porter
Carnegie Mellon University

Vice-Chair
Daniel Wasserman
University of Texas at Austin

Secretary
Adrienne Stiff-Roberts
Duke University

Treasurer
William Wong
University of Waterloo

ELECTRONIC MATERIALS
SCIENCE AND TECHNOLOGY

Contacts to Semiconductor Epilayers, Nanostructures, and Organic Films
Leonard Brillson, The Ohio State University
Shadi Dayeh, University of California, San Diego
Suzanne Mohney, The Pennsylvania State University
Lisa Porter, Carnegie Mellon University
Tae-Yeon Seong, Korea University
Jerry Woodall, University of California, Davis

Epitaxial Materials and Devices
Seth Bank, The University of Texas at Austin
Kurt Eyring, Air Force Research Laboratory
Archie Holmes, The University of Texas at Austin
Siriram Krishnamoorthy, University of California, Santa Barbara
Charles Lutz, Lumeneum Operations LLC
Nadeemullah Mahdik, U.S. Naval Research Laboratory
Kyle McNicholas, Lincoln Laboratory, Massachusetts Institute of Technology

Siddharth Rajan, The Ohio State University
Shadi Shadepour-Sandvik, State University of New York Polytechnic Institute
Stephanie Tomaso, U.S. Naval Research Laboratory
Christine Wang, Lincoln Laboratory, Massachusetts Institute of Technology
Dan Wasserman, The University of Texas at Austin
Kun-Man Yu, City University of Hong Kong

Hetero-Integration, Interconnects and Packaging
Guohai Chen, National Institute of Advanced Industrial Science and Technology
Mona Ebrish, U.S. Naval Research Laboratory
Daniel Ewing, Department of Energy’s Kansas City National Security Campus
Michael Hamilton, Auburn University
Jamie Phillips, University of Delaware

Materials Discovery
Anderson Janotti, University of Delaware
Siriram Krishnamoorthy, University of California, Santa Barbara
Patrick Shea, Northrop Grumman Corporation
Angel Yanguas-Gil, Argonne National Laboratory

Materials Processing and Integration
Daniel Ewing, Department of Energy’s Kansas City National Security Campus
Mark Goorsky, University of California, Los Angeles
Doug Hall, University of Notre Dame
Karl Hobart, U.S. Naval Research Laboratory
Becky (R.L.) Peterson, University of Michigan
Nate Quitoriano, McGill University
Steve Ringel, The Ohio State University
Patrick Shea, Northrop Grumman Corporation
Jerry Woodall, University of California, Davis

Metamaterials and Materials for THz, Plasmonics and Polaritons
Joshua Coldwell, Vanderbilt University
Kurt Eyring, Air Force Research Laboratory
Rachel Goldman, University of Michigan
Anthony Hoffman, University of Notre Dame
Stephanie Law, University of Delaware
Thomas Searles, University of Illinois at Chicago
Berardi Sensale Rodriguez, The University of Utah
Jason Valentine, Vanderbilt University
Daniel Wasserman, The University of Texas at Austin
Huili Grace Xing, Cornell University

Micro-LEDs and -Displays—Materials, Fabrication and Characterization
Steven DenBaars, University of California, Santa Barbara
Zetian Mi, University of Michigan
Tae-Yeon Seong, Korea University
Jerry Woodall, University of California, Davis

Nanofabrication and Processing
Bruno Azeredo, Arizona State University
Kris Bertness, National Institute of Standards and Technology
Mona Ebrish, U.S. Naval Research Laboratory
Muinho Kim, Nanyang Technological University, Singapore
Xiuling Li, The University of Texas at Austin
Parisa Mohseni, Rochester Institute of Technology
Angel Yanguas-Gil, Argonne National Laboratory

Nanomagnetic, Magnetic Memory and Spintronic Materials
Hemant Dixit, Wolfspeed
Michael Flatté, The University of Iowa
Cheng Gong, University of Maryland
Jean Anne Incorvia, The University of Texas at Austin
Roland Kawakami, The Ohio State University
Xinyu Liu, University of Notre Dame
Pawan Tyagi, University of the District of Columbia
Angel Yanguas-Gil, Argonne National Laboratory

Solar Bandgap Materials and Devices
Ganesh Balakrishnan, The University of New Mexico
Suprem Das, Kansas State University
Shanti Iyer, North Carolina Agricultural and Technical State University
Sanjay Krishna, The Ohio State University
André Lenert, University of Michigan
Kris Bertness, National Institute of Standards and Technology

Point Defects, Doping and Extended Defects
Andrew Armstrong, Sandia National Laboratories
Ramon Collazo, North Carolina State University
Rachel Goldman, University of Michigan
Lincoln Lauhon, Northwestern University
Kunal Mukherjee, Stanford University
Steve Ringel, The Ohio State University
Shadi Shadepour-Sandvik, State University of New York Polytechnic Institute
Jun Suda, Kyoto University and Nagoya University
Christian Wetzel, Rensselaer Polytechnic Institute
Jerry Woodall, University of California, Davis

Quantum, Strongly Correlated and Topological Materials
Matthew Doty, University of Delaware
Rachel Goldman, University of Michigan
Anthony Hoffman, University of Notre Dame
Stephanie Law, University of Delaware
Connie Li, U.S. Naval Research Laboratory
Jeremy Robinson, U.S. Naval Research Laboratory
Thomas Searles, University of Illinois at Chicago
Chakrapani Varanasi, U.S. Army Research Office—Materials Science Division

ENERGY STORAGE AND CONVERSION MATERIALS

Electrochemical Energy Storage and Conversion
Susan Fullerton, University of Pittsburgh
David Gundlach, National Institute of Standards and Technology
Jung-Hyun Kim, The Ohio State University
Zetian Mi, University of Michigan
Edward Yu, The University of Texas at Austin

Energy Harvesting
Alan Doolittle, Georgia Institute of Technology
Deidra Hodges, Florida International University
Ken Jones, U.S. Army Research Laboratory
Suzanne Mohney, The Pennsylvania State University
Jamie Phillips, University of Delaware
Shadi Shadepour-Sandvik, State University of New York Polytechnic Institute

Solar Cell Materials and Devices
Geoffrey Bradshaw, Air Force Research Laboratory
Rachel Goldman, University of Michigan
Mark Goorsky, University of California, Los Angeles
André Lenert, University of Michigan
Steve Ringel, The Ohio State University
Oleg Rubel, McMaster University
Jae-Hyun Ryu, University of Houston
Mike Scarpulla, The University of Utah
Christian Wetzel, Rensselaer Polytechnic Institute
Mark Wistey, Texas State University
Jerry Woodall, University of California, Davis

Thermoelectrics and Thermal Transport
Kris Bertness, National Institute of Standards and Technology
Samuel Graham, Georgia Institute of Technology
Ferdinand Poudeau, University of Michigan
Xiaojia Wang, University of Minnesota
Yaguo Wang, The University of Texas at Austin
Joshua Zide, University of Delaware
The Ohio Union at The Ohio State University

First Floor
- Registration ......................................................... Great Hall Foyer
- Exhibit ................................................................. Performance Hall
- Welcome Reception ................................................ Performance Hall
- Posters ................................................................. Performance Hall
- Refreshment Breaks ................................................. Performance Hall
- Technical Session .................................................. U.S. Bank Conference Theater
- Technical Session .................................................. Great Hall Meeting Room 1 & 2
- Technical Session .................................................. Great Hall Meeting Room 3

Second Floor
- EMC Awards Ceremony & Plenary Session ................ Archie M. Griffin Ballroom
- Technical Session ................................................... Archie M. Griffin West Ballroom
- Conference Dinner Reception ................................ Archie M. Griffin East Ballroom
- Technical Session .................................................. Ohio Staters Inc. Traditions Room
- Technical Session .................................................. Ohio Staters Inc. Founders Room
- Technical Session ................................................... Senate Chamber

Third Floor
- Technical Session ................................................... Cartoon Room 1
- Technical Session .................................................. Rosa M. Allabouni Room
Susan Trolier-McKinstry
The Pennsylvania State University

New Materials for Three Dimensional Ferroelectric Microelectronics

Susan Trolier-McKinstry is an Evan Pugh University Professor and Steward S. Flaschen Professor of Ceramic Science and Engineering and professor of electrical engineering. Her main research interests include thin films for dielectric and piezoelectric applications. She directs both the Center for Dielectrics and Piezoelectrics and the Center for Three-Dimensional Ferroelectric Microelectronics. She is a member of the National Academy of Engineering, a fellow of the American Ceramic Society, IEEE and the Materials Research Society, and an academician of the World Academy of Ceramics. She currently serves as an associate editor for Applied Physics Letters. She was 2017 President of the Materials Research Society; previously she served as president of the IEEE Ultrasonics, Ferroelectrics and Frequency Control Society, as well as Keramos.
**DAILY SCHEDULE OF EVENTS**

**TUESDAY**

**Registration** 3:00 pm – 5:00 pm  First Floor, Great Hall Foyer

**WEDNESDAY**

**Registration** 7:30 am – 5:00 pm  First Floor, Great Hall Foyer

EMC Awards Ceremony and Plenary Session 8:20 am – 9:20 am  Second Floor, Archie M. Griffin West Ballroom

Exhibit 9:00 am – 12:30 pm  First Floor, Performance Hall

BREAK 9:20 am – 10:00 am  First Floor, Performance Hall

Poster Set-up 9:30 am – 3:00 pm  First Floor, Performance Hall

A: Group III-Nitrides—Power Diodes 10:00 am – 12:00 pm  First Floor, Great Hall Meeting Room 3

B: Silicon Carbide—Devices and Reliability 10:00 am – 12:00 pm  Second Floor, Archie M. Griffin West Ballroom

C: Wearable Electronics and Biosensors 10:00 am – 12:00 pm  Second Floor, Ohio Staters Inc. Founders Room

D: Gallium Oxide Devices 10:00 am – 12:00 pm  Second Floor, Ohio Staters Inc. Traditions Room

E: Dielectrics and Multifunctional Oxides 10:00 am – 12:00 pm  Second Floor, Senate Chamber

F: Point Defects, Doping and Extended Defects 10:00 am – 12:30 pm  Third Floor, Rosa M. Allabroom Room

DRC Session 11: Heterogeneous Integration 10:00 am – 12:30 pm  First Floor, U.S. Bank Conference Theater

Lunch 12:00 pm – 1:30 pm  (Not provided by Conference)

DRC Session 12: Wide Bandgap III – III-N HEMTs 1:20 pm – 3:00 pm  First Floor, U.S. Bank Conference Theater

G: 2D Material Devices and Sensors 1:30 pm – 5:10 pm  First Floor, Great Hall Meeting Room 1 & 2

H: Group III-Nitrides—Power Diodes and HEMTs 1:50 pm – 5:10 pm  First Floor, Great Hall Meeting Room 3

I: Silicon Carbide Materials and Characterization 1:30 pm – 3:10 pm  Second Floor, Archie M. Griffin West Ballroom

K: Metasurfaces and Structured Photonics 1:30 pm – 2:50 pm  Second Floor, Ohio Staters Inc. Founders Room

L: Gallium Oxide Growth 1:30 pm – 5:10 pm  Second Floor, Ohio Staters Inc. Traditions Room

M: Solar Cell Materials and Devices 1:30 pm – 4:30 pm  Second Floor, Senate Chamber

Exhibit 1:30 pm – 4:30 pm  First Floor, Performance Hall

BREAK 1:30 pm – 3:30 pm  First Floor, Performance Hall

Poster Viewing 3:30 pm – 5:10 pm  First Floor, Performance Hall

J: Nanoscale Characterization 3:30 pm – 5:10 pm  Second Floor, Archie M. Griffin West Ballroom

Exhibit 6:00 pm – 8:00 pm  First Floor, Performance Hall

Welcome Reception/Poster Session 6:00 pm – 8:00 pm  First Floor, Performance Hall

**THURSDAY**

**Registration** 8:00 am – 5:00 pm  First Floor, Great Hall Foyer

N: 2D Materials Growth and Surfaces 8:20 am – 11:40 am  First Floor, Great Hall Meeting Room 1 & 2

O: Group III-Nitrides—MOCVD Growth 8:20 am – 12:00 pm  First Floor, Great Hall Meeting Room 3

P: Quantum, Strongly Correlated and Topological Materials 8:20 am – 12:00 pm  First Floor, U.S. Bank Conference Theater

Q: Oxide Semiconductor Devices, Defects and Transport 8:20 am – 11:40 am  Second Floor, Ohio Staters Inc. Traditions Room

R: Detectors and Narrow Bandgap Materials 8:20 am – 12:00 pm  Second Floor, Senate Chamber

S: Emerging Epitaxial Materials 8:20 am – 10:00 am  Third Floor, Cartoon Room 1

Exhibit 9:00 am – 12:30 pm  First Floor, Performance Hall

BREAK 10:00 am – 10:20 am  First Floor, Performance Hall

BREAK 10:00 am – 12:00 am  First Floor, Performance Hall

T: Epitaxial Growth of Highly Mismatched Alloys 10:20 am – 12:00 pm  Third Floor, Cartoon Room 1

Lunch 12:00 pm – 1:30 pm  (Not provided by Conference)

U: Nano-Magnetic, Magnetic Memory and Spintronic Materials 1:30 pm – 5:10 pm  First Floor, Great Hall Meeting Room 1 & 2

V: Group III-Nitrides—Light Emitting Diodes 1:30 pm – 2:50 pm  First Floor, Great Hall Meeting Room 3

X: Low-Dimensional Materials and Nanofabrication 1:30 pm – 4:50 pm  First Floor, U.S. Bank Conference Theater

Y: Materials Processing and Integration 1:30 pm – 3:10 pm  Second Floor, Ohio Staters Inc. Traditions Room

AA: Plasma- and Surface Phonon Polaritons 1:30 pm – 5:10 pm  Second Floor, Senate Chamber

BB: Electrochemical Energy Storage and Conversion 1:30 pm – 5:30 pm  Third Floor, Cartoon Room 1

BREAK 3:10 pm – 3:30 pm  First Floor, Performance Hall

Exhibit 3:30 pm – 4:00 pm  First Floor, Performance Hall

Poster Viewing 3:30 pm – 3:30 pm  First Floor, Performance Hall

Poster Tear-down Deadline 5:30 pm  First Floor, Performance Hall

Conference Dinner Reception 6:00 pm – 8:30 pm  Second Floor, Archib M. Griffin East Ballroom

**FRIDAY**

**Registration** 8:00 am – 12:00 pm  First Floor, Great Hall Foyer

CC: Neuromorphic + Late News 8:20 am – 12:00 pm  First Floor, Great Hall Meeting Room 1 & 2

DD: Group III-Nitrides—Contacts and HEMTs 8:20 am – 11:20 am  First Floor, Great Hall Meeting Room 3

EE: Flexible, Printed and Organic Electronic Materials and Devices 8:20 am – 12:00 pm  First Floor, U.S. Bank Conference Theater

FF: Gallium Oxide—Material Processing, Characterization and Defects 8:20 am – 12:00 pm  Second Floor, Ohio Staters Inc. Traditions Room

GG: Epitaxial Growth on Patterned Substrates 8:20 am – 10:00 am  Third Floor, Cartoon Room 1

BREAK 10:00 am – 10:20 am  First Floor, Performance Hall

HT: Lattice Mismatched Epitaxial Growth 10:20 am – 12:00 pm  Third Floor, Cartoon Room 1

**TRAVEL RESOURCES**

The Conference does not endorse or sponsor any of the listings below. Information is provided as a courtesy to attendees.

**PARKING**

Visitors and guests to The Ohio State University are required to purchase parking any time they park on campus.

The closest parking available to the Conference is the Ohio Union South Parking Garage.

Located near the eastern corridor of the academic campus, the Ohio Union South Garage offers visitor and limited permit parking.

Visitors can park in this garage any time. All garage fees are due upon exit. Pay-on-foot machines accept cash, credit, and validations.

For more information on CampusParc, visit osu.campusparc.com.

**INTERNET ACCESS**

The Ohio Union offers free wireless internet. Connect to Wifi@OSU and open your browser to accept the terms of service.

No password is required.

Wireless internet service is typically available in the residence halls, but due to maintenance schedules, is not always guaranteed.

**OHIO STATE UNIVERSITY SMOKE-FREE AND TOBACCO-FREE POLICY**

Ohio State has adopted a tobacco-free policy that supports a healthy environment for all. Effective January 1, 2014, the use of all types of tobacco products is prohibited in all university buildings and on all university-owned properties, including parking lots, garages, and all outside areas.

**DINING OPTIONS**

Inside the Ohio Union you’ll find the Union Market, a fast, casual option offering a variety of grab-and-go food choices; Woody’s Tavern, a pub-style restaurant serving wood-fired pizza and Ohio’s finest beer and wine; and Espresso-OH, a coffee shop serving specialty drinks, breakfast items, and gelato. In addition, there are many dining options within walking distance.

Summer hours for dining options inside the Ohio Union are as follows:

- Express-OH is open Monday – Friday 8:00 am–4:00 pm; Weekends 10:00 am–4:00 pm
- Union Market is open Monday – Thursday 10:30am-7:00 pm; Friday 10:30am-5:00 pm; Closed Saturday and Sunday
- Woody’s Tavern is open Monday – Friday 4:00 pm–7:00 pm; Closed Saturday/Sunday
<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:20 am</td>
<td>Susan Troler-McKinsty</td>
<td>New Materials for Three Dimensional Ferroelectric Microelectronics</td>
<td>Archie M. Griffin West Ballroom</td>
</tr>
<tr>
<td>8:30 am</td>
<td></td>
<td><strong>Awards Ceremony</strong></td>
<td>Great Hall Meeting Room 3</td>
</tr>
<tr>
<td>9:20 am</td>
<td></td>
<td><strong>BREAK</strong></td>
<td></td>
</tr>
<tr>
<td>10:00 am</td>
<td>Lincoln Lauhon</td>
<td>Correlated Nanoscale Imaging of Doping, Conductivity, and Cathodoluminescence in GaN p-n Junctions Prepared by Selected Area Regrowth</td>
<td>Archie M. Griffin West Ballroom</td>
</tr>
<tr>
<td>10:20 am</td>
<td>Russell Dupuis</td>
<td>1.3 kV Vertical GaN p-i-n Rectifier with Nitrogen-Implanted Field Guard Ring Edge Terminal</td>
<td>Archie M. Griffin West Ballroom</td>
</tr>
<tr>
<td>10:40 am</td>
<td>Andrew M. Armstrong</td>
<td>1.6 kV Etched-and-Regrown GaN pn-Diode Realized by Mitigation of Plasma Etch-Enhanced Deep Level Defects</td>
<td>Archie M. Griffin West Ballroom</td>
</tr>
<tr>
<td>11:00 am</td>
<td>Matthew Alexander Porter</td>
<td>(Student) Design, Manufacturability and Optimization of Hybrid Guard Ring-JTE Edge Terminations via Nitrogen Implantation in Epitaxial GaN PN Power Diodes</td>
<td>Archie M. Griffin West Ballroom</td>
</tr>
<tr>
<td>11:20 am</td>
<td>Christopher M. Matthews</td>
<td>(Student) AIN Homojunction PN Diodes—The Highest Bandgap Semiconductor Diodes Ever Demonstrated</td>
<td>Archie M. Griffin West Ballroom</td>
</tr>
<tr>
<td>11:40 am</td>
<td>Vincent E. Meyers</td>
<td>(Student) Defect Microstructural and Diffusion Studies of Implant-Gyrotron Microwave Annealed GaN:Mg—Effect of Sequential High- and Moderate-Temperature Annealing</td>
<td>Archie M. Griffin West Ballroom</td>
</tr>
<tr>
<td>10:00 am</td>
<td>Sami El Hageali</td>
<td>(Student, Late News) Structural and Optical Characterization of Trapezoidal Defects in 4H-SiC Epilayers and Their Effect on MOSFETs Reliability</td>
<td>Ohio States Inc. Traditions Room</td>
</tr>
<tr>
<td>10:20 am</td>
<td>Shengnan Zhu</td>
<td>(Student) JFET Region Design for 650 V 4H-SiC Planar Power MOSFETs</td>
<td>Ohio States Inc. Founders Room</td>
</tr>
<tr>
<td>10:40 am</td>
<td>Suman Das</td>
<td>(Student) Channel Hole Scattering Processes in 4H-SiC MOSFETs</td>
<td>Ohio States Inc. Traditions Room</td>
</tr>
<tr>
<td>11:00 am</td>
<td>Suvendu Nayak</td>
<td>(Student) Process-Induced Variability of SiC DMOSFET Short Circuit Capability</td>
<td>Ohio States Inc. Traditions Room</td>
</tr>
<tr>
<td>11:20 am</td>
<td>Hema Lata Rau Maddi</td>
<td>B05 Characterization of SiC-SiO₂ Interface States in Commercial 4H-SiC Power MOSFETs from Cryogenic to High Temperature</td>
<td>Ohio States Inc. Traditions Room</td>
</tr>
<tr>
<td>11:40 am</td>
<td>Ashton Purcell</td>
<td>(Student) Recombination Centers in 4H-SiC pin Diodes Observed by Electrically Detected Magnetic Resistance and Near-Zero Field Magnetoresistance</td>
<td>Ohio States Inc. Founders Room</td>
</tr>
<tr>
<td>10:00 am</td>
<td>Nam-In Kim</td>
<td>(Student) Stress Hormone Detection by Single-Crystalline III-N Piezoelectric Thin-Film-Based Sensor</td>
<td>Ohio States Inc. Traditions Room</td>
</tr>
<tr>
<td>10:20 am</td>
<td>Dongseop Lee</td>
<td>(Student) Recessed AlGaN/GaN HEMT Bionicsensors with High Sensitivity and Linearity for Detection of Microystin-LR Made of Ultrawide-Bandgap III-N Thin Film</td>
<td>Ohio States Inc. Traditions Room</td>
</tr>
<tr>
<td>10:40 am</td>
<td>Nam-In Kim</td>
<td>(Student) Pressure Monitoring at Extremely High-Temperature Range Using Highly Flexible Piezoelectric Sensor Made of Ultrawide-Bandgap III-N Thin Film</td>
<td>Ohio States Inc. Traditions Room</td>
</tr>
<tr>
<td>11:00 am</td>
<td>Julia Isidora Salas Toledo</td>
<td>C04 Flexible Modified Carbon Nanotube/Nanofiber-Based Triboleric Nanogenerator</td>
<td>Ohio States Inc. Traditions Room</td>
</tr>
<tr>
<td>11:20 am</td>
<td>Lauren Brady</td>
<td>C05 Student Detection of the Nitrogen Cycle Using the Metabolic Activity of Shewanella Oneidensis MR-1</td>
<td>Ohio States Inc. Traditions Room</td>
</tr>
<tr>
<td>11:40 am</td>
<td>Nam-In Kim</td>
<td>C06 Student Wearable Eye Movement Sensors Using Flexible and Biocompatible III-N Thin Films for Personal Safety, Healthcare Monitoring and Abnormality Diagnosis</td>
<td>Ohio States Inc. Traditions Room</td>
</tr>
<tr>
<td>10:00 am</td>
<td>Nidhin Kurian Kalarickal</td>
<td>D01 Demonstration of Self-Aligned Delta Doped MISFETs with Current Density &gt; 550 mA/mm</td>
<td>Ohio States Inc. Traditions Room</td>
</tr>
<tr>
<td>10:20 am</td>
<td>Marko Tadjer</td>
<td>D02 Growth and Electrothermal Characterization of β-(AlₓGa₁₋ₓ)₂O₃/Ga₂O₃ Heterostructure Field-Effect Transistors</td>
<td>Ohio States Inc. Traditions Room</td>
</tr>
<tr>
<td>10:40 am</td>
<td>Ashok Vedantam Dheenan</td>
<td>D03 (Student) β-Ga₂O₃_MESFETs with Insulating Mg-Doped Buffer Grown by MBE</td>
<td>Ohio States Inc. Traditions Room</td>
</tr>
<tr>
<td>11:00 am</td>
<td>Zhenwei Wang</td>
<td>D04 Electrical Characteristics and Band Alignment of n-Si/In-Ga₂O₃ Heterojunction Fabricated by Surface-Activated Bonding</td>
<td>Ohio States Inc. Traditions Room</td>
</tr>
<tr>
<td>11:20 am</td>
<td>Joseph Spencer</td>
<td>D05 (Student) Beta-Gallium Oxide Oxide Junction Barrier Schottky Diodes with Sputtered P-Type Nickel Oxide</td>
<td>Ohio States Inc. Traditions Room</td>
</tr>
<tr>
<td>11:40 am</td>
<td>Zhe Ashley Jian</td>
<td>D06 (Student, Late News) Heterogeneous Integration of Single-Crystal β-Ga2O3 and N-Polar GaN Substrates with ZnO Interlayer Deposited by Atomic Layer Deposition</td>
<td>Ohio States Inc. Traditions Room</td>
</tr>
<tr>
<td>10:00 am</td>
<td>Aminat Oyiza Suleiman</td>
<td>E01 The Role of Thermal Vibrational Disorder in the Structural Phase Transition of VO2 Probed by Raman Spectroscopy</td>
<td>Senate Chamber</td>
</tr>
<tr>
<td>10:20 am</td>
<td>Samuel Marks</td>
<td>E02 High Transparent Conductive Mercury of SrVO₃ Grown by Solid-Phase Epitaxy</td>
<td>Senate Chamber</td>
</tr>
<tr>
<td>10:40 am</td>
<td>Kamila J Thompson</td>
<td>E03 (Student) Correlation of Native Point Defects with Piezoelectric Voltage in Strained ZnO Microvires</td>
<td>Senate Chamber</td>
</tr>
<tr>
<td>11:00 am</td>
<td>Brenton A Noesges</td>
<td>E04 (Student) Controlling Charge Distributions Near Complex Oxide Interfaces via Defect Engineering</td>
<td>Senate Chamber</td>
</tr>
<tr>
<td>11:20 am</td>
<td>Lyndon E Smith</td>
<td>E05 (Student, Late News) Mechanothermal Synthesis and Characterization of Ti-Doped Bismuth Ferrite Using Nano-Agitator Milling Process</td>
<td>Senate Chamber</td>
</tr>
<tr>
<td>11:40 am</td>
<td>Tetyana V. Torchynska</td>
<td>E06 On the Impact of Impurities’ Nature and Annealing Conditions on Structural and Optical Properties of Hafnia-Based Thin Films</td>
<td>Senate Chamber</td>
</tr>
<tr>
<td>10:00 am</td>
<td>Rafael Jaramillo</td>
<td>F01 Small Defects, Big Deal—Using Point Defects to Control Giant Opto-Mechanical Effects and to Engineer New Resistive Switches</td>
<td>Rosa M. Alabouni Room</td>
</tr>
<tr>
<td>10:20 am</td>
<td>Eamonn T Hughes</td>
<td>F02 (Student) Dislocations Altering the Microstructure and Luminescence of InAs Quantum Dots on Silicon</td>
<td>Rosa M. Alabouni Room</td>
</tr>
<tr>
<td>10:40 am</td>
<td>Yekan Wang</td>
<td>F03 (Student) Defects with Mg Segregation in Mg-implanted GaN After Ultra-High-Pressure Annealing</td>
<td>Rosa M. Alabouni Room</td>
</tr>
<tr>
<td>11:00 am</td>
<td>Fatih Furkan Ince</td>
<td>F04 (Student) Growth of High Indium Percentage InGaSb on InP Substrates Using the Interfacial Misfit Dislocation Array Growth Mode</td>
<td>Rosa M. Alabouni Room</td>
</tr>
<tr>
<td>11:20 am</td>
<td>Chunyi Huang</td>
<td>F05 (Student) Remote Si Doping of InGaAs Nanowires for Topological Quantum Computing</td>
<td>Rosa M. Alabouni Room</td>
</tr>
<tr>
<td>11:40 am</td>
<td>Joshua Ferrigno</td>
<td>F06 Irradiation Effects on Phonon Mediated Thermal Transport and Defect Evolution in GaAs</td>
<td>Rosa M. Alabouni Room</td>
</tr>
</tbody>
</table>
**CONFERENCE BADGE**

Badges must be worn at all times within the Conference venue, including all receptions.

**RECORDING/PHOTO POLICY**

Recording or photographing Conference presentations, posters or displays is strictly prohibited without prior permission of the presenter.

---

**PROGRAM AT-A-GLANCE**

**WEDNESDAY PM**

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Topic</th>
<th>Venue</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:30 pm</td>
<td>Sarbhashis Das</td>
<td>G01 (Student) Multifunctional MoTe₂ Transistors for Analog, Digital, Neuromorphic and Modulation Primitives</td>
<td></td>
</tr>
<tr>
<td>1:50 pm</td>
<td>Akhil Dodda</td>
<td>G02 (Student) Near Sensor Security Based on Multifunctional Monolayer MoS₂ FETs</td>
<td></td>
</tr>
<tr>
<td>2:10 pm</td>
<td>Zhihu Cheng</td>
<td>G03 The (Mostly) Unwelcome Guest in Transition Metal Chalcogenides—Native Oxidation and the Effects of Oxygen During Processing MoS₂, TiS₂, and Zr(S,Se)₂</td>
<td></td>
</tr>
<tr>
<td>2:30 pm</td>
<td>Rafael Jaramillo</td>
<td>G04 (Late News) What Limits Electronic Transport in 2D Transition Metal Dichalcogenides—Phonons or Defects?</td>
<td></td>
</tr>
<tr>
<td>2:50 pm</td>
<td>Yuan Yue Liu</td>
<td>G05</td>
<td></td>
</tr>
<tr>
<td>3:10 pm</td>
<td></td>
<td>BREAK</td>
<td></td>
</tr>
<tr>
<td>3:30 pm</td>
<td>Jennifer R Hajus</td>
<td>G06 Comparison of Epitaxial Graphene Electrodes for Electrochemical Detection and Identification of Heavy Metals in Seawater</td>
<td></td>
</tr>
<tr>
<td>3:50 pm</td>
<td>Sooram Kim</td>
<td>G07 Lattice Strain Induced Biosensing of SARS-CoV-2 Enabled by Quasi-Freestanding Epitaxial Graphene</td>
<td></td>
</tr>
<tr>
<td>4:10 pm</td>
<td>Hirandeep Reddy Kuchoor</td>
<td>G08 Improved Density of GaAsSb Nanowires on Monolayer Graphene/SiO₂/Si for Near-Infrared Photodetector Application</td>
<td></td>
</tr>
<tr>
<td>4:30 pm</td>
<td>Elisabeth Mansfield</td>
<td>G09 Degradation of CVD-Grown MoS₂ Subjected to DC Electrical Stress</td>
<td></td>
</tr>
<tr>
<td>4:50 pm</td>
<td>Emanuel Ber</td>
<td>G10 (Student, Late News) Reducing Schottky Barrier Height vs Width—Which is Most Effective in Improving Contact Resistance to Atomically Thin Semiconductors?</td>
<td></td>
</tr>
<tr>
<td>1:30 pm</td>
<td>Yekan Wang</td>
<td>H01 (Student) Defect Characteristics Under Devices and Reverse Leakage Current Investigated Using X-ray Topography</td>
<td></td>
</tr>
<tr>
<td>1:50 pm</td>
<td>Yafei Liu</td>
<td>H02 (Student) Investigation of the Nature and Origins of Area Defects in Gallium Nitride Substrate Wafers</td>
<td></td>
</tr>
<tr>
<td>2:10 pm</td>
<td>James C Gallagher</td>
<td>H03 Effects of Surface Defects on Vertical GaN Diode Performance</td>
<td></td>
</tr>
<tr>
<td>2:30 pm</td>
<td>Yuxuan Zhang</td>
<td>H04 (Student) Correlating Optical Characteristics and Electrical Performance of Vertical GaN-on-GaN PN Diodes</td>
<td></td>
</tr>
<tr>
<td>2:50 pm</td>
<td></td>
<td>BREAK</td>
<td></td>
</tr>
<tr>
<td>3:30 pm</td>
<td>Caleb Glaser</td>
<td>H05 (Student) Interface Trap Density Characterization of ALD Gate Dielectrics for GaN Power MOSFETs</td>
<td></td>
</tr>
<tr>
<td>3:50 pm</td>
<td>Mahlet Molla</td>
<td>H06 Thermodynamic and Band Structure Study of Sc₅Al₁₋₅N</td>
<td></td>
</tr>
<tr>
<td>4:10 pm</td>
<td>Md Didarul Alam</td>
<td>H07 (Student) Fabrication of Flexible AlGaN/GaN HEMTs Using Laser Lift-off</td>
<td></td>
</tr>
<tr>
<td>4:30 pm</td>
<td>Alan G Jacobs</td>
<td>H08 Efficient N-Type Ion Implantation Activation in GaN with High Mobility</td>
<td></td>
</tr>
<tr>
<td>4:50 pm</td>
<td>Zexuan Zhang</td>
<td>H09 (Student) N-Polar GaN/AlGaN High Electron Mobility Transistor Structures on Single-Crystal AlN Substrates</td>
<td></td>
</tr>
<tr>
<td>1:30 pm</td>
<td>Daniel J Pennachio</td>
<td>I01 Exploring SiC CVD Growth Parameters Compatible with Remote Epitaxy on Epitaxial Graphene Substrates</td>
<td></td>
</tr>
<tr>
<td>1:50 pm</td>
<td>Nadeemullah Mahadik</td>
<td>I02 Expansion of BPDs from Star-Shaped Defects in 4H-SiC</td>
<td></td>
</tr>
<tr>
<td>2:10 pm</td>
<td>Zeyu Chen</td>
<td>I03 (Student) Analysis of Strain Gradient in High Energy Implanted 4H-SiC Epi Wafer by Synchrotron X-ray Rocking Curve Topography</td>
<td></td>
</tr>
<tr>
<td>2:30 pm</td>
<td>Hongyu Peng</td>
<td>I04 Analysis of Dislocations in 4H-SiC Wafers Using Synchrotron X-ray Topography</td>
<td></td>
</tr>
<tr>
<td>2:50 pm</td>
<td>Qianyu Cheng</td>
<td>I05 (Student) Determination of Effective Penetration Depths on Synchrotron X-ray Topographic Images of Dislocations Lying on the Basal Plane in 4H-SiC Crystals</td>
<td></td>
</tr>
<tr>
<td>3:10 pm</td>
<td></td>
<td>BREAK</td>
<td></td>
</tr>
<tr>
<td>3:30 pm</td>
<td>Luis Maja Avila</td>
<td>J01 EUV Pulsed Atom Probe Tomography of β-Ga₂O₃ Semiconductor Materials</td>
<td></td>
</tr>
<tr>
<td>3:50 pm</td>
<td>Moritz Hansmann</td>
<td>J02 (Student) STM Simulation of High Aspect Ratio Tunneling Behavior on the Example of in Situ Harvested GaAs Nanowire</td>
<td></td>
</tr>
<tr>
<td>4:10 pm</td>
<td>Seth Shields</td>
<td>J03 (Student) Atomic Resolution Scanning Tunneling Microscopy Studies of Oxidized Cu(100) Surfaces</td>
<td></td>
</tr>
<tr>
<td>4:30 pm</td>
<td>Dorothee Sophie Rosenzweig</td>
<td>J04 (Student) GaAs(110) Surface Modifications by Adsorption Hydrogen at Room Temperature and Above</td>
<td></td>
</tr>
<tr>
<td>4:50 pm</td>
<td>Fedor V Sharov</td>
<td>J05 (Student) A Near-Adiabatic Rapid-Sweep (NARS) Approach to Electrically Detected Magnetic Resonance (EDMR) and Near-Zero-Field Magnetoresistance (NZFMR)</td>
<td></td>
</tr>
</tbody>
</table>

---

**Americans with Disabilities Act (ADA) Compliance**

The Materials Research Society (MRS), its meeting partners and event venues, are responsible for complying with the Americans with Disabilities Act (“ADA”) including the “readily achievable” removal of physical barriers to access meeting rooms, sleeping rooms and common areas. This may also include reasonable provisions for auxiliary aids and services when necessary and where achievable without undue burden. MRS will make every effort to ensure that disabled individuals are accommodated so that they can receive the full benefit of participation in our events, and will modify, where possible, the policies, practices and procedures as necessary to provide goods and services to disabled individuals. On-site needs will be met to the extent possible.
### K: Metasurfaces and Structured Photonics
Ohio Staters Inc. Founders Room

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:30 pm</td>
<td>Hanyu Zheng</td>
<td>K02 (Student) Meta-Optic Accelerators for Object Classifiers</td>
</tr>
<tr>
<td>1:50 pm</td>
<td>Milan Palei</td>
<td>K03 Probing Long-Range Coupling in Plasmonic Metasurfaces via Far-Field Diffraction</td>
</tr>
<tr>
<td>2:10 pm</td>
<td>Raymond C Rumpf</td>
<td>K04 Electromagnetics and Photonics in the Age of Digital Manufacturing</td>
</tr>
<tr>
<td>2:30 pm</td>
<td>Anjali Chaudhary</td>
<td>K05 Electroplated Helical Slow-Wave Structures for Millimeter-Through-Thz Vacuum Electronic Devices</td>
</tr>
</tbody>
</table>

### L: Gallium Oxide Growth
Ohio Staters Inc. Traditions Room

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:30 pm</td>
<td>Takeki Itoh</td>
<td>L01 (Student) Epitaxial Growth on β-Ga2O3 (110) Substrate by Plasma-Assisted Molecular Beam Epitaxy</td>
</tr>
<tr>
<td>1:50 pm</td>
<td>Thaddeus J Asel</td>
<td>L02 Source Material Oxidation Challenges in Ge-Doped β-Ga2O3 Grown via Plasma-Assisted Molecular Beam Epitaxy</td>
</tr>
<tr>
<td>2:10 pm</td>
<td>Tianchen Yang</td>
<td>L03 (Student) Characterization of β-Phase MgGaO Thin Films Grown by Molecular Beam Epitaxy</td>
</tr>
<tr>
<td>2:30 pm</td>
<td>A F M Anhar Uddin Bhuian</td>
<td>L04 (Student) MOCVD growth of Si Doped (010) β-(Al0.5Ga0.5)2O3 Films—Structural and Electrical Properties</td>
</tr>
<tr>
<td>2:50 pm</td>
<td>Lingyu Meng</td>
<td>L05 (Student) MOCVD Epitaxy of β-Ga2O3 Thin Films on (100) β-Ga2O3 Substrate</td>
</tr>
</tbody>
</table>

### M: Solar Cell Materials and Devices
Senate Chamber

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:30 pm</td>
<td>Bora Kim</td>
<td>M01 (Student, Late News) GaAs Laser Power Converters for Cryogenic Applications</td>
</tr>
<tr>
<td>1:50 pm</td>
<td>Kevin Ye</td>
<td>M02 (Student) Time-Resolved Photoluminescence Studies of Perovskite Chalcogenides</td>
</tr>
<tr>
<td>2:10 pm</td>
<td>Mohammed Alaani</td>
<td>M03 (Student) An Optical Response Analysis of Cadmium Telluride-Based Solar Cell Structures Incorporating High Resistivity Transparent Layers of Magnesium-Zinc Oxide</td>
</tr>
<tr>
<td>2:30 pm</td>
<td>Intuon Chatratin</td>
<td>M04 (Student) Group-V Acceptors and Their AX Centers in CdTe</td>
</tr>
<tr>
<td>2:50 pm</td>
<td>Marzieh Savadkoohi</td>
<td>M05 (Student) Investigation of Spin-Based Photovoltaic Effect in a Magnetic Tunnel Junction-Based Molecular Spintronic Devices (MTJ-MSDs)</td>
</tr>
</tbody>
</table>

### DRC Session 11: Heterogeneous Integration
U.S. Bank Conference Theater

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>10:00 am</td>
<td>Mario Lanza</td>
<td>11.1 Hybrid 2D/CMOS Microchips</td>
</tr>
<tr>
<td>10:40 am</td>
<td>Marko Radosavljevic</td>
<td>11.2 Large-Scale Heterogeneous Device Integration</td>
</tr>
<tr>
<td>11:20 am</td>
<td>Rahul Pendurthi</td>
<td>11.3 Monolithic and Heterogeneous Integration of Atomically Thin Semiconductors for non-von Neumann CMOS</td>
</tr>
<tr>
<td>11:40 am</td>
<td></td>
<td>11.4 LATE NEWS</td>
</tr>
</tbody>
</table>

### DRC Session 12: Wide Bandgap III - III-N HEMTs
U.S. Bank Conference Theater

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:20 pm</td>
<td>Siddharth Rajan</td>
<td>12.1 Ultra-Wide Bandgap Semiconductor Transistors for mm-wave Applications</td>
</tr>
<tr>
<td>2:00 pm</td>
<td>Bohao Wu</td>
<td>12.2 Modeling of the Charge-Voltage Characteristics of AlSb/CdS/GaSe Heterostructures</td>
</tr>
<tr>
<td>2:20 pm</td>
<td>Tuofu Zhama</td>
<td>12.3 Improved On/Off Current Ratio of TiO2/AlGaN/GaN MIS-HEMTs with N2O Surface Treatment on TiO2 Layer</td>
</tr>
<tr>
<td>2:40 pm</td>
<td>Eungkyun Kim</td>
<td>12.4 First demonstration of N-polar GaN/AlGaN/AInN HEMT on Single Crystal AlN Substrates</td>
</tr>
</tbody>
</table>
General Viewing

Wednesday 3:10 pm – 3:30 pm

Poster Session
6:30 pm – 8:30 pm

Thursday, no later than 5:30 pm

Remaining posters will be discarded.

Poster Set-up

Wednesday, 9:30 am – 3:00 pm

Poster presenters should be standing with their poster.
Student poster presenters must attend from 6:00 pm to 8:00 pm to present poster and answer questions to be eligible for the Best Student Poster Presentation award.

<table>
<thead>
<tr>
<th>Presenter</th>
<th>Paper #</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>Majid Aalizadeh</td>
<td>PS01</td>
<td>(Student) Growth and Characterization of High-Temperature Nitrogen-Polar InAlN Films and HEMTs Using Plasma Assisted Molecular Beam Epitaxy</td>
</tr>
<tr>
<td>Elizabeth Favela</td>
<td>PS02</td>
<td>(Student) Ni/Au and Co/Au Schottky Contacts on β-Ga$_2$O$_3$ and Effects of Annealing</td>
</tr>
<tr>
<td>Farmood Mirhosravi</td>
<td>PS03</td>
<td>(Student) Leveraging Thermoelectric Anisotropy in Single Crystal Antimony for Novel Heat Flux Sensing Devices</td>
</tr>
<tr>
<td>Kenneth McAfee</td>
<td>PS04</td>
<td>(Student) Growth of Iron Selenide Thin Films on c-Al$_2$O$_3$(0001) via Molecular Beam Epitaxy</td>
</tr>
<tr>
<td>Ryan Schalip</td>
<td>PS05</td>
<td>(Student) A Machine Learning Attack Resilient True Random Number Generator Based on Stochastic Programmability in Two-Dimensional Transistors</td>
</tr>
<tr>
<td>Akshay Wali</td>
<td>PS06</td>
<td>(Student) In situ Chemical Analysis of Complex Oxide Interfaces via Auger Electron Spectroscopy</td>
</tr>
<tr>
<td>Harish Kumarasubramanian</td>
<td>PS07</td>
<td>(Student) Design and Fabrication of ITO Based Transparent and Flexible Electrode Array for Simultaneous 2-Photon Imaging and Electrophotolithography</td>
</tr>
<tr>
<td>Hayden Brown</td>
<td>PS09</td>
<td>(Student) Impact of Biquadratic Exchange Coupling via Molecule on Magnetic Tunnel Junction Based Molecular Spintronics Devices with Competing Molecule Induced Inter-Electrode Coupling</td>
</tr>
<tr>
<td>Andrew Christopher Grizzle</td>
<td>PS10</td>
<td>(Student) Spin Fluctuations in Molecule-Electrode Magnetic Tunnel Junction-Based Spintronics Devices</td>
</tr>
<tr>
<td>Andominaia Mariah Randriambololona</td>
<td>PS11</td>
<td>(Student) A Comparison Between Heisenberg and Biquadratic Exchange Coupling Effects on Magnetic Tunnel Junction Molecular Spintronics Devices (MTJMSDs)</td>
</tr>
<tr>
<td>Pranshu Tyagi</td>
<td>PS12</td>
<td>(Student) A Monte Carlo Study of Paramagnetic Nanostructure Coupled with Two Ferromagnetic Electrodes of a Cross-Junction Shaped Spintronics Device At Different Thermal Energies</td>
</tr>
<tr>
<td>Katja Sofia Diaz-Granados</td>
<td>PS13</td>
<td>(Student) Influence of Crystallographic Orientation on the Asymmetric Emission of Calcite</td>
</tr>
<tr>
<td>Bishnu R Dahal</td>
<td>PS14</td>
<td>Magnetic Anisotropy Effect on the Magnetic Tunnel Junction-Based Molecular Spintronics Devices</td>
</tr>
<tr>
<td>Summayya Kouser</td>
<td>PS15</td>
<td>Control of the Color Centers in Diamond Through Surface Encapsulation</td>
</tr>
<tr>
<td>Rodnecia Taylor</td>
<td>PS16</td>
<td>(Student) Spatial and Thermal Properties of Magnetic Tunnel Junction Based Molecular Spintronics Device (MTJMSD) Due to Magnetic Anisotropy</td>
</tr>
<tr>
<td>Joseph T. Race</td>
<td>PS17</td>
<td>(Student) The Design and Synthesis of Lead-Free Layered Hybrid Perovskites as Room-Temperature Ferroelectrics</td>
</tr>
<tr>
<td>Annatoma Arif</td>
<td>PS18</td>
<td>(Student) Characterization of Aqueous Lead Sensing Performance of Bismuth Functionalized 3D Inkjet Printed Electrochemical Electrodes</td>
</tr>
<tr>
<td>Arush Guliani</td>
<td>PS19</td>
<td>(Student) Spin Fluctuation Effect on Magnetic Tunnel Junction-Based Molecular Spintronics Devices (MTJMSD)</td>
</tr>
<tr>
<td>Yao Li</td>
<td>PS20</td>
<td>(Student) Phase Equilibria in the Metal-Sc-N Systems and Their Relevance for Contacts to ScN, ScGaN and ScAlN</td>
</tr>
<tr>
<td>A B M Hamidul Islam</td>
<td>PS21</td>
<td>Effect of Distributed Bragg Reflectors on the Optical Crosstalk in InGaN-Based Flip-Chip Micro-LED Arrays</td>
</tr>
<tr>
<td>Terje Gunnar Finstad</td>
<td>PS22</td>
<td>Zinc Multi-Princogen Semiconductors—Cu Doping and Thermoelectric Characteristics</td>
</tr>
<tr>
<td>Rabin Pokharel</td>
<td>PS23</td>
<td>Epitaxial GaAs/GaAsSb Separate Absorption Multiplication (SAM) Avalanche Nanowire Photodetector</td>
</tr>
<tr>
<td>Rebekeh De Penning</td>
<td>PS24</td>
<td>(Student) Flexible Electrochemically Reduced Graphene Oxide Sensors for Lead and Cadmium Detection</td>
</tr>
<tr>
<td>Ghasanay Das Varma</td>
<td>PS25</td>
<td>Superconducting Properties of Fe (Te, Se) Thin Film on YSZ Substrate Using Pulsed Laser Deposition (PLD) Technique</td>
</tr>
<tr>
<td>Paul Gaurav G. Nalam</td>
<td>PS26</td>
<td>(Student) Phase-Control Enabled Tunable Optical Properties of Nanostructured GeO$_2$, Wide Band Gap Semiconductor Thin Films</td>
</tr>
<tr>
<td>Kendall Deon Dawkins</td>
<td>PS27</td>
<td>(Student) Optimized Light Absorption in GaAsSb(N) Nanowires for Photodetector Application</td>
</tr>
<tr>
<td>Tetyana V. Torchynska</td>
<td>PS28</td>
<td>Impact of Double Donor In and Ga Doping on Self-Compensating Process in ZnO Nanocrystal Films</td>
</tr>
<tr>
<td>Brahmin El Filali</td>
<td>PS29</td>
<td>(Student) Structure, Emission and Resistivity Variation with AL and In Co-Doping of ZnO Films Grown by Spray Pyrolysis</td>
</tr>
<tr>
<td>Benjamin L Dutton</td>
<td>PS30</td>
<td>(Student) Growth and Characterization of (Ba$<em>x$Ca$</em>{1-x}$)$_2$TiO$_4$, Single Crystals in Ir, Pt, and Mo Crucibles</td>
</tr>
<tr>
<td>Sang Hoon Lee</td>
<td>PS31</td>
<td>Fabrication of a Roll-to-Roll Printed Cantilever Type Touch Sensing and Actuating Device</td>
</tr>
<tr>
<td>M. Jasim Uddin</td>
<td>PS32</td>
<td>Force Spun PVD/TMU/Au Nanofiber Based TENG for Flexible Energy Harvesting and Bio Mechanical Motion Sensor</td>
</tr>
<tr>
<td>Bhog Gautam</td>
<td>PS33</td>
<td>Effect of Radical on Morphology and Charge Generation in Polymer Non-Fullerene Solar Cells</td>
</tr>
<tr>
<td>Jian Liu</td>
<td>PS34</td>
<td>(Student) Micro-Sized Si-Based Anodes Characterization and Optimization Using in situ Atomic Force Microscopy</td>
</tr>
</tbody>
</table>
The Journal of Electronic Materials reports monthly on the science and technology of electronic materials, while examining new applications for semiconductors, magnetic alloys, dielectrics, nanoscale materials and photonic materials. The Journal welcomes articles on methods for preparing and evaluating the chemical, physical, electronic and optical properties of these materials. Specific areas of interest are materials for state-of-the-art transistors, nanotechnology, electronic packaging, detectors, emitters, metallization, superconductivity and energy applications. Review papers on current topics enable individuals in the field of electronics to keep abreast of activities in areas peripheral to their own.

Manuscripts for the EMC 2022 collection will be evaluated according to the same high standards as would be applied to any article submitted to the Journal. Authors are encouraged to read carefully and comply with the “Instructions for Authors” on the springer.com/journal/11664. Submission of a manuscript implies that the work described has not been previously published and is not under consideration for publication elsewhere.

A special issue of the Journal of Electronic Materials (JEM)* will be published with peer-reviewed papers from the 64th Electronic Materials Conference.

- Article submission date is August, 31, 2022.
- Contact the 2022 Special Issue Editors listed below.

The Journal of Electronic Materials reports monthly on the science and technology of electronic materials, while examining new applications for semiconductors, magnetic alloys, dielectrics, nanoscale materials and photonic materials. The Journal welcomes articles on methods for preparing and evaluating the chemical, physical, electronic and optical properties of these materials. Specific areas of interest are materials for state-of-the-art transistors, nanotechnology, electronic packaging, detectors, emitters, metallization, superconductivity and energy applications. Review papers on current topics enable individuals in the field of electronics to keep abreast of activities in areas peripheral to their own.

Manuscripts for the EMC 2022 collection will be evaluated according to the same high standards as would be applied to any article submitted to the Journal. Authors are encouraged to read carefully and comply with the “Instructions for Authors” on the springer.com/journal/11664. Submission of a manuscript implies that the work described has not been previously published and is not under consideration for publication elsewhere.

Presenter | Paper # | Title
--- | --- | ---
Adesewa Oluwaseun Maselugbo | PS35 | (Student) Magnetic Modification of Boron Nitride Nanotubes for Alignment in Thermal Interface Composite
Andres Vercik | PS36 | A Universal Expression for Transport in Nanostructured Materials and Devices
Pius Suh | PS37 | (Student) Intra-Molecular Coupling on the Magnetic Properties of Magnetic Tunnel Junction-Based Molecular Spintronics Devices
Sk Md Ali Zaker Shawon | PS38 | Modified ZnSnO3 Structure in the Smart Helmet as a Promising Human Motion Sensor
Debabrata Das | PS39 | Tunable Optical Response by Anion Engineering in Crystalline Gallium Oxynitride Thin Film
Mahir Abrar | PS40 | (Student) A Numerical Study of Perovskite Solar Cells by Bandgap Tuning of Active Materials and Operating Temperature Variances
Mauro Caballero Victorio | PS41 | (Student) Towards a High-Modulation Reconfigurable Filter for Photodetectors via an Electrochromic Device
Luis F Hernandez Camas | PS42 | Simulation and Modeling of Perovskite Solar Cells for Renewable Energy Application
Mohammed Mohammed Abdullah Al-Ghorbani | PS43 | 2D Material Based Ag-ZnO-CeO3 Heterostructure for Solar-Driven CO2 Reduction
Xavier Mathew | PS44 | (Late News) Depth-Dependent Photoluminescence Analysis of the Inhomogeneities in Perovskite Solar Cell
Irina Buyanova | PS45 | (Late News) Wurtzite Crystalline Structure Enhances Second-Harmonic Generation in GaAs Nanowires
Rahayana Ruth Bautista | PS46 | (Student, Late News) Revealing the Electronic Heterogeneity and Inhomogeneity in Perovskite CsPbBr3 Nanowires Using Contactless Dielectric Force Microscopy
Narges Masouni | PS47 | (Late News) Thickness Dependence of Electronic Properties of GaN Slabs: A Density Functional Study
Nini Rose Mathews | PS48 | (Late News) Effects of Ge doping on the properties of CuZnSnS4 thin film solar cells
Narin Sunthornpan | PS49 | (Student, Late News) Realizing an atomically flat surface of Ge (111) thin film at low temperature (220°C) by gold-induced layer exchange
Sanjee Lamsal | PS50 | (Student, Late News) Aerosol Printed Asymmetric Coupled Stripline (ACS) fed Microstrip Antenna for Biomedical Applications
Wondwosen Fekadu Demisse | PS51 | (Student, Late News) Design and development of additively manufacture passive heat sink for electronics cooling
Nabil AlZaqri | PS52 | (Late News) Rhodium Nanoparticles Incorporated Mesoporous Silica as an Active Catalyst for Cyclohexene Hydrogenation under Ambient Conditions

Journal of Electronic Materials

A special issue of the Journal of Electronic Materials (JEM)* will be published with peer-reviewed papers from the 64th Electronic Materials Conference.

- Article submission date is August, 31, 2022.
- Contact the 2022 Special Issue Editors listed below.

The Journal of Electronic Materials reports monthly on the science and technology of electronic materials, while examining new applications for semiconductors, magnetic alloys, dielectrics, nanoscale materials and photonic materials. The Journal welcomes articles on methods for preparing and evaluating the chemical, physical, electronic and optical properties of these materials. Specific areas of interest are materials for state-of-the-art transistors, nanotechnology, electronic packaging, detectors, emitters, metallization, superconductivity and energy applications. Review papers on current topics enable individuals in the field of electronics to keep abreast of activities in areas peripheral to their own.

Manuscripts for the EMC 2022 collection will be evaluated according to the same high standards as would be applied to any article submitted to the Journal. Authors are encouraged to read carefully and comply with the “Instructions for Authors” on the springer.com/journal/11664. Submission of a manuscript implies that the work described has not been previously published and is not under consideration for publication elsewhere.

2022 Special Issue Editors

Joshua Caldwell
josh.caldwell@vanderbilt.edu

Jennifer Hite
Jennifer.hite@nrl.navy.mil

Nadeem Mahadik
nadeem.mahadik@nrl.navy.mil

Parsian Mohseni
pkmohseni@rit.edu

Jamie Phillips
jphilli@udel.edu

Shadi Shahedipour-Sandvik
sshahedipour-sandvik@sunypoly.edu

Randy Tompkins
randy.p.tompkins.civ@mail.mil

Editor-in-Chief—Shadi Shahedipour-Sandvik
### PROGRAM AT-A-GLANCE

#### THURSDAY AM

<table>
<thead>
<tr>
<th>Time</th>
<th>Name</th>
<th>ID</th>
<th>Summary</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:20 am</td>
<td>Cooper Augustus Voigt</td>
<td>N01</td>
<td>Molecular Beam Epitaxy Synthesis of In$_3$Se$_5$ Thin-Films on Graphite in the Temperature Range 150°C – 250°C and 500°C – 700°C</td>
</tr>
<tr>
<td>8:40 am</td>
<td>Yuan Li</td>
<td>N02</td>
<td>Molecular Beam Epitaxy Growth of Monolayer Hexagonal Boron Nitride on Nickel Substrates Incorporated with Oxygen Atoms</td>
</tr>
<tr>
<td>9:00 am</td>
<td>Nicholas Trainor</td>
<td>N03</td>
<td>Kinetics of Wafer-Scale Epitaxial Growth of MoS$_2$ on Sapphire</td>
</tr>
<tr>
<td>9:20 am</td>
<td>Shanchuan Li</td>
<td>N04</td>
<td>(Student, Late News) Facile Integration of Giant Exchange Bias in 2D Magnet/Oxide Heterostructures</td>
</tr>
<tr>
<td>9:40 am</td>
<td>Wouter Mortelmans</td>
<td>N05</td>
<td>Fast and Easy Optical Imaging and Epitaxial Growth Control of Rotational Domains in SnSe Thin Films</td>
</tr>
<tr>
<td>10:00 am</td>
<td>BREAK</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10:20 am</td>
<td>Daniel Lewis</td>
<td>N06</td>
<td>Electron Emission Sources from Quasi-Freestanding Epitaxial Graphene Planar Devices</td>
</tr>
<tr>
<td>10:40 am</td>
<td>Subrata Das</td>
<td>N07</td>
<td>Hot Electron Laser Assisted Cathode Using Electronically Tunable Negative Electron Affinity Silicon Surface</td>
</tr>
<tr>
<td>11:00 am</td>
<td>Tony Varghese</td>
<td>N08</td>
<td>Additive Manufacturing of Interface Engineered Colloidal 2D-Crystals for Flexible Thermoelectric Energy Harvesting</td>
</tr>
<tr>
<td>11:20 am</td>
<td>William Henry Koll</td>
<td>N09</td>
<td>Scanning Tunneling Microscopy of Monolayer Hexagonal Boron Nitride Monolayer Nanoribbons on Graphene</td>
</tr>
<tr>
<td>8:20 am</td>
<td>Jack Almeter</td>
<td>O01</td>
<td>Facet Control by Supersaturation in III-Nitrides</td>
</tr>
<tr>
<td>8:40 am</td>
<td>Bingjun Li</td>
<td>O02</td>
<td>Growth Evolution in Non-Planar GaN Selective Area Epitaxy</td>
</tr>
<tr>
<td>9:00 am</td>
<td>Yuto Ando</td>
<td>O03</td>
<td>Crack Suppression in High Al-Mole-Fraction AlGaN Beyond the Critical Layer Thickness via Non-Planar Growth Approach on Patterned GaN Platforms</td>
</tr>
<tr>
<td>9:20 am</td>
<td>Benjamin McEwen</td>
<td>O04</td>
<td>Effect of Growth Parameters on Be Incorporation Efficiency in MOCVD GaN:Be</td>
</tr>
<tr>
<td>9:40 am</td>
<td>Shashwat Rathkanthiwar</td>
<td>O05</td>
<td>Chemical Potential Control in p-Type N-Polar GaN</td>
</tr>
<tr>
<td>10:00 am</td>
<td>BREAK</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10:20 am</td>
<td>Wenbo Li</td>
<td>O06</td>
<td>Characterization of Traps in High-Growth-Rate MOCVD GaN</td>
</tr>
<tr>
<td>10:40 am</td>
<td>Bingjun Li</td>
<td>O07</td>
<td>High-Speed MOCVD Growth of GaN Assisted by TBCI</td>
</tr>
<tr>
<td>11:00 am</td>
<td>Vineeta R Muthuraj</td>
<td>O08</td>
<td>High to Ultrahigh Si-Doped GaN Grown by Metalorganic Chemical Vapor Deposition at 550°C for Heterogeneous Integration</td>
</tr>
<tr>
<td>11:20 am</td>
<td>Tianhai Wu</td>
<td>O09</td>
<td>Demonstration of Single Crystal InN and GaN/InN Heterostructures by MOCVD</td>
</tr>
<tr>
<td>11:40 am</td>
<td>Tim Mirabito</td>
<td>O10</td>
<td>Effects of Pre-Metallization on the MOCVD Growth and Properties of Ge-Doped AlGaN on AlN Templates</td>
</tr>
<tr>
<td>8:40 am</td>
<td>Jennifer E DeMell</td>
<td>P01</td>
<td>Nonlocal Measurement as a Probe of the Spin Hall Effect in Topological Insulators</td>
</tr>
<tr>
<td>9:00 am</td>
<td>Denis R Candido</td>
<td>P02</td>
<td>Magnon-Mediated Entanglement of Solid-State Spin Qubit</td>
</tr>
<tr>
<td>9:20 am</td>
<td>Ian C Nodurft</td>
<td>P03</td>
<td>Entanglement of circularly polarized light with the Quantum Zeno Effect</td>
</tr>
<tr>
<td>9:40 am</td>
<td>Mahnaz Islam</td>
<td>P04</td>
<td>Visible Light Emission During Electrical Threshold Switching of NbO$_2$ Mott Switches</td>
</tr>
<tr>
<td>10:00 am</td>
<td>BREAK</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10:20 am</td>
<td>Patrick Taylor</td>
<td>P05</td>
<td>MBE Growth of Bi$_2$Se$_3$ with Reduced Twin Defect Density</td>
</tr>
<tr>
<td>10:40 am</td>
<td>Shuyu Cheng</td>
<td>P06</td>
<td>Epitaxial Growth of Kagome Ferromagnet Fe$_3$S$_9$ and Sn-Modulated Heterostructures</td>
</tr>
<tr>
<td>11:00 am</td>
<td>Logan Riney</td>
<td>P07</td>
<td>Fermi Level Tuning and Band Alignment in Mn Doped InAs/GaSb</td>
</tr>
<tr>
<td>11:20 am</td>
<td>Quoc Dai Ho</td>
<td>P08</td>
<td>Confinement-Induced Topological Phase Transition in Thin-Film Rare-Earth Pnictides</td>
</tr>
<tr>
<td>11:40 am</td>
<td>Dhrav Chimanhbai Desai</td>
<td>P09</td>
<td>Charge Transport in a Dirac Semimetal, Na,Bi</td>
</tr>
<tr>
<td>Time</td>
<td>Speaker</td>
<td>Title</td>
<td>Room</td>
</tr>
<tr>
<td>------------</td>
<td>--------------------------</td>
<td>----------------------------------------------------------------------</td>
<td>-----------------------</td>
</tr>
<tr>
<td>8:20 am</td>
<td>Sarah L Swisher</td>
<td>Q01 Large-Area Photonic Lift-off Process for Flexible Thin-Film Transistors</td>
<td>Ohio Staters Inc. Traditions Room</td>
</tr>
<tr>
<td>8:40 am</td>
<td>Dong Hun Lee</td>
<td>Q02 (Student) Facile Processing and Properties of P-Type SnO\textsubscript{x} and Oxide-Based p-n Heterojunction Application with n-InGaZnO</td>
<td>Ohio Staters Inc. Traditions Room</td>
</tr>
<tr>
<td>9:00 am</td>
<td>Eli Powell</td>
<td>Q03 (Student) Separation of Defect States and Intrinsic Channel Mobility on the Electrical Operation of IGZO TFTs</td>
<td>Ohio Staters Inc. Traditions Room</td>
</tr>
<tr>
<td>9:20 am</td>
<td>Kishwar Mashhoq</td>
<td>Q04 (Student) Investigation of p-Type SnO Sub-Bandgap Defects by Comparing Experimental Transistor Data to Numerical Device Simulations</td>
<td>Ohio Staters Inc. Traditions Room</td>
</tr>
<tr>
<td>9:40 am</td>
<td>Rajashtree Bhattacharya</td>
<td>Q05 (Student) Materials Characterization of LaCoO\textsubscript{3} Grown by Optimized Reactive DC Magnetron Sputtering and Evaluation of Contact Metal Resistivities by Transmission Line Measurement Technique</td>
<td>Ohio Staters Inc. Traditions Room</td>
</tr>
<tr>
<td>10:00 am</td>
<td>BREAK</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10:20 am</td>
<td>Kingsley Egbo</td>
<td>Q06 Controlling the p-Type Conductivity of SnO (001) Films by Group-III Doping During Molecular Beam Epitaxy</td>
<td>Senate Chamber</td>
</tr>
<tr>
<td>10:40 am</td>
<td>Jade Cowsky</td>
<td>Q07 (Student) Defects, Doping and Electronic Structure Correlations of Indium Tin Oxide (ITO) Thin Films</td>
<td>Senate Chamber</td>
</tr>
<tr>
<td>11:00 am</td>
<td>Jaesung Jo</td>
<td>Q08 (Student) Study of Hole Scattering Mechanisms in P-Type Cu\textsubscript{2}O</td>
<td>Senate Chamber</td>
</tr>
<tr>
<td>11:20 am</td>
<td>Yaopiao Hu</td>
<td>Q09 (Student) Electron Transport Mechanism and Mobility Prediction in Amorphous In\textsubscript{2}O\textsubscript{3} for BEOL Transistors</td>
<td>Senate Chamber</td>
</tr>
<tr>
<td>8:20 am</td>
<td>Mark Wisley</td>
<td>R01 Undoing Band Anticrossing in Highly Mismatched Alloys</td>
<td>Senate Chamber</td>
</tr>
<tr>
<td>8:40 am</td>
<td>Ellie Yiliien Wang</td>
<td>R02 (Student) Growth and Characterization of Al\textsubscript{1-x}In\textsubscript{x},As\textsubscript{y}Sb\textsubscript{1-y}, Digital Alloys Grown on InP</td>
<td>Senate Chamber</td>
</tr>
<tr>
<td>9:00 am</td>
<td>Jarod Meyer</td>
<td>R03 (Student) Exploring the Impact of Sn Alloying on Structure and Luminescence in PbSnSe Epitaxial Films on GaAs</td>
<td>Senate Chamber</td>
</tr>
<tr>
<td>9:20 am</td>
<td>Rachel Corey White</td>
<td>R04 (Student) Growth of InAsSbBi on InSb Towards Lattice-Matched Longwave-Infrared Optoelectronics</td>
<td>Senate Chamber</td>
</tr>
<tr>
<td>9:40 am</td>
<td>Amberly Ricks</td>
<td>R05 (Student) Growth and Characterization of AlInSbBi for Wide-Bandgap Barriers on InSb</td>
<td>Senate Chamber</td>
</tr>
<tr>
<td>10:00 am</td>
<td>BREAK</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10:20 am</td>
<td>Leland Joseph Nordin</td>
<td>R06 Low Growth Temperature Epitaxial PbSe for Heterogeneous Mid-Infrared Emitters</td>
<td>Senate Chamber</td>
</tr>
<tr>
<td>10:40 am</td>
<td>Mariah Lauren Schwartz</td>
<td>R07 (Student) Investigation of Polarity of Unintentionally Doped AlGaAsSb and AlInAsSb Avalanche Photodiodes on InP Substrates</td>
<td>Senate Chamber</td>
</tr>
<tr>
<td>11:00 am</td>
<td>Alexander Timothy Newell</td>
<td>R08 (Student) Majority Carrier Concentration and Minority Carrier Lifetime in Mid-wave Infrared InGaAs/InAsSb and InAs/InAsSb Superlattice nBn Detectors</td>
<td>Senate Chamber</td>
</tr>
<tr>
<td>11:20 am</td>
<td>Abhilasha Kamboj</td>
<td>R09 (Student) Guided-Mode Resonance Enhanced Room-Temperature Infrared Detectors</td>
<td>Senate Chamber</td>
</tr>
<tr>
<td>11:40 am</td>
<td>Yinan Wang</td>
<td>R10 (Student) High-Speed Long-Wave Infrared Ultrathin nBn T2SL Detectors</td>
<td>Senate Chamber</td>
</tr>
<tr>
<td>8:20 am</td>
<td>Ke Zou</td>
<td>S01 Wafer-Scale Ferromagnetic Fe\textsubscript{3}Ge\textsubscript{2}Te\textsubscript{2} Thin Films by Molecular Beam Epitaxy</td>
<td>Cartoon Room 1</td>
</tr>
<tr>
<td>8:40 am</td>
<td>Yuxing Ren</td>
<td>S02 (Student) MBE Growth of Cr:Bi\textsubscript{1-x}Sb\textsubscript{x},Te for Enhancing Spin-Orbital-Torque Switching and Stabilizing Quantum Anomalous Hall Effect</td>
<td>Cartoon Room 1</td>
</tr>
<tr>
<td>9:00 am</td>
<td>Mythili Surendran</td>
<td>S03 (Student) Epitaxial Thin Films of Chalcogenide Perovskites and Related Phases</td>
<td>Cartoon Room 1</td>
</tr>
<tr>
<td>9:20 am</td>
<td>Yongchen Liu</td>
<td>S04 (Student) High-Quality van der Waals Material on a Semiconductor Substrate</td>
<td>Cartoon Room 1</td>
</tr>
<tr>
<td>9:40 am</td>
<td>Rafael Jaramillo</td>
<td>S05 Making Chalcogenide Perovskite Semiconductor Thin Films by Gas-Source Molecular Beam Epitaxy</td>
<td>Cartoon Room 1</td>
</tr>
<tr>
<td>10:00 am</td>
<td>BREAK</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10:20 am</td>
<td>Narges Masoumi</td>
<td>T01 Critical Evaluation of Thermal and Compositional Dependences in a Finite Strain Model of Ge-Si-Sn Alloys on Ge(100) and GeSn Buffer Layers from DFT</td>
<td>Cartoon Room 1</td>
</tr>
<tr>
<td>10:40 am</td>
<td>Tuhin Dey</td>
<td>T02 (Student) Molecular Beam Epitaxy Growth of Highly Tensile Strained GeSnC Alloys up to 4% Sn and 3% C</td>
<td>Cartoon Room 1</td>
</tr>
<tr>
<td>11:00 am</td>
<td>Augustus Arbogast</td>
<td>T03 (Student) MBE Growth and Characterization of GeSnC/Ge Multiple Quantum Well Structure</td>
<td>Cartoon Room 1</td>
</tr>
<tr>
<td>11:20 am</td>
<td>Qian Meng</td>
<td>T04 (Student) Mechanical and Electronic Effect of B on the Band Structure of BGaAs Alloys</td>
<td>Cartoon Room 1</td>
</tr>
<tr>
<td>11:40 am</td>
<td>Harry Lewis</td>
<td>T05 (Student, Late News) Impact Ionization Coefficients and Excess Noise in Al\textsubscript{1-x}Ga\textsubscript{x},As\textsubscript{y}Sb\textsubscript{1-y}, Avalanche Photodiodes</td>
<td>Cartoon Room 1</td>
</tr>
<tr>
<td>Time</td>
<td>Speaker</td>
<td>Title</td>
<td>Location</td>
</tr>
<tr>
<td>---------</td>
<td>--------------------------</td>
<td>-------------------------------------------------------------------------------------------------</td>
<td>---------------------------------</td>
</tr>
<tr>
<td>1:30 pm</td>
<td>Alexander J Bishop U01</td>
<td>Spin-Polarized Scanning Tunneling Microscopy of Epitaxial Fe₃GeTe₂</td>
<td>Great Hall Meeting Room 1 &amp; 2</td>
</tr>
<tr>
<td>1:50 pm</td>
<td>Wenyi Zhou U02</td>
<td>(Student) Kinetically-Controlled Epitaxial Growth of vdW Fe₃GeTe₂ Ferromagnets and Their Heterostructures with Topological Insulators</td>
<td></td>
</tr>
<tr>
<td>2:10 pm</td>
<td>Brad Goff U03</td>
<td>(Student) Spin Polarized STM Imaging of Magnetic Skyrmions in Metallic Thin-Film Heterostructures</td>
<td></td>
</tr>
<tr>
<td>2:30 pm</td>
<td>Shuyu Cheng U04</td>
<td>(Student) Tuning Magnetic Properties of [Pt/Co/Cu] Multilayers</td>
<td></td>
</tr>
<tr>
<td>2:50 pm</td>
<td>Richard Harry U05</td>
<td>(Student, Late News) Electromagnetic Interference (EMI) Shielding Techniques for Simulated PVDF-TrFE/Fe₃O₄ Multiferroic Monopolar Antenna</td>
<td></td>
</tr>
<tr>
<td>3:10 pm</td>
<td>BREAK</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3:30 pm</td>
<td>Marzieh Savadkoohi U06</td>
<td>(Student) The Effect of Spin Fluctuations on Temporal and Spatial Evolution of Magnetic Moment in A Magnetic Tunnel Junction-Based Molecular Spintronic Device (MTJMSD)</td>
<td></td>
</tr>
<tr>
<td>3:50 pm</td>
<td>Eva Mutunga U07</td>
<td>Design of Experiment Approach for Harnessing Robust Molecular Spintronic Devices</td>
<td></td>
</tr>
<tr>
<td>4:10 pm</td>
<td>Igor Lyalin U08</td>
<td>(Student) Spin–Orbit Torque in Bilayers of Kagome Ferromagnet Fe₃Sn₂ and Pt</td>
<td></td>
</tr>
<tr>
<td>4:30 pm</td>
<td>Yueguang Shi U09</td>
<td>(Student) Magnetic Properties of Doped and Undoped Organic Magnetic Semiconductors—V(TCNE)_2, Cr(TCNE)_2 and Nb(TCNE)_2</td>
<td></td>
</tr>
<tr>
<td>4:50 pm</td>
<td>Weimin Chen U10</td>
<td>(Late News) Generating Room-Temperature Electron Spin Polarization Exceeding 90% in an Opto-Spintronic Semiconductor Nanostructure</td>
<td></td>
</tr>
<tr>
<td>1:30 pm</td>
<td>Jeong-Hwan Park V01</td>
<td>(Student) Enhancing the External Quantum Efficiency of Micro-LEDs via Optimized Dry Etching Condition</td>
<td></td>
</tr>
<tr>
<td>1:50 pm</td>
<td>Mohammad Awwad V02</td>
<td>(Student) Impact of Photon Recycling on Absorption Losses in Tunnel Junction-Based III-Nitride LEDs</td>
<td></td>
</tr>
<tr>
<td>2:10 pm</td>
<td>Wentao Cai V03</td>
<td>(Student) High In-Content InGaN Platelets as Underlayer for Light-Emitting Diodes Toward Long Wavelength Application</td>
<td></td>
</tr>
<tr>
<td>2:30 pm</td>
<td>Miad Yarali V04</td>
<td>(Student) Significant Improvement in Quantum Efficiencies and Wall-Plug Efficiency of Flexible AlGaN-Based Deep-Ultraviolet Light-Emitting Diodes</td>
<td></td>
</tr>
<tr>
<td>3:30 pm</td>
<td>Keisuke Motoki W01</td>
<td>(Student) Observation of Compositional Modulation in AlGaN Self-Assembled Superlattices by Transmission Electron Microscopy</td>
<td></td>
</tr>
<tr>
<td>3:50 pm</td>
<td>Gihua Zhang W02</td>
<td>(Student) Molecular Beam Epitaxial Growth of AlGaN Epilayers on Si Using a Nanowire Template</td>
<td></td>
</tr>
<tr>
<td>4:10 pm</td>
<td>Mina Moradnia W03</td>
<td>(Student) Transition-Metal-Alloyed Group-III-Nitride Piezoelectric Thin Films Grown by Hybrid Chemical Vapor Deposition and Sputtering Deposition Techniques</td>
<td></td>
</tr>
<tr>
<td>4:30 pm</td>
<td>Morton Greenslit W04</td>
<td>(Student) Use of a TiN Seed Layer to Enhance (0002) Epitaxy and Piezoelectric Coupling of AlN Thin Films</td>
<td></td>
</tr>
<tr>
<td>4:50 pm</td>
<td>Joshua Nordlander W05</td>
<td>(Student) Sputter Deposition of III-N Thin Films</td>
<td></td>
</tr>
<tr>
<td>1:30 pm</td>
<td>Ruiqi Hu X01</td>
<td>(Student) Density Functional Theory Calculations of Rare-Earth Mono-Phosphides Embedded in III-Vs</td>
<td></td>
</tr>
<tr>
<td>1:50 pm</td>
<td>Sadihvikas Addamane X02</td>
<td>Ga(As)Sb Nanostructures Formed by Arsenic-Induced Etching of III-Sb Surfaces</td>
<td></td>
</tr>
<tr>
<td>2:10 pm</td>
<td>Takafumi Moriyama X03</td>
<td>(Student) Structural Analysis of Highly Luminescent and Narrow Bandwidth Cl-Doped InP/ZnSe/ZnS Quantum Dot Heterostructures</td>
<td></td>
</tr>
<tr>
<td>2:30 pm</td>
<td>Priyanka Ramaswamy X04</td>
<td>Study of Al₂O₃ Dielectric on Ga-Assisted MBE Grown GaAs₁₋ₓSbx Nanowires</td>
<td></td>
</tr>
<tr>
<td>2:50 pm</td>
<td>Alireza Abrand X05</td>
<td>(Student) Tuning Selective Narrowband Infrared Absorption Using Coaxial InAs-GaAsₓSbx Nanowires with Partial Shell Segment Coverage</td>
<td></td>
</tr>
<tr>
<td>3:10 pm</td>
<td>BREAK</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3:30 pm</td>
<td>Michael Pedowitz X06</td>
<td>(Student) Growth and Transformation of Mixed Valence Manganese Oxide Nanostructures on Epitaxial Graphene-Silicon Carbide Heterostructures</td>
<td></td>
</tr>
<tr>
<td>3:50 pm</td>
<td>Kyle G Tezanos X07</td>
<td>(Student) Enhancement of Visible Photoluminescence Through Atomic Layer Deposition Surface Passivation of Porous Silicon Nanowire Arrays Fabricated by Metal-Assisted Chemical Etching</td>
<td></td>
</tr>
<tr>
<td>4:10 pm</td>
<td>Benjamin Diroll X08</td>
<td>Intrapband Optical Gain in Colloidal Nanoplates</td>
<td></td>
</tr>
<tr>
<td>4:30 pm</td>
<td>Laura Biedermann X09</td>
<td>Development of Granular Metals for High Voltage Applications</td>
<td></td>
</tr>
<tr>
<td>1:30 pm</td>
<td>Glenn Packard Y01</td>
<td>(Student) Chromium Segregation in Silicon Thin Films During Wide Area Sub-Millisecond Melting and Recrystallization</td>
<td></td>
</tr>
<tr>
<td>1:50 pm</td>
<td>Michael Evan Liao Y02</td>
<td>(Student) Interfacial Thermal Transport of Thinned and Chemical Mechanical Polished (-201) β-Ga₂O₃ Direct Wafer Bonded to (001) Si</td>
<td></td>
</tr>
<tr>
<td>2:10 pm</td>
<td>Martin Gregorio Reyes-Banda Y03</td>
<td>Ionic Exchange in Perovskite Thin Films Using Solid-State Reactions</td>
<td></td>
</tr>
<tr>
<td>2:30 pm</td>
<td>Leuam Fernandez-Tizuerdo Y04</td>
<td>Planar and 3D Microstructured CsPbBr₃ Perovskite Devices for Neutron Detection</td>
<td></td>
</tr>
<tr>
<td>2:50 pm</td>
<td>Cagri Aydinkarahaliloglu Y05</td>
<td>(Student) Predicting Premature Failure of Quantum Cascade Lasers Using Supervised Machine Learning</td>
<td></td>
</tr>
<tr>
<td>3:10 pm</td>
<td>BREAK</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
# PROGRAM AT-A-GLANCE

## THURSDAY PM

### Z: Heterogeneous Integration Technologies

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>3:30 pm</td>
<td>Chenziyi Mi</td>
<td>Z01 (Student) Heterogeneous Integration of Blue GaN Laser Diode Using Electrochemical Etching</td>
<td></td>
</tr>
<tr>
<td>3:50 pm</td>
<td>Sherman Peek</td>
<td>Z02 (Student) Electronic Packaging and Interconnect Technologies for Cryogenic and Superconducting Applications</td>
<td></td>
</tr>
<tr>
<td>4:10 pm</td>
<td>Rebecca A Wheeling</td>
<td>Z03 Indium Microbump Interface Evolution with Varying Underbump Metallurgy Stack-Ups</td>
<td></td>
</tr>
<tr>
<td>4:30 pm</td>
<td>Yuri Piro</td>
<td>Z04 (Student) UV Curable Ink Composition for Novel Direct Ink Writing Processes</td>
<td></td>
</tr>
<tr>
<td>4:50 pm</td>
<td>Bhushan Lohani</td>
<td>Z05 (Student) Additive Microfabrication of System in Package for Heterogenous Integration with Semiconductor Dies</td>
<td></td>
</tr>
</tbody>
</table>

### AA: Plasmon and Surface Phonon Polaritons

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:30 pm</td>
<td>Angela Cleri</td>
<td>AA01 (Student) Lateral Permittivity Patterning by Ion Irradiation in CdO Thin Films for Mid-IR Plasmonics</td>
<td></td>
</tr>
<tr>
<td>1:50 pm</td>
<td>Kurt Eyink</td>
<td>AA02 MBE Growth of Delta Doped Si:InAsSb/GaSb HMM and Their Hyperbolic Response</td>
<td></td>
</tr>
<tr>
<td>2:10 pm</td>
<td>Seyedeh Maryam Vaghfei Esfidi</td>
<td>AA03 (Student) Understanding Organ Pipe Resonances in SPhP Trenches for Spectroscopic Sensing</td>
<td></td>
</tr>
<tr>
<td>2:30 pm</td>
<td>Ryan Spangler</td>
<td>AA04 (Student) Physical Vapor Transport Growth of α-MoO3 Sheets for Hypersonic Thermal Transport via Hyperbolic Phonon Polaritons</td>
<td></td>
</tr>
<tr>
<td>2:50 pm</td>
<td>Sean McSherry</td>
<td>AA05 (Student) Control of Thermal Transport at Ultrahigh Temperatures by Immiscible Oxide Heterostructures</td>
<td></td>
</tr>
<tr>
<td>3:10 pm</td>
<td>BREAK</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3:30 pm</td>
<td>Aaron J. Muhowski</td>
<td>AA06 Plasmon-Enhanced Distributed Bragg Reflectors</td>
<td></td>
</tr>
<tr>
<td>3:50 pm</td>
<td>Morgan Berghold</td>
<td>AA07 (Student) All-Epitaxial Ultra-Thin Long-Wave Infrared Plasmonic Detectors</td>
<td></td>
</tr>
<tr>
<td>4:10 pm</td>
<td>Wilder Acuna</td>
<td>AA08 (Student) ErAs:InGaAlBiAs for 1.55 µm-pumped Terahertz Photoconductive Switches</td>
<td></td>
</tr>
<tr>
<td>4:30 pm</td>
<td>Quang To</td>
<td>AA09 Plasmon-Phonon-Intersubband Transition Interactions at THz Frequency in Bi2Se3-GaAs Heterostructures</td>
<td></td>
</tr>
<tr>
<td>4:50 pm</td>
<td>Saadia Nasir</td>
<td>AA10 (Student) In-Plane Plasmon Coupling in Topological Insulator Bi2Se3 Thin Films</td>
<td></td>
</tr>
</tbody>
</table>

### BB: Electrochemical Energy Storage and Conversion

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:30 pm</td>
<td>Soonil Lee</td>
<td>BB01 (Student) High Performance Wafer-Scale Metal-Insulator-Semiconductor Photoanodes for Solar-Driven Water Splitting</td>
<td></td>
</tr>
<tr>
<td>1:50 pm</td>
<td>Amjad Hussain</td>
<td>BB02 Highly Robust Solid Oxide Fuel Cells—Prevention of Chemical Inter-Diffusion by Introducing a Buffer Layer</td>
<td></td>
</tr>
<tr>
<td>2:10 pm</td>
<td>Song Xu</td>
<td>BB03 PiFM (Photo Induced Force Microscopy) Based Nanoscale IR Spectroscopy and Imaging in Energy Research</td>
<td></td>
</tr>
<tr>
<td>2:30 pm</td>
<td>Michael Lee</td>
<td>BB04 (Student) Porous Current Collector Network Materials for High-Loading Li-Ion Battery Cathodes</td>
<td></td>
</tr>
<tr>
<td>2:50 pm</td>
<td>Lalith Rao</td>
<td>BB05 (Student) Strategy to Passivate High-Voltage Spinel Cathode-Electrolyte Interfaces (CEI)</td>
<td></td>
</tr>
<tr>
<td>3:10 pm</td>
<td>BREAK</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3:30 pm</td>
<td>Pablo Rosas Martinez</td>
<td>BB06 (Student) Study of V2O5/LiPON Interface Using Depth-Resolved Cathodoluminescence Spectroscopy</td>
<td></td>
</tr>
<tr>
<td>3:50 pm</td>
<td>Jun Wei Yap</td>
<td>BB07 (Student) Comparing Performance Enhancement by Different Carbon Additives for Si Anodes in Lithium-Ion Batteries</td>
<td></td>
</tr>
<tr>
<td>4:10 pm</td>
<td>Yuxuan Zhang</td>
<td>BB08 (Student) Enabling High-Rate Long-LifeSpan Lithium-Sulfur Batteries via Stereolithography Technique and Oxidative Chemical Vapor Deposition</td>
<td></td>
</tr>
<tr>
<td>4:30 pm</td>
<td>Zhenghuan Tang</td>
<td>BB09 (Student) Optimization of LiBO2 Interlayer for Garnet-Based All-Solid-State Lithium Metal Batteries</td>
<td></td>
</tr>
<tr>
<td>4:50 pm</td>
<td>Edward Gillan</td>
<td>BB10 (Late News) Rapid Thermochromical Solvent-Free Synthesis of Crystalline Metal Borides and Their Investigation as Water Splitting Electrocatalysts</td>
<td></td>
</tr>
<tr>
<td>5:10 pm</td>
<td>Yuanyue Liu</td>
<td>BB11 (Late News) Atomistic Simulations of Reaction Kinetics at Electrochemical Interface</td>
<td></td>
</tr>
</tbody>
</table>
### PROGRAM AT-A-GLANCE

#### FRIDAY AM

#### CC: Neuromorphic + Late News

<table>
<thead>
<tr>
<th>Time</th>
<th>Name</th>
<th>Topic</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:20 am</td>
<td>Yiyang Li</td>
<td>CC01 Nonvolatile Analog Electrochemical Random Access Memory for In-Memory Computing</td>
</tr>
<tr>
<td>8:40 am</td>
<td>Colton Duprey</td>
<td>CC02 (Student, Late News) Effects of Small Molecule Dopants in Piezoresistive Sensing PAAMPSA/PANI/PA Polymer Complex</td>
</tr>
<tr>
<td>9:00 am</td>
<td>Fei Qin</td>
<td>CC03 (Student) Influence of Oxygen Vacancy and Top Electrode on Switching Behavior of InGaZnO Based Resistive Random Access Memory</td>
</tr>
<tr>
<td>9:20 am</td>
<td>Sanghyeon Choi</td>
<td>CC04 (Student) SiOx Nanorod Memristive Neuron for Probabilistic Inference Applications</td>
</tr>
<tr>
<td>9:40 am</td>
<td>Joshua Gabriel</td>
<td>CC05 (Late News) Silicon Carbide Growth Reaction Engineering for Quantum Sensing—Impact of Thermodynamic Model Uncertainty on Product Distributions</td>
</tr>
<tr>
<td>10:00 am</td>
<td></td>
<td>BREAK</td>
</tr>
<tr>
<td>10:20 am</td>
<td>Akhil Doddha</td>
<td>CC06 (Student) A Low-Power, Bio-inspired, Adaptive Machine Vision Based on Atomically Thin Memristors</td>
</tr>
<tr>
<td>10:40 am</td>
<td>Dipanjan Sen</td>
<td>CC07 (Student) Spike-Timing Based Adaptive Photo Encoder Considering Monolayer MoS₂ Based Memristors</td>
</tr>
<tr>
<td>11:00 am</td>
<td>Ragib Ahsan</td>
<td>CC08 (Student) Ultralow-Power Photoactivated Spiking Silicon Neurons</td>
</tr>
<tr>
<td>11:20 am</td>
<td>James C Carter</td>
<td>CC09 Atomic Layer Deposition of Antimony(III) Telluride</td>
</tr>
<tr>
<td>11:40 am</td>
<td>Wondwosen Demisse</td>
<td>CC10 (Student, Late News) Electrochemical Additive Manufacturing Producing Composite Materials for Electronics</td>
</tr>
</tbody>
</table>

#### DD: Group III-Nitrides—Contacts and Novel Devices

<table>
<thead>
<tr>
<th>Time</th>
<th>Name</th>
<th>Topic</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:20 am</td>
<td>Cristyan E Quiñones García</td>
<td>DD01 (Student) Role of Point Defects and Compensation in the Formation of Ohmic Contacts to Mg-Doped GaN</td>
</tr>
<tr>
<td>8:40 am</td>
<td>Amit P Shah</td>
<td>DD02 Effect of Rhenium Layer Thickness and Annealing Temperature on the Surface Microstructure of Re-Al-Ni-Au Based Ohmic Contacts on n-Type GaN</td>
</tr>
<tr>
<td>9:00 am</td>
<td>Taoufik Slimani Tiemcani</td>
<td>DD03 Development of Low Resistance Ohmic Contacts with Bilayer Ni/Al-Doped ZnO Thin Films to p-Type GaN</td>
</tr>
<tr>
<td>9:20 am</td>
<td>Nathaniel O’Neal</td>
<td>DD04 (Student, Late News) HTOL Reliability of Novel Re-GaN Schottky Diodes</td>
</tr>
<tr>
<td>9:40 am</td>
<td>Subhajit Mohanty</td>
<td>DD05 (Student, Late News) N-Polar GaN HEMTs with ALD HIO₃ as Gate Dielectric</td>
</tr>
<tr>
<td>10:00 am</td>
<td></td>
<td>BREAK</td>
</tr>
<tr>
<td>10:20 am</td>
<td>Emma Rocco</td>
<td>DD06 (Student) N-Polar GaN Photocathodes Stabilized with h-BN</td>
</tr>
<tr>
<td>10:40 am</td>
<td>Kaitian Zhang</td>
<td>DD07 (Student) Pulsed-Mode MOCVD Growth of ZnSn(Ga)N₃ and Determination of the Valence Band Offset with GaN</td>
</tr>
<tr>
<td>11:00 am</td>
<td>Elaheh Kheirandish</td>
<td>DD08 Novel Treatment of Raman and Photoluminescence Spectroscopy Analysis for Assessment of Electrical Characteristics of Mg Implanted-Annealed GaN</td>
</tr>
</tbody>
</table>

#### EE: Flexible, Printed, and Organic Electronic Materials and Devices

<table>
<thead>
<tr>
<th>Time</th>
<th>Name</th>
<th>Topic</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:20 am</td>
<td>William J Scheideler</td>
<td>EE01 Liquid Metal Printing of High Mobility 2D In₃O₂ for Flexible Electronics</td>
</tr>
<tr>
<td>8:40 am</td>
<td>Hyunwoo Choi</td>
<td>EE02 (Student) Surface Morphology Effects of Inkjet-Printed Silver Electrodes on the Contact Resistance of Printed Organic Thin-Film Transistors</td>
</tr>
<tr>
<td>9:00 am</td>
<td>Emma J. Renteria</td>
<td>EE03 Semiconductor Nanomembranes for Electromagnetic Interference Shielding Applications</td>
</tr>
<tr>
<td>9:20 am</td>
<td>Pushpa Raj Paudel</td>
<td>EE04 (Student) Substrate-Free Organic Electrochemical Transistors Based on Ionic Liquid Crystal Elastomer</td>
</tr>
<tr>
<td>9:40 am</td>
<td>Sheida Faraji</td>
<td>EE05 Exploration of New Classes of Solution-Processed High-K Dielectric Materials for Low-Power Electronics</td>
</tr>
<tr>
<td>10:00 am</td>
<td></td>
<td>BREAK</td>
</tr>
<tr>
<td>10:20 am</td>
<td>Benjamin K. Chang</td>
<td>EE06 (Student) Bandlike and Polaronic Charge Transport in Organic Crystals from First-Principles</td>
</tr>
<tr>
<td>10:40 am</td>
<td>Song Xu</td>
<td>EE07 PiFM—Nanoscale Chemical Mapping and Spectroscopy via AFM-IR for Ultrathin Organic Films</td>
</tr>
<tr>
<td>11:00 am</td>
<td>Tyler James Wiegand</td>
<td>EE08 (Student) Assessing the Contribution to OPV Efficiency of Energy Transfer in Charge Transfer Coupled H-Aggregates</td>
</tr>
<tr>
<td>11:20 am</td>
<td>Buang Zhang</td>
<td>EE09 (Student) Impact of Surfactant Choice on Polymer Emulsions, Thin-Film Morphology and LED Performance</td>
</tr>
<tr>
<td>11:40 am</td>
<td>Lucas Beagle</td>
<td>EE10 (Late News) Microwave-Facilitated Few-Layer COF/Monolayer TMD Heterostructures</td>
</tr>
<tr>
<td>Time</td>
<td>Name</td>
<td>Code</td>
</tr>
<tr>
<td>-------</td>
<td>-----------------------</td>
<td>------</td>
</tr>
<tr>
<td>8:20</td>
<td>Sushovan Dhara</td>
<td>FF01</td>
</tr>
<tr>
<td>8:40</td>
<td>Ming-Hsun Lee</td>
<td>FF02</td>
</tr>
<tr>
<td>9:00</td>
<td>Joseph Spencer</td>
<td>FF03</td>
</tr>
<tr>
<td>9:40</td>
<td>Michael Evan Liao</td>
<td>FF05</td>
</tr>
<tr>
<td>10:00</td>
<td>BREAK</td>
<td></td>
</tr>
<tr>
<td>10:20</td>
<td>Giulia Carini</td>
<td>FF06</td>
</tr>
<tr>
<td>10:40</td>
<td>Alan G Jacobs</td>
<td>FF07</td>
</tr>
<tr>
<td>11:00</td>
<td>Jacqueline Cooke</td>
<td>FF08</td>
</tr>
<tr>
<td>11:20</td>
<td>Daram N Ramdin</td>
<td>FF09</td>
</tr>
<tr>
<td>11:40</td>
<td>Cassandra Remple</td>
<td>FF10</td>
</tr>
<tr>
<td>8:20</td>
<td>Alec Mason Skipper</td>
<td>GG01</td>
</tr>
<tr>
<td>8:40</td>
<td>Subhashree Seth</td>
<td>GG02</td>
</tr>
<tr>
<td>9:00</td>
<td>Jun Tao</td>
<td>GG03</td>
</tr>
<tr>
<td>9:20</td>
<td>Ashlee Garcia</td>
<td>GG04</td>
</tr>
<tr>
<td>9:40</td>
<td>Yiteng Wang</td>
<td>GG05</td>
</tr>
<tr>
<td>10:00</td>
<td>BREAK</td>
<td></td>
</tr>
<tr>
<td>10:20</td>
<td>Mijung Kim</td>
<td>HH01</td>
</tr>
<tr>
<td>10:40</td>
<td>Hyun Uk Chae</td>
<td>HH02</td>
</tr>
<tr>
<td>11:00</td>
<td>Trent Garrett</td>
<td>HH03</td>
</tr>
<tr>
<td>11:20</td>
<td>Madison D Drake</td>
<td>HH04</td>
</tr>
<tr>
<td>11:40</td>
<td>Fatih Furkan Ince</td>
<td>HH05</td>
</tr>
</tbody>
</table>
**EXHIBITOR PROFILES**

**PERFORMANCE HALL**

<table>
<thead>
<tr>
<th>Wednesday</th>
<th>Thursday</th>
</tr>
</thead>
<tbody>
<tr>
<td>9:00 am – 12:00 pm</td>
<td>9:00 am – 12:00 pm</td>
</tr>
<tr>
<td>1:30 pm –  4:00 pm</td>
<td>1:30 pm –  4:00 pm</td>
</tr>
<tr>
<td>6:00 pm –  8:00 pm</td>
<td></td>
</tr>
</tbody>
</table>

---

**Gatan EDAX**  
[www.gatan.com](http://www.gatan.com)  
[www.edax.com](http://www.edax.com)

Gatan is the world’s leading manufacturer of instrumentation and software used to enhance and extend the operation and performance of electron microscopes. EDAX is a leading provider of innovative materials characterization systems encompassing Energy Dispersive Spectroscopy, Wavelength Dispersive Spectrometry, Electron Backscatter Diffraction, and X-ray Fluorescence. Gatan and EDAX are members of AMETEK’s Materials Analysis business unit.

---

**Klar Scientific, Inc.**  
[www.klarscientific.com](http://www.klarscientific.com)

**Key Products:** Point-and-shoot confocal spectroscopic microscopes; scanning, autofocus microscopes for mapping photoluminescence and Raman emissions; wavelength kits for 266nm through 975nm illumination; test and measurement services

Klar Scientific develops compact, affordable instruments designed for scientists who need spectral information with high spatial resolution. Klar microscopes provide photoluminescence (PL) and Raman mapping for excitation wavelengths from the deep-UV to near-IR. Klar also offers measurement services to provide clients with spectral maps of their samples.

---

**Lake Shore Cryotronics**  
[www.lakeshore.com](http://www.lakeshore.com)

**Key Products:** source measurement systems; cryogenic probe stations; hall effect measurement systems & instruments; modular characteristic systems; electromagnets; superconducting magnet systems; AC/DC current & voltage sources

A leading innovator of solutions for electronic material research, Lake Shore Cryotronics offers modular multichannel lock-in measurement systems for highly synchronized DC, 100 kHz AC and mixed DC + AC sourcing and measuring; cryogenic probe stations; systems and instruments for fast, highly precise Hall measurements; and modular characterization systems for electronic/electro-transport measurements.
Nextron Corporation  
www.microprobesystem.com

Key Products: Micro Probe System; Micro Optical Chamber; Humidity Control System; MFC Gas Control Stage; Pressure Control System; External XYZ Micropositioner.

Nextron has developed researcher-centered equipment, which is highly valuable. Micro Probe System is suitable to measure and analyze the electrical and optical properties of the materials under various environmental conditions; temperature, vacuum, humidity, gas flow, and irradiation of light.

United Mineral and Chemical Corp.  
www.umccorp.com

Key Products: MBE Source Materials; MBE Equipment; Dopants; PLD systems

United Mineral and Chemical Corporation is a leading supplier of ultra high purity, MBE grade ingots and metal sources including Arsenic, Red Phosphorus, Indium, Gallium, Aluminum, Antimony, Magnesium, Selenium, Silicon and Tellurium. Compounds of III-V materials are offered as well. UMC also represents Dr. Eberl MBE-Komponenten for MBE effusion cells, crackers, doping and sublimation sources as well as ancillary equipment and components. In additional, UMC also represents TSST for PLD systems and components used for thin film research.

Vacuum One (Veeco, Edwards, and MDC)  
www.vacuumone.com

Key Products: MBE Equipment and Sources; Vacuum Pumps and Gauges; Vacuum Components; Cryostats

Renishaw is a recognized leader in Raman spectroscopy, producing high performance Raman systems for a range of applications. We have decades of experience developing flexible Raman systems that give reliable results, even for the most challenging measurements. Whatever your Raman analysis requirements, Renishaw’s teams of scientists and engineers are here to provide you with expert advice, as well as product, technical, and applications support.

Wafer Technology  
www.wafertech.co.uk

Key Products: III-V Materials; GaAs; InAs; GaSb; InSb; InP; Polycrystal

Wafer Technology Ltd. is a U.K.-based producer of III-V materials and epitaxy-ready substrates, offering the widest product range in Europe. Wafer Technology’s unrivalled choice of material types and forms enables it to support almost any customer application.
We report correlated nanoscale-resolution imaging of doping and spatially-resolved analysis of composition and properties. Uniquely, our marker-layer approach enables the direct comparison of the laterally and vertically grown regions of non-planar junctions at a given point in time. In the laterally grown p-n junction each contribute to non-ideal behaviors of regrown p-n diodes, particularly excessive leakage current. However, a component of the regrowth interface. The unprecedented integration of spatially spreading resistance microscopy (SSRM) was used to generate a two-dimensional map of conductance with nanometer resolution. Cathodoluminescence (CL) mapping and spectroscopy provide about the wake-up, fatigue, and retention processes. Those that closely couple memory and logic. The talk will cover the rising energy consumption of computing, major gains are worldwide energy consumption. In the U.S., data centers alone are a "bottleneck" in moving instructions and data between separate logic and memory circuits. Computing accounts for 5 – 15% of the 3rd dimension in microelectronics for functions beyond microelectronics. These new materials, including Hf1-xZrxO2, Al1-xScxN, and Mg depletion in the limits is the quality of the regrowth interface, which is a significant present, the main challenge to achieving expected performance power diodes have been predicted for non-planar junction.
64th Electronic Materials Conference

EMC Awards Ceremony and Plenary Session
Session Chairs: Lisa Porter and Daniel Wasserman
Wednesday Morning, June 29, 2022
Arlie M. Griffin West Ballroom

8:20 AM EMC Awards Ceremony

8:30 AM *PL01
New Materials for Three-Dimensional Ferroelectric Microelectronics
Susan Trolle-McKinstry; The Pennsylvania State University, United States

In the last decade, there have been major changes in the families of ferroelectric materials available for integration with CMOS electronics. These new materials, including HfO₂, ZrO₂, Al₂O₃, AIN, AlₓOₓN, and Zn₁₋ₓMgₓO, offer the possibility of new functionalities. This talk will discuss the possibility of exploiting the 3rd dimension in microelectronics for functions beyond the present, the main challenge to achieving expected performance geometries that can be fabricated using selected area regrowth. At power diodes have been predicted for non-planar junction specific applications. High theoretical breakdown voltages in GaN play a crucial role in optimizing performance metrics tailored to electronics due to its intrinsic properties, but device geometry and memory circuits. Computing accounts for 5 – 15% of worldwide energy consumption. In the U.S., data centers alone are projected to consume approximately 73 billion kWh in 2020. While recent efficiency gains in hardware have partially mitigated the rising energy consumption of computing, major gains are achievable in a paradigm shift to 3D computing systems, especially those that closely couple memory and logic. The talk will cover the relevant materials, their deposition conditions, and what is known about the wake-up, fatigue, and retention processes.

9:20 AM Refreshment Break

SESSION A: Group III-Nitrides—Power Diodes
Session Chairs: Theeradetch Detchprohm and Russell Dupuis
Wednesday Morning, June 29, 2022
Great Hall Meeting Room 3

10:00 AM A01
Correlated Nanoscale Imaging of Doping, Conductivity and Cathodoluminescence in GaN p-n junctions Prepared by Selected Area Regrowth
Alexander Chang, Bingun Lu, Sizhen Wang, Sam Frisone, Rachel S. Goldman, Jung Hahn, and Lincoln Lauhon; Northwestern University, United States; Yale University, United States; University of Michigan, United States

GaN is an excellent platform for high-power high-frequency electronics due to its intrinsic properties, but device geometry plays crucial role in optimizing performance metrics tailored to specific applications. High theoretical breakdown voltages in power diodes have been predicted for non-planar junction geometries that can be fabricated using selected area regrowth. At present, the main challenge to achieving expected performance limits is the quality of the regrowth interface, which is a significant source of current leakage in regrown diodes. Prior studies have shown that unintentional donors, defects, and Mg depletion in the p-n junction each contribute to non-ideal behaviors of regrown p-n diodes, particularly excessive leakage current. However, a complete understanding of their relative impacts in distinct regions within the junction cannot be achieved without correlated, spatially-resolved analysis of composition and properties.

We report correlated nanoscale-resolution imaging of doping and conductivity in Mg-doped p-GaN regrowth that reveals how position-dependent non-idealities of the non-planar regrowth interface impact local electronic properties and ultimately the performance of devices. p-GaN was selectively regrown in n-GaN trenches formed by inductively coupled plasma etching with SiO₂ masks of variable mask-to-trench-width ratio. Atom probe tomography (APT) was used to analyze intentional and unintentional impurity distributions as a function of growth time and location by reconstructing the evolving shape of the growth surface with A1 marker layers, and cross-sectional scanning spreading resistance microscopy (SSRM) was used to generate a two-dimensional map of conductance with nanometer resolution. Cathodoluminescence (CL) mapping and spectroscopy provide further insights into the nature of Mg donors and the distribution of unintentional dopants. Uniquely, our marker-layer approach enables the direct comparison of the laterally and vertically grown regions of non-planar junctions at a given point in time. In the lateral junctions that form at the edges of the c-plane trenches, reduced Mg doping and unintentional oxygen doping create a compensation region that further broadens the junction and may contribute to increased tunnelling current under reverse bias. The spatial and temporal dependence of the oxygen concentration revealed by APT point to the SiO₂ mask as the source of the unintentional dopant. We identify that mask退mask materials, and maskless approaches are needed. We also conclude that residual sub-surface etching damage below the regrowth interface induces both n-type and p-type conductivity through carrier tunneling, broadening the p-n junction and establishing leakage pathways at the regrowth interface. The unprecedented integration of spatially resolved mapping of dopants, impurities, conductivity, and carrier type is a powerful approach to discriminating distinct factors that limit the performance of regrown diodes, enabling the rational optimization of process and device design.

10:20 AM A02
1.3 kV Vertical GaN p-i-n Rectifier with Nitrogen-Implanted Field Guard Ring Edge Termination
Minkyu Cho, Marzieh Bakhtiary-Noodeh, Chiyu Xu, Theeradetch Detchprohm, Russell Dupuis, and Shyh-Chiang Shen; Georgia Institute of Technology, United States

Vertical GaN p-i-n diodes with 1.3 kV breakdown voltage are presented. An AIXTRON 6 x 2" closely-coupled showerhead (CCS) metalorganic chemical vapor deposition (MOCVD) reactor was used for the epitaxial growth. The epitaxial structure was grown on a bulk GaN substrate with a low-dislocation density < 10⁶ cm⁻². The growth structure consists of 0.5 μm of n-GaN:Si ([n] = 6x10¹⁸ cm⁻³), 8.5 μm of GaN:uid drift layer, 0.45 μm of p-GaN:Mg ([p] = 1x10²⁰ cm⁻³), and 20 nm of p+GaN:Mg ([Mg] = 1x10²⁰ cm⁻³). Floating guard ring (FGR) structures were implemented in the study to prevent premature device breakdown under reverse bias. Both FGR widths and gaps were designed based on TCAD simulation to achieve a smooth potential profile during reverse breakdown. Multiple GaN p-i-n rectifiers were fabricated and characterized. The fabricated devices achieved forward voltage drop of 2.6 V and reverse breakdown voltage of 1.3 kV. Floating guard ring (FGR) structures were implemented in the study to prevent premature device breakdown under reverse bias. Both FGR widths and gaps were designed based on TCAD simulation to achieve a smooth potential profile during reverse breakdown. Multiple GaN p-i-n rectifiers were fabricated and characterized. The fabricated devices achieved forward voltage drop of 2.6 V and reverse breakdown voltage of 1.3 kV.
along the perpendicular direction to the device surface, and the depth was defined as a relative position from the p-n interface in the drift layer. The free carrier concentration in the drift layer increased as the position was located away from the p-n interface varying from $6 \times 10^{15}$ cm$^{-3}$ at 0.75 mm to $9 \times 10^{16}$ cm$^{-3}$ at 2.46 mm. The forward bias I-V characteristics showed a 3.3 V turn-on voltage at 100 A/cm$^2$ and a specific-on-resistance of 0.25 ohm cm$^2$. The minimum ideality factor was 1.24 at 2.74 V. The breakdown voltage was 1360 V as evaluated at the reverse current density of 0.01 A/cm$^2$. The Baliga Figure of Merit (BFOM) of the device is 7.4 GW/cm$^2$. M ore detailed statistical breakdown voltage distribution of the devices and analysis will be presented at the conference.

10:40 AM A03
1.6 kV Etched-and-Regrown GaN pn-Diodes Realized by Mitigation of Plasma Etch-Enhanced Deep Level Defects
Andrew M. Armstrong, Andrew Allerman, Mary H. Crawford, Greg Pickrell, Vincent A bate, Caleb Glaser and Trevor Smith; Sandia National Laboratories, United States

GaN offers increased power density for power electronics due to its larger band gap energy compared to Si. However, difficulties in selective area epitaxy limit the development of p-type GaN vertical devices. Ion implantation of Mg to form selective regions of p-type GaN has been demonstrated, but high operation with low leakage remains elusive. Selective-area epitaxy can also form p-regions in n-GaN by using inductively coupled plasma (ICP) etching followed by p-GaN regrowth, but etch-induced defects cause severe leakage.

Here, we show that ICP etching increases reverse leakage by increasing the concentration of a deep level defect, however, a slow reactive ion etching (RIE) following ICP etch can achieve low leakage and high voltage performance for etched-and regrown GaN diodes by removing ICP-enhanced defects. Steady-state photocapacitance (SSPC) measured an increased concentration of a defect state with an energy level at 1.9 eV below the conduction band for ICP etched-and-regrown pn-diodes compared to continuously-grown diodes. Increased defectivity correlated with increased reverse leakage. When the ICP etch was followed by the RIE etch, both the concentration of the 1.9 eV deep level and the reverse leakage in etched-and-regrown diodes were reduced to levels observed for continuously-grown diodes. Upon demonstrating improved performance with the RIE treatment, we fabricated etched-and-regrown diodes with a multi-step junction termination extension (JTE) to demonstrate high breakdown voltage (1610 V), excellent forward characteristics (ideality factor ~1.5), and lower specific-on-resistance (1.1 mohm cm$^2$).

GaN pn-diodes were grown by metal-organic chemical vapor deposition on free-standing n-GaN. The n-GaN drift region was 10 microns thick with a net donor density of $3 \times 10^{16}$ cm$^{-3}$. Following n-GaN growth, the surface was etched using Cl$_2$/BCl$_3$/Ar ICP. For one sample, termed ICP, a 0.4 micron thick p-GaN epi-layer with a M g concentration of $3 \times 10^{19}$ cm$^{-3}$ was regrown without any post-ICP treatment. Another sample, termed ICP+RIE+KOH, had nominally the same n-GaN drift growth, ICP etch, and p-GaN regrowth conditions, except that a slow RIE etch and subsequent KOH surface treatment was applied prior to p-GaN regrowth. The RIE etch depth was 270 nm using 45 sccm CF$_4$ + 5 sccm O$_2$, with 8 W RF power, resulting in a 0.3 A/s etch rate. The surface was then treated with KOH at 80 °C for 10 minutes. A continuously-grown pn-diode, termed CT, was also grown as a control sample. M esa diodes were studied using SSPC to correlate ICP-enhanced deep level defects and increased reverse leakage. A n ICP etch was used to form a mesa extending into the n-GaN drift with Pd/Au p-contacts on the p-GaN and a Ti/Ai n-contact on the wafer backside. Comparing the SSPC deep level spectra of the CT and ICP+RIE+KOH diodes revealed a $20 \times$ increase in concentration of the 1.9 eV deep level for the former. The reverse leakage for the ICP diode at 500 V also increased $>100 \times$ vs. CT. We attribute the increase in reverse leakage with ICP etch to recombination-generation current mediated by the ICP-enhanced 1.9 eV deep level. For the ICP+RIE sample, the 1.9 eV deep level concentration was 20x lower than for ICP, i.e., it recovered to the level in the as-grown CT sample. Further, the reverse leakage at 500 V for the ICP+RIE device was almost the same as the CT device. We conclude that the ICP-enhanced 1.9 eV deep level is the primary contributor to increased reverse leakage in etched-and-regrown GaN pn-diodes, and this deep level can be mitigated by post-ICP etch by RIE to recover epilayer quality and reverse leakage equivalent to that of continuously-grown diodes.

Finally, a multi-step JTE was included for another ICP+RIE sample, termed ICP+RIE+JTE, to maximize electrical performance, yielding the forward and reverse characteristics reported above.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA-0003525.

11:00 AM A04
(Student) Design, Manufacturability and Optimization of Hybrid Guard Ring-JTE Edge Terminations via Nitrogen Implantation in Epitaxial GaN PN Power Diodes
Matthew A. Porter, Mona Ebrish, Alan G. Jacobs, James C. Gallagher, Karl Hobart and Travis Anderson; Naval Postgraduate School, United States; U.S. Naval Research Laboratory, United States

Recent advances in bulk GaN substrate growth have enabled the wafer-scale fabrication of high current, high voltage vertical power devices with performance competitive with similar devices fabricated from SiC. However, significant work remains on optimization of vertical GaN power devices, specifically in the design and implementation of edge terminations which enable high voltage operation. As it is difficult to implement successfully activated p-type implants in GaN, vertical GaN power devices are typically fabricated after epitaxial growth of junctions. Wafer-level variations in doping and junction characteristics have been observed via long range optical techniques, which can greatly impact the performance and design of edge terminations. This work examines the design, manufacturability and optimization, using parametric TCAD simulation, of a novel hybrid bilayer junction termination extension with guard ring extensions, henceforth termed the hybrid GR-JTE in a 1.2 kV GaN PN power device design. The termination structure is formed via nitrogen implantation into the edge region of the junction. An exploration into the manufacturability of the hybrid GR-JTE was carried out with a focus upon the sensitivity of the breakdown voltage of the device as a function of the effective JTE dose remaining after nitrogen implant through variation of the effective anode thickness with a fixed doping of $1 \times 10^{12}$ cm$^{-3}$. Realistic implant damage profiles were derived from SRIM simulations of nitrogen implantation into GaN and modelled in TCAD as mid-gap states. A similar study of dose variation was also carried out through variation of anode doping at a fixed anode thickness of 500 nm. As a basis for comparison, both studies were repeated with a single implant bilayer JTE design. It was found that the hybrid GR-JTE decreased the sensitivity of the breakdown voltage to dose variation by 24% at a 1000 V threshold in comparison to the bilayer JTE design, using an experimental maskset as a basis for guard ring placement. The addition of guard-ring extensions to the JTE structure specifically decreases the dose sensitivity of the edge termination when the dose falls below the optimum for the JTE structure, due to the excess charge available within the guard ring structures. Further study of the influence of interface charge at the device surface demonstrates that breakdown voltage sensitivity is reduced in the hybrid GR-JTE structure due to screening effects of depletion at the top of guard ring structures. A comparison between experimental results on fabricated devices with either bilayer JTE or hybrid GR-JTE terminations is carried out to compare the predicted yield variation between the two designs. Additionally, a study of the optimization of the placement of
At 6.1 eV, aluminum nitride (AlN) boasts one of the widest known band gaps, which gives this material the unique potential to address needs in the fields of deep ultraviolet optoelectronics, high performance power conversion devices, radio frequency devices, and extreme environment semiconductor devices. Compared to other commonly used semiconductors (i.e., Si, SiC, GaN, and β-Ga2O3), AlN has the highest critical electric field and theoretical breakdown voltage, which lead to the highest Baliga’s and Johnson’s figures-of-merit (BFOM & JFOM). AlN also has the second highest saturation velocity and thermal conductivity. However, AlN is an insulator and has shown little promise to be converted to a semiconductor via doping during the long history of its study. Prior to this work, the main obstacle preventing the realization of many of AlN’s potential applications was the difficulty doping this material. N-type AlN has been reported in near surface regions and with bulk electron concentrations up to $10^{18}$ cm$^{-3}$, and p-type AlN ($p=3.1 \times 10^{18}$ cm$^{-3}$), 2) the highest ever reported bulk Si-defect reconfiguration, we have demonstrated: 1) substantial bulk p-type AlN ($p=6\times10^{18}$ cm$^{-3}$), 2) the highest ever reported bulk Si-doped n-type AlN ($n=6\times10^{18}$ cm$^{-3}$), and 3) the first AlN homojunction PN diode, with a nearly ideal turn-on voltage of $-6$ V.

Recently, we achieved Be-doped p-type AlN films with bulk hole concentrations up to $3.1 \times 10^{19}$ cm$^{-3}$ via the improved growth kinetics of metal modulated epitaxy (MME) demonstrating high quality films at low substrate temperatures, replicating our successes with p-type doping of GaN. Be is better suited for AlN due to the similar size of Al and Be and thus, reduced strain when substituting on a cation site. MME utilizes low substrate temperatures during growth to lower contamination normally resulting from outgassing of structural components in the growth chamber and controls the surface chemistry and kinetics to facilitate proper incorporation of the dopants on the cation sites. Additionally, we have demonstrated Si-doped n-type AlN films with bulk electron concentrations up to $6 \times 10^{18}$ cm$^{-3}$, completing the set of essential components needed for homojunction AlN diodes. Presently, low temperatures are believed to play a vital role in Si doping in that it may inhibit the formation of the Si-DX center, and similarly to the p-type case, the use of MME uniquely enables the realization of these highly doped n-type films with reduced compensation of Si.

Highly crystalline material is a pre-requisite for the growth of semiconducting AlN films and devices, but the well-known formation of surface oxides on AlN can result in a dense layer of stacking faults that create dislocations at the growth interface. We additionally report an eradication of these stacking faults by Al-assisted surface cleaning, which should further improve the electrical characteristics of the AlN films and devices. While excellent ohmic contacts have been developed to as-grown films, early PN diodes show high sheet resistance due to contact to plasma etched surfaces. Nevertheless, the PN diodes show $-6$ decades of rectification and turn on voltages of $-6$V as expected for a 6.1 eV semiconductor. The potential role of interface defects will also be detailed.

References

11:40 AM A06
(Student) Defect Microstructural and Diffusion Studies of AlGaN/GaN Microwave Anode—The Highest Bandgap Semiconductor Diodes Ever Demonstrated
Christopher M. Matthews, Habib Ahmad, Zachary Engel, Keisuke M otoki, Sangho Lee and W. Alan Doollittle; Georgia Institute of Technology, United States

The material properties of the $A$ AlGaN system, including its high band gaps, which gives this material the unique potential to produce fewer compensating impurities and reduce metastable defect reconfiguration, have been demonstrated: 1) substantial bulk p-type AlN ($p=3.1 \times 10^{18}$ cm$^{-3}$), 2) the highest ever reported bulk Si-doped n-type AlN ($n=6\times10^{18}$ cm$^{-3}$), and 3) the first AlN homojunction PN diode, with a nearly ideal turn-on voltage of $-6$ V. The material properties of the (Al)GaN system, including its high band gaps, which gives this material the unique potential to produce fewer compensating impurities and reduce metastable defect reconfiguration, have been demonstrated: 1) substantial bulk p-type AlN ($p=3.1 \times 10^{18}$ cm$^{-3}$), 2) the highest ever reported bulk Si-doped n-type AlN ($n=6\times10^{18}$ cm$^{-3}$), and 3) the first AlN homojunction PN diode, with a nearly ideal turn-on voltage of $-6$ V.

Recently, we achieved Be-doped p-type AlN films with bulk hole concentrations up to $3.1 \times 10^{19}$ cm$^{-3}$ via the improved growth kinetics of metal modulated epitaxy (MME) demonstrating high quality films at low substrate temperatures, replicating our successes with p-type doping of GaN. Be is better suited for AlN due to the similar size of Al and Be and thus, reduced strain when substituting on a cation site. MME utilizes low substrate temperatures during growth to lower contamination normally resulting from outgassing of structural components in the growth chamber and controls the surface chemistry and kinetics to facilitate proper incorporation of the dopants on the cation sites. Additionally, we have demonstrated Si-doped n-type AlN films with bulk electron concentrations up to $6 \times 10^{18}$ cm$^{-3}$, completing the set of essential components needed for homojunction AlN diodes. Presently, low temperatures are believed to play a vital role in Si doping in that it may inhibit the formation of the Si-DX center, and similarly to the p-type case, the use of MME uniquely enables the realization of these highly doped n-type films with reduced compensation of Si.

Highly crystalline material is a pre-requisite for the growth of semiconducting AlN films and devices, but the well-known formation of surface oxides on AlN can result in a dense layer of stacking faults that create dislocations at the growth interface. We additionally report an eradication of these stacking faults by Al-assisted surface cleaning, which should further improve the electrical characteristics of the AlN films and devices. While excellent ohmic contacts have been developed to as-grown films, early PN diodes show high sheet resistance due to contact to plasma etched surfaces. Nevertheless, the PN diodes show $-6$ decades of rectification and turn on voltages of $-6$V as expected for a 6.1 eV semiconductor. The potential role of interface defects will also be detailed.

References
The stacking sequences of some of the faults were determined as (...2, 3, 2, 3,...) and (...2, 3, 2,...) in the Zhdanov’s notation by high-resolution TEM (Fig. 3) showed that the high density of SFS in these towers act as strong sites of carrier recombination which is likely to have an impact on the on-state transfer characteristics of SiC devices. Furthermore, device electrical measurements have shown that this type of defect impacts the electrical performance of MOSFETs via an increase in the on-state resistance and a reduction of the breakdown voltage depending on the coverage percentage of the tower of defects in the active area of the device.

This study uses a multi-scale luminescence characterization approach coupled to a structural and electrical analysis to provide a detailed understanding of the optoelectronic properties, structural nature of this defect, and its adverse impact on 4H-SiC MOSFETs. The complete understanding of this defect is necessary to develop mitigation strategies and fulfill the potential advantages that 4H-SiC has to offer.

Summary

Silicon Carbide (SiC) MOSFETs, especially the 600 V class, are gaining increasing attention in the electric vehicles (EVs) market. The design of the JFET region is critical for the static and dynamic performances of the SiC power MOSFET. This work studies the impact of JFET region designs on the I-V and C-V performance of 650 V planar SiC MOSFETs. The ON-resistance, breakdown voltage, the gate to drain capacitance (Cgd), and oxide electric field during the off-state of the 650 V MOSFETs are studied through device characterization and TCAD simulation. The results suggest that the shortest possible JFET region and the smallest possible cell pitch combined with improved JFET doping leads to the lowest ON-resistance and Cgd.

Device Fabrication

The MOSFETs are fabricated on two 6-inch SiC wafers by a state-of-the-art commercial SiC foundry. A 7 µm, 2×1018 cm-3 doped n-type epitaxial layer on a 2×1019 cm-3 doped p-type substrate is used as the starting material. The substrate has been thinned to 170 µm after the front-side fabrication. The body of the MOSFET is defined by ion implantation. The n+ and p+ implanted doping concentrations are 1×1017 cm-2 and 1×1016 cm-2, respectively.

Experimental and Simulation Results

The 650 V MOSFETs are designed with JFET width of 0.8 µm, 1.0 µm, 1.2 µm, and 1.5 µm, which are named as A1 to A4 for devices on wafer I and B1 to B4 for devices on wafer II. For JFET width equals 1.2 µm, a tight design (A5 and B5) is applied by shrinking the channel length to 0.5 µm and reducing the ON-resistance of the devices. The orthogonal P+ layout topology is used for all devices. On-wafer measurements have been conducted on all devices. The transfer, output, and blocking characterizations are measured using the Keysight 1506A at room temperature. The threshold voltages are extracted using the linear extrapolation method. The measurement results show that the threshold variation is less than 1 V for devices on both wafers. The Ron,sp decreases with the increasing JFET width. With a specific JFET width, MOSFET on wafer I has higher Ron,sp compared with wafer II.

In this study, trapezoidal defects in 4H-SiC epitaxial layers were investigated by photoluminescence (PL) imaging, cathodoluminescence spectrum imaging (CLS), electron beam induced current (EBIC) imaging and by transmission electron microscopy (TEM) observation. The bar-shaped stacking faults were identified by the PL and CL measurements with peak emission wavelengths of ~420 nm and ~450 nm (Figs. 1, 2). The nature of the stacking faults is discussed using the luminescence results combined with movies showing expanding dislocations via the recombination enhanced dislocation glide mechanism. The expanding dislocations show that these towers of defects are made of a combination of Shockley-type and Frank-type stacking faults. The TEM analysis combined with movies of expanding stacking faults showed that trapezoidal defects come from the substrate and are present on multiple basal layers. The origin of this defect in the substrate is speculated based on our results and previous reports.
demands n- and p-channel MOSFETs is very appealing as its potential to operate efficiently at temperatures greater than 300 °C. Comprehensive investigations are needed.

Lower mobilities. But studies on such devices are scarce and more improvement of channel conductivity, and device stability.

Acknowledgment: This work is supported in part by the Block Gift Grant from II-VI Foundation.

10:00 AM 003 (Student) Channel Hole Scattering Processes in 4H-SiC MOSFETs Sunan Das, Ayaye A Hy, Marcello Kuruda and Sari Dhar; Auburn University, United States

Silicon Carbide (4H-SiC) has become the principal semiconductor of power electronics and extreme environment applications because of its physical properties such as wide bandgap, high breakdown electric field, and high thermal conductivity. 4H-SiC discrete devices such as diodes and metal-oxide semiconductor-field-effect transistors (MOSFETs) are currently very popular in high voltage power conversion in hybrid/electric vehicles and in various high-temperature sensor applications. On the other hand, the development of an integrated circuit (IC) technology based on 4H-SiC is relatively immature. 4H-SiC IC technology demands n- and p-channel MOSFETs is very appealing as its potential to operate efficiently at temperatures greater than 300 °C would enable various functions that are not accessible to conventional silicon-based technology. It has been established that, on n-channel 4H-SiC MOSFETs, nitridation of the SiO2/4H-SiC interface results in a reduction of near-interface trap density, improvement of channel conductivity, and device stability. Their p-channel counterparts, in contrast, have been reported to have lower mobilities. But studies on such devices are scarce and more comprehensive investigations are needed.

In this study, Hall measurements are used to determine the primary scattering processes for inversion layer holes in n-doped p-channel 4H-SiC MOSFETs produced on a moderately doped (6.2 × 10^15 cm^-3) substrate. Specifically, analysis of the Hall mobility (μ_Hall) by varying the body (substrate) bias and temperature was employed to determine the effective field (E_eff) dependence of μ_Hall for holes. Under strong inversion, mobility is characterized at a constant carrier concentration in order to keep the screening effect constant, yielding a surface roughness limited mobility with a power-law dependence on E_eff as -2.4, comparable to that of holes in silicon p-channel MOSFETs. At very low E_eff attained at a low negative body bias, i.e., near the onset of inversion, phonon scattering is observed to limit mobility, as evidenced by a temperature-dependent study. These new findings emphasize the importance of improved interface state density and fixed positive charge passivation in p-channel FETs, which would result in a lower threshold voltage for strong inversion, resulting in better channel conduction due to reduced E_eff.

Acknowledgment: The authors gratefully acknowledge the support from the National Renewable Energy Laboratory/US Department of Energy sub-contract NREL-AHL-9-92362-01.

References:

11:00 AM 004 (Student) Process-Induced Variability of SiC DMOSFET Short Circuit Capability Suvenu Nayak, Hema Lata Rao Mad Doshi, Swaroop Ganguly and Anant K. Agarwal; IIIT BOM BAY, India, The Ohio State University, United States

Summary: Among compound semiconductors, Silicon Carbide (SiC) is useful especially in the high voltage, fast switching applications. Like with all technology areas, as SiC MOSFET technology matures in terms of performance, questions of reliability and failure take on a more central role[1]. The short circuit (SC) capability addresses a key failure mechanism in these devices. The current and the lattice temperature of the device increase tremendously with the voltage stress leading to the device burning out. Among various reasons reported for this, the conducting paths created due to the melting of contacts (Aluminum) may be considered the most important factor [1]. This work, we investigate the effect of possible process-induced variability on SC capability by 2-D simulation.

Device and Simulation Setup: A generic 1200 V vertical SiC DMOSFET structure, shown in Fig. 1, is simulated in a non-isothermal environment of the TCAD platform to study the short circuit capability of the device. Thus, we have used the thermodynamic model in addition to the usual drift-diffusion for electrons and holes. The parameters for bulk and interface mobility, its degradation with temperature, and thermal parameters such as thermal conductivity and specific heat capacity have been taken from the experimental literature. The acceptor type interface trap (Q_a = 1.5 × 10^12 cm^-2) at E_c-E_f = 0.18 eV) and oxide fixed charge density 2 × 10^12 cm^-2 are defined at SiC/SiO2 for the simulation. The device is normally off type, and the important parameters are tabulated in Table 1.

Results: We consider the variability arising from two possible processes for self-aligned channel formation. The first, illustrated in Fig. 2.a, arises from the dry etch process used to form an oxide spacer which follows the p-well implant defined by the oxide hard mask. The spacer then acts as a hard mask during the n+-source region implant so as to define the channel (subtractive). The distance between the two p-well, in this case, is fixed. Thus, channel length variability, in this case, is towards the n-source side ('1'). The second, illustrated in Fig. 3.a, arises from a wet etch process to move back the oxide hard mask, which is used for the n-source implant. The shortened oxide now constitutes a hard mask for the p-well implant and thereby defines the channel (subtractive). The distance between the two n-source implants, in this case, is fixed. The channel length variability, in this case, is therefore from the JFET region side ('2'). The total cell pitch remains constant in both cases. We consider both a decrease and an increase of channel length from each side. Fig. 2.b shows the variability of type '1', while Fig. 3.b shows the variability of type '2'. The effect of these variability types on the SC capability is different and depends on the effective channel length, which here ranges from 0.3 to 0.7 μm. For type '1', the effective channel length increases and decreases with n-source, and most of the other device parameters are not affected as shown in Table 1. For type '2', the varied channel length is effectively changing the JFET dimensions. The combined effect is more pronounced which can be observed from the resulting SC curves. The SC capability of the device worsens with a decrease in channel length since that leads to higher currents. The results indicate that the additive method of fabrication is preferable for the SiC-based DMOSFET for reproducible SC performance.
Acknowledgement
This work was supported by the IIT Bombay-Ohio State Frontier Science and Engineering Research Center under "Towards the rugged SiC technology for electric transportation" project.

Reference

11:20 AM B05
Characterization of SiC-SiO2 Interface States in Commercial 4H-SiC Power MOSFETs from Cryogenic to High Temperature Hema Lata Rao M addi, Suvendu Nayak, J iashu Qian, Vishank Talesara, Y ibo Xu, M arvin H. White, Wu Lu and A nant K. Agarwal; The Ohio State University, United States

Summary
High-power Silicon Carbide (SiC) metal-oxide-semiconductor field-effect transistors (MOSFETs) have created considerable interest due to their high-speed switching capabilities, avalanche capability, and low on-resistance. In previous research [1], it was shown that the density of SiC/SiO2 interface states (Dit) which increases exponentially towards the conduction band edge (E_c) was primarily responsible for poor inversion layer electron mobility. D_c closer to the conduction band edge (E_c) can be determined at low temperatures by monitoring the deterioration of the subthreshold slope in the drain current versus gate voltage (ID-VGS) characteristics of MOSFETs. Alternatively, it may also be assessed from the change in threshold voltage (Vth) caused by temperature changes. The governing characteristics of planar gate MOSFETs at room and high temperatures have been studied in a number of studies, but few have looked at their performance at cryogenic temperatures. In this work, D_c near the E_c (E_c-E_F = 0.01eV) is measured for two different commercially available 1.2 kV MOSFETs using the threshold voltage change (ΔV th) caused by temperature variation. The temperature is varied from 80 K to 500 K using liquid nitrogen cryostat. The experimental setup includes a cryogenic probe station, a liquid nitrogen dewar, and B 1506A parameteric analyzer. The static characteristics (I_D-V GS) were measured, and the threshold voltage is extracted using the linear extrapolation method. The vendors with their respective voltage and current ratings are tabulated in Table 1.

Results and Discussion
Interface traps per unit area, ΔNint, can be calculated by the following equation,

\[ \Delta N_{int} = \frac{1}{2} \int \Delta D_T(\phi) \, d\phi = \frac{1}{2} \int (\Delta V_{th})_T \, d\phi \]

where \( \Delta V_{th} \) is determined at \( \phi = \phi_{th} \). The energy band diagram for low temperature (\( \phi_{th1} \) and room temperature (\( \phi_{th2} \)) in Fig. 1, represents the Fermi potential change (\( \Delta \phi_F \)) for the corresponding temperatures.

At low temperature, the Fermi level (E_f) moves closer to the valence band (E_v) in the p-type bulk. Consequently, at \( \phi = \phi_{th} \), more band bending is necessary to induce sufficient carrier density at the surface. Conversely, at high temperatures, E_f moves away from the valence band and therefore the required band bending is less. As the temperature increases, electron concentration in the conduction band increases due to the detrapping of the carriers from the interface states above E_f. This results in fewer negative charges at the interface, leading to a decrease in threshold voltage. The I_D-V GS and \( V_{th} \) variation within a temperature range of 80 K to 500 K for vendors “C” and “E” is shown in Fig.2, Fig.3, and Fig.4 respectively. D_c distributions of devices from vendors “C” and “E” are shown in Fig.5. Lowering the temperature leads to an increase in \( V_{th} \), as expected. The exponential increase in \( D_c \) towards the conduction band edge is visible as the temperature is lowered to 80 K. The Fermi level enters the conduction band around 100K based on the electrostatic calculations. In our study, due to the lack of process information from vendors, our estimation of the gate oxide thickness was based on the ramp-to-breakdown measurement and an assumption of 2 x 1015/cm² for P-base doping. As observed, the \( D_c \) value for vendor “C” is higher than vendor “E” which can also be predicted from a higher threshold voltage variation (\( \Delta V_{th} \)) in vendor “C” as compared to 3.64 V in vendor “E” for the entire range of measured temperatures, attributing to the process of gate oxide formation and annealing.

References:

Acknowledgment: The funding from the Vehicle Technology Office at the US Department of Energy, Washington DC is gratefully acknowledged.

11:40 AM B06
(Student) Recombination Centers in 4H-SiC pin Diodes Observed by Electrically Detected Magnetic Resistance and Near-Zero Field Magnetoresistance A. Ashton Purcell3, Fedor V. Sharov4, Patrick M. Lelahni4 and Jacob Biju2; 1The Pennsylvania State University, United States; 2GE Global Research, United States

Over the last two decades there has been a growing interest in the implementation of 4H-SiC in high power and high temperature applications. This is primarily due to its relatively large bandgap of 3.26 eV. A device of particular interest in high field applications is the pin diode. Although recombination centers play an important role in these devices, relatively little is known about their chemical and physical nature. We report on the observation of recombination centers in 4H-SiC based pin diodes using electrically detected magnetic resonance (EDMR) and near-zero field magnetoresistance (NZFM R). Our results show the presence of at least two physically distinct recombination centers. Our EDMR measurements utilize spin dependent recombination induced changes in device current associated with electron-hole recombination in these devices. EDMR spectra have significant analytical power because they closely match that of well understood conventional EPR spectra. In these magnetic resonance measurements, defect identification is possible due to perturbations to the environment of unpaired electrons in point defects, such as deep level recombination centers. An unpaired electron which is otherwise unaffected by its environment would have a magnetic resonance condition described by a microwave frequency expressed by \( h \nu = g \mu_B \) Here, \( g \) is a constant called the Landé g factor, \( h \) is Planck’s constant, and \( \mu_B \) is the Bohr magneton. For a defect in a semiconductor this simple expression is altered by the local environment. For the situation of interest in our study, the two main perturbations to the isolated electron case come from spin-orbit coupling and electron-nuclear hyperfine interactions.

In our study, we report on EDMR associated with recombination events caused by magnetic resonance at deep level defects involved in electron-hole recombination; this type of EDMR is called spin dependent recombination (SDR). In SDR the rate of electron-hole recombination events is increased by the magnetic resonance induced “flipping” of unpaired electrons at deep level sites [1]. This electron spin flipping results in measurable changes in device current. We report X-band (9.5GHz) EDMR as well as on the physically related NZFMR response of 4H-SiC pin diodes. The EDMR spectra exhibit a nearly isotropic () spectrum which is almost certainly due to silicon vacancies [2]. We observe an additional strong EDMR spectrum which has a magnetic field orientation dependent which has somewhat higher values which extend to at least 0. We tentatively ascribe this spectrum to an intrinsic defect but cannot yet provide a more specific identification. In addition, we report on NZFMR results which
provide information about the bias-dependent kinetics of the SDR process within the intrinsic region of the diodes. The results may be of particular use for the fields of deep-space and quantum magnetometry.


consumption. Flexibility is one of the key properties for expanded applications. For example, in gas pressure sensing, the closed-loop in gas inlet or outlet network can be utilized using a flexible sensor located on the diaphragm. The flexible piezoelectric sensors have been reported with several materials for normal condition utilization. However, for extremely high-temperature regions, above 500 °C, sensing materials are limited. Although lead zirconate titanate (PZT) is the most dominant piezoelectric material by its high piezoelectric coefficients, which enable to generate higher output voltages, it is not available for high-temperature operation due to its low Curie temperature (T_{C}). Zinc oxide (ZnO) and polyvinylidene fluoride (PVDF)-based piezoelectric materials have another barrier for sensing at high temperatures. ZnO is reported to increase oxygen vacancies as the temperature rises and PVDF has low melting (~200 °C) and boiling point (375 °C). III-N thin films offer the potential for high-temperature operation thanks to their wide bandgap energy, permanent spontaneous polarization, and low electrical conductivity. Especially, single-crystalline gallium nitride (GaN) piezoelectric thin film has been reported to show excellent output voltage up to 400 °C, indicating outstanding sensitivity, rapid response time by a high electromechanical coupling factor, chemical and mechanical long-term stability, high thermal resistance, and excellent biocompatibility. With wider bandgap III-N materials, the benefit is expected to be further extended to higher temperatures.

In this study, we developed and demonstrated piezoelectric AlN thin-film sensors with high flexibility for the detection of gas pressures at extremely high temperatures. Crack-free AlN epitaxial layer was grown by metalorganic chemical vapor deposition. Flexible III-N thin films were fabricated by a layer transfer method from the rigid silicon to flexible copper foil substrate. They were analyzed by X-ray diffraction to reveal their crystalline quality without phase defect or defects. The single sensor was attached to the diaphragm of the fitting tool and located in the furnace. The operating condition of the sensor was controlled from low to high temperature with various gas pressures. The long-term stability of the sensor was evaluated using fixed temperature and pressure levels. The simulation was conducted by software to support the results at each temperature and pressure. The flexible III-N piezoelectric sensors with high endurance at extreme conditions can be further applied in several applications such as aerospace and defense fields.

11:00 AM C04
(Student) Flexible Modified Carbon Nanotube/Nanofiber-Based Triboelectric Nanogenerator | Julia I. Salas Toledo, Karen Lozano and M. Jaimi Uddin; The University of Texas Rio Grande Valley, United States

Flexible triboelectric nanogenerators (TENGs) are the next generation of devices for energy harvesting on wearable and portable electronics. This study presents how the properties of carbon nanotubes (CNT) can enhance the performance of flexible and stretchable triboelectric nanogenerators (TENGs), when it is incorporated into one of the nanofiber layers. These nanofiber layers consisted in Polyvinylidene fluoride (PVDF), which was considered as the negative triboelectric layer, and Thermoplastic Polyurethane (TPU) as the positive, and in which the CNT was incorporated. Both nanofiber layers used were prepared using the Forcespinning® technique. The morphology and structure were characterized through SEM, EDX and XRD and triboelectric properties were characterized, and produced a maximum of 164V in an open circuit at 180 bpm, in contact area of 2.0 x 2.0 in square. PVDF/TPU-CNT, shows potential and versatility in the application of everyday energy harvesting from its flexibility and stretchability.

11:20 AM C06
(Student) Detection of the Nitrogen Cycle Using the Metabolic Activity of Shewanella Oneidensis MR-1 | Lauren Brady, James Lozano and M. Jasmin Uddin; Rensselaer Polytechnic Institute, United States

The presence of excess nutrients in freshwater and marine ecosystems can have significant detrimental effects including altering the dynamics of microbial communities and food-webs, and promoting the formation of harmful algal blooms which can produce toxins that are harmful for fish, wildlife, and humans. Scientists in diverse fields including chemistry, microbiology, and engineering have noted the capacity to detect the presence and concentration of many of these nutrients, or other chemicals of environmental concern, by electrochemically interfacing with microbes that metabolize these chemicals. The dissimilatory metal-reducing bacterium *Shewanella oneidensis* MR-1 is a particularly versatile model organism capable of both aerobic and anaerobic respiration, dissimilatory metal reduction, participation in the microbial nitrogen cycle, and direct electron transfer to or from a biased electrode. In this study, a porous carbon fiber electrode capable of supporting 3D biofilm growth is combined with several correlated electrochemical techniques to detect nitrogen cycle activity via the metabolic activity of *Shewanella*.

*Shewanella oneidensis* MR-1 was grown in 800mL batch culture jars each containing a working, reference, and counter electrode. Batches containing *Shewanella* inoculum were compared to a sterile control. The jars were left at room temperature for 24 days, with no clear indication of biofilm formation. Next, a 0.2V bias voltage was applied in accordance with prior studies indicating that this bias voltage would activate *Shewanella* cytochrome gene expression [1][2]. Cyclic Voltammetry (CV) was used to electrochemically investigate the electron transfer processes within the system. A DC biocurrent appeared in the inoculated batches that did not occur in the sterile batches. It is believed that the increase in biocurrent was based on reduction by *Shewanella*’s nitrate and nitrite reductases. Results also showed evidence of a CV peak at +180mV vs. Ag/AgCl Electrode which could also be represented as +790 mV vs. Standard Hydrogen Electrode that occurred in batches inoculated with *Shewanella* but not in sterile batches. This peak matches the reduction potential of denitrification (NO₂⁻ reduction to N₂) and concurs with earlier studies indicating the capacity for *Shewanella* to engage in denitrification [3][4]. Thus, the preliminary results indicate that a DC biocurrent is created in the presence of *Shewanella* and the nitrogen cycle processes can be identified using electrochemical measurement techniques such as cyclic voltammetry to verify the reduction of nitrates. Ultimately this work may lead to more cost-effective and versatile chemical sensors for detecting various environmental pollutants in-situ.

References:

11:40 AM C06
(Students) Wearable Eye Movement Sensors Using Flexible and Biocompatible III-N Thin Films for Personal Safety, Healthcare Monitoring and Abnormality Diagnosis Nam-In Kim, Jie Chen, Mina Moadminia, Sara Pouladi and Jae-Hyun Ryu; University of Houston, United States

Personal healthcare is increasingly important in the medical field to detect the symptoms from specific diseases for the diagnosis of early-stage disorders. A biorural physiological signals including pulse rate, blood pressure, body temperature, muscle movement, and respiration can be the source for symptoms. For example, real-time pulse monitoring is a possible technique for people with a high risk of cardiovascular diseases. Likewise, among the signals, abnormal eye movement and blinking are related to several brain-related disorders, such as attention deficit hyperactivity disorder (ADHD), stroke, autism, Alzheimer’s disease (AD), and Parkinson’s disease (PD). Thus, monitoring of eye-related motions and movements opens a way to diagnose at an early stage from the symptoms of the slow eye movement, sluggish blinking from external stimulus. Current eye-tracking systems (ETSs) for sensing eye movements and blinking demand complex devices such as helmets, headgear, or goggles, high-resolution cameras, and image processing software. These requirements are the main limitation for monitoring eye-related motion at home with a user-friendly system.

Flexible epidermic sensors can address the shortcomings of present ETS. Specifically, piezoelectric sensors with skin-attachability and wearability have inherent merits in size, weight, power, and cost. Thin-film-based piezoelectric skin-attachable sensors using lead zirconate titanate (PZT) and zinc oxide (ZnO) are inappropriate due to their disadvantages. The toxic lead element is one of the components for PZT crystal and lead can be absorbed in human skin, which is poisonous. Sensors attached to the skin have to contain non-toxic elements. ZnO-based sensors exhibit relatively low output value, sensitivity, and resolution, which requires post-processing steps. As an alternative material, group III-N thin films are very promising to detect physical motion. Furthermore, a single piezoelectric sensor with single-crystalline gallium nitride (GaN) was reported with attachment on the temple area to monitor the eye blinking and lateral eyeball movement. In this study, our skin-attachable and wearable sensors were fabricated as array format developing the single sensor. A rayable sensors were attached to 3 different temple areas (upper, middle, and lower temple) to monitor the several types of eyeball movements including lateral, vertical, diagonal, and rotational direction. All the results from each sensor are distinguishable, which indicates that the sensors generated different values of output signals from each position with varied stimuli.

SESSION D: Gallium Oxide Devices

10:00 AM D01
(Students) Demonstration of Self-Aligned Delta Doped MISFETs with Current Density > 550 mA/mm Nidhin Kurian Kalarickal, A shok V. Dheenan, Joe F. Mclgone, Andreas Fiedler, Sushovan Dhara, Mark Brenner, Steven A. Ringel and Siddharth Rajan; The Ohio State University, United States

We report on the design and demonstration of β-Ga2O3 self aligned delta doped MISFETs with current density exceeding 550 mA/mm using plasma assisted MBE growth. Self aligned devices were fabricated using gate recess of heavily doped β-Ga2O3 access regions using in-situ etching, followed by formation of spacer layers using ALD Al2O3.

With a high theoretical breakdown field of 8 MV/cm, β-Ga2O3 is highly promising for applications in power switching and high power RF electronics. High-performance devices require high current density and low on-resistance, but previously reported β-Ga2O3 based transistors fabricated on native substrates were limited to ~300 mA/mm. In this report we demonstrate the use of self-aligned gate structure to enable state-of-art current densities exceeding 550 mA/mm.

The growth was carried out in a Riber M7 MBE system equipped with a Vecco O2 plasma source. The epitaxial structure consists of 30 nm Mg doped β-Ga2O3 layer, 500 nm UID β-Ga2O3 layer, 2 Si delta doped channels separated by 5 nm, 45 nm UID β-Ga2O3 cap layer and 45 nm n++ β-Ga2O3 layer. The device fabrication was initiated by ohmic contact formation to the n++ β-Ga2O3 layer using Ti/Au (30/100 nm) followed by annealing at 470 under N2 for 1 min. Device isolation was later carried out by using BCl3/Ar based dry etch. 200 nm PECVD SiN x was then deposited to form the hard mask for the gate recess etch. The recess etch of 60 nm was carried out using Ga etching using atomic Ga flux in an MBE chamber [Applied Physics Letters 119.12 (2021): 123503] at a Tsub of 500 °C. Following the recess etch, Tsub was lowered to 400 °C and 10 nm of Al2O3 was deposited as the gate dielectric. To form the sidewall dielectric spacers, 60 nm Al2O3 was deposited followed by RIE etching and wet etching (1:10 BOE) to remove it from the gate region, leaving 50 nm of Al2O3 on the gate-side walls. Gates were then defined using 150 nm Ni to partially cover the source and drain access regions.

Transfer length measurements showed a contact resistance of 0.2 Ω.mm for metal to n++ access region and low sheet resistance of 122 Ω/sq for the n++ access region. In addition, contact resistance of ~1 Ω.mm is estimated as the contact resistance between the delta doped channel and n++ access region. The channel sheet resistance post gate recess etch is measured to be 3170 Ω/sq indicating complete removal of the access region above the channel. Capacitance-voltage measurements (100 kHz) indicate a distance of ~52 nm from the gate electrode to the 1st delta doped channel. Transistors I-V characteristics show high current density of 560 mA/mm for devices with gate length of 0.6 μm and source-drain spacing of 2 μm, similar to the two-terminal (un gated) current density. This is the highest reported current density obtained in lateral β-Ga2O3 transistors on native substrates. Significant self heating effects causing drop in current density is also observed above 5 V of drain voltage. Due to the high channel charge density, low on/off ratio between 2 and 3 orders is obtained in the present study, suggesting that further engineering of the channel and dielectric layers is necessary to improve this. In summary, we demonstrated β-Ga2O3 self aligned delta doped MISFETs using a novel low-damage atomic Ga-flux etching.
The promise of Ga2O3 to deliver high power, high efficiency, low breakdown, fast switching, and high output power. Following our demonstration of delta-doped (AlxGa1-x)2O3/Ga2O3 heterojunction field-effect transistors (HFETs) held exceptional promise for a new generation of high power electronics due to its high theoretical electric breakdown field of 8 MV/cm, availability of native melt-grown substrates and ease of n-type doping across a wide range of concentrations [App. Phys. Lett. 112.6 (2018): 064041]. Although p-type conductivity is unfeasible due to a large hole effective mass, doping with deep acceptor-like impurities suitable for device applications. Despite the ultra-wide energy gap of Ga2O3 alloys, shallow donors (e.g. Si) have enabled n-type doping of these films. Furthermore, a two-dimensional electron gas (2DEG) can form via the delta doping approach, similar to early AIGaS/GaAs heterostructures. Thus, Ga2O3-based delta-doped heterojunction field-effect transistors (HFETs) grown via the ozone-assisted molecular beam epitaxy technique (O3-MBE) [3], in this follow-up work we have performed the following experiments. We have performed O3-MBE growth of β-(AlxGa1-x)2O3 (010) and (100) β-Ga2O3 simultaneously in order to evaluate critical thickness limits for β-(AlxGa1-x)2O3 as a function of substrate orientation, Al mole fraction (5-20%) and β-(AlxGa1-x)2O3 film thickness (50-400 nm). Above a certain thickness, epitaxial AIGaO suffered from cracks whose density increased as the AIGaO film grew thicker. Films grown on (100) Ga2O3 exhibited cracking at much lower thickness than films grown on (100) Ga2O3. This observation agreed with the work of Mu et al. [4, 5], who suggested an Griffith criterion in order to provide a critical thickness lower bound for β-AIGaO/GO based on crystal fracture strength g, elastic constants Gxy and strain components ε.

For HFET device fabrication, samples of β-(AlxGa1-x)2O3/Ga2O3 with (AlxGa1-x)2O3 barrier layer thickness of 21 nm and Al mole fraction x of 16.8-18.8% were grown via O3-MBE [6]. Electrochemical capacitance-voltage measurements, performed on calibration samples grown on conductive substrate, showed a single carrier peak with concentration of 2x10^{19} cm^{-3}. Room temperature Hall measurements performed on HFET structures grown on Fe-doped substrate resulted in sheet resistance Rs = 10763 Ω sq^{-1}, sheet carrierg concentration of 9.55x10^{13} cm^{-2}, with mobility of 61 cm²/V s. Ohmic contacts with specific contact resistivity of 4.6x10^{-4} Ω cm² were formed via Si ion implantation and activation annealing at 925 °C for 30 min in N2, followed by Ti/Au lift-off and contact anneal on 47 °C for 1 min in N2. Prior to metal deposition, HFET devices did not utilize ion implantation and were observed to have severely degraded over the course of several months, likely due to interfacial TiO2 formation as reported by Lee and Peterson for the case of Ga2O3 [7]. Lateral HFETs were processed with a 20 nm thick ALD Al2O3 gate dielectric layer and 150 nm of Ti/Au metal stack. Current-voltage characteristics, and Fig. 3 shows open-gated average channel temperature as a function of drain bias (VDS = 0 V) measured via scanning thermal microscopy. [1] S. J. Higashigushi, K. Jensen, Appl. Phys. Lett. 112, 064041 (2018). [3] M. J. Tadjer et al., J. Vac. Sci. Technol. A 39, 033402 (2021). [4] A. A. Griffith, Philos. Trans. R. Soc. London, Ser. A 221, 163 (1921). [5] S. Mu et al., APL Mater. 8, 091105 (2020). [6] Y. Oshima et al., Appl. Phys. Expr. 9, 061102 (2016). [7] M. H. Lee, R. L. Peterson, ACS Appl. Mater. Interfaces 2020, 12, 41, 46277-46287.
pinch-off voltage of -5 V. On/off ratio was 10^6 and limited by the gate leakage, indicating that the Mg delta-doping at the substrate-growth interface was successful in suppressing the source leakage. In summary, we have demonstrated well-controlled Mg doping over a range of concentrations in β-Ga2O3 grown by MBE. Mg doping was also shown to compensate unintentional donors and form insulating buffer layers for lateral FETs.

This work was funded by Department of Energy / National Nuclear Security Administration under Award Number(s) DE-NA000392 and the AFOSR GAME MURI Award No. FA9550-18-1-0479, program manager Dr. Ali Sayri.

11:00 AM D04
Electrical Characteristics and Band Alignment of n-Si/n-Ga2O3 Heterojunction Fabricated by Surface-Activated Bonding
Zhenwei Wang1, Daiki Takasaki1, Jinho Liang3, Takahiro Kitaoka1, Mototeru Shigekawa4 and Masatada Higashikawa1
1National Institute of Information and Communications Technology, Japan; 2Osaka City University, Japan

β-Ga2O3-based power devices have been studied intensively in recent years, owing to its wide bandgap of 4.5 eV and the availability of single-crystal wafers produced from melt-grown bulks. On the other hand, the lack of p-type conductivity is one of the serious technical challenges in terms of its physical properties in developing a variety of Ga2O3 devices. Utilization of other p-type semiconductors as components of the Ga2O3 device structures would be one of the possible solutions for this fundamental issue. Fabrication of high-quality heterostructures between Ga2O3 and dissimilar material by epitaxial growth, however, is often hindered by large mismatches in lattice constant and thermal expansion coefficient. In this work, for the first time, we fabricated n-Si/n-Ga2O3 heterostructures by using room-temperature surface-activated bonding (SAB) process instead of epitaxial growth and studied their electrical characteristics to investigate the quality and band alignment of the heterojunction. It is expected that in the case of two semiconductors with fully different lattice parameters, the SAB can provide better-quality heterojunctions compared with epitaxial growth, because it is free from limitations of the mismatches. Note that this is the first step to explore the possibility of using n- and/or p-Si as components of Ga2O3 device structures.

The n-Si/n-Ga2O3 heterostructures were fabricated by SAB using an n-Ga2O3 (001) substrate and an n-Si (100)-on-insulator substrate. For characterization of electrical properties, the bonded substrate was processed into test structures with n-Si pillars on the n-Ga2O3 substrate. Ohmic electrodes were fabricated on top n-Si and bottom n-Ga2O3 sides. Cross-sectional transmission electron microscopy observation revealed that an intermediate amorphous layer with a thickness of about 2 nm was formed at the bonding interface. Rectifying current density–voltage (J–V) characteristics were obtained, suggesting that there was an energy barrier in the electron transport path due to negative charges existing at the interface. Furthermore, depletion regions were formed in both n-Si and n-Ga2O3 layers due to the negative charge at the interface. This study proposes that SAB can be an alternative technique to epitaxial growth for fabricating Ga2O3-based heterostructures with dissimilar material having major differences in lattice parameters, and that the SAB heterostructures would expand the design possibility of Ga2O3 device structures.

This work was supported in part by JSPS KAKENHI Grant Number 19H01282.

11:20 AM D05
(Student) Beta-Gallium Oxide Junction Barrier Schottky Diodes with Sputtered P-Type Nickel Oxide
Joseph Spencer1,2, Boyan Wang3, Ming Xiao3, Alan G. Jacobs3, Alyssa M. Cook3, James C. Gallagher4, Karl Hobart5, Khoi Sasaki6, Akito Kuramata7, Yuhao Zhang4 and Margo Tadjar3
1Virginia Tech, United States; 2U. S. Naval Research Laboratory, United States; 3Weber State University, United States; 4Novel Crystal Technology, Japan

Gallium oxide (GO) has become a widely researched ultra-wide bandgap semiconductor in both the material and electronic power device fields. The popularity of GO is due in part to its ability for melt growth, growth of high quality homoepitaxial drift layers on native substrates, and the prospect of higher breakdown strength than other wide band gap materials such as gallium nitride (GaN) and silicon carbide (SiC). However, one key disadvantage of GO is the inability to achieve p-type doping due to its flat valence band structure and self-trapping of holes [1]. This fundamental limitation of GO technology precludes the development of PN junctions for this material. Recently, p-type nickel oxide (NiO) heterojunctions with GO were reported for the first time by Afonso et al. [2]. For this paper, we report the development of p-type NiO via sputtering and demonstrate GO/NiO Junction Barrier Schottky (JBS) diodes with high forward current density and a breakdown voltage of around 600V.

Prior to device fabrication, NiO thin films were RF-sputtered on silicon substrates and modeled using spectroscopic ellipsometry to confirm bandgap, optical constants, and film thickness. NiO thin films were sputtered on p-type Si to characterize carrier type and free carrier concentration using the capacitance-voltage technique and a Hg probe instrument. Hall effect measurements were employed for resistivity characterization using evaporated Ni/Au Ohmic contacts. However, determining carrier concentration and mobility using Hall effect technique was found to be unreliable due to low mobility and very low Hall voltage values.

JBS diodes were fabricated on ~10 μm thick high dielectric oxide phase (GO) films that were doped around 2×10^16 cm^-3. The GO was etched using inductively-coupled BC1 plasma to produce 400 nm deep trenches before NiO deposition by RF sputtering at room temperature and lift-off. NiO-filled GO trenches were 2 μm wide; GO trench pitch was 2, 4, and 6 μm. In addition, NiO was deposited for edge termination around the annular devices. Schottky and PIN diodes were fabricated alongside the JBS diodes as control devices used to confirm proper JBS diode operation.

Initial I–V testing of devices under forward bias showed a JBS diode with a turn-on voltage nearly identical to the Schottky diode. PIN diodes displayed a higher turn-on voltage than both the Schottky and JBS diodes, as expected. All three types of diodes reached a current density of 100 A/cm² before either series resistance or testing compliance limited forward current density. Reverse bias testing was carried out in Fluorinert, where the best performing JBS diodes reached a reverse bias of 600 V at which point the reverse compliance of 10 μA was reached. Catastrophic breakdown was not reached for the best performing device. PIN diodes reached breakdown voltages up to -650 V before breaking down or reaching compliance. However, these PIN diodes exhibited substantial reverse leakage with increasing reverse bias and need to be investigated further. The best performing Schottky diodes achieved V_{BR} - 500 V before compliance was reached.

Further device testing and analysis of both the PIN and Schottky diodes is needed in order to better characterize the JBS diodes. An immediate area of concern is the quality of the sputtered NiO as
Recently, β-Ga2O3 has attracted great attention as a promising candidate for high power switching applications. However, two main challenges of β-Ga2O3 are its relatively low electron mobility (180 cm²V⁻¹s⁻¹) and low thermal conductivity (10-30 W/m-K) [1], [2]. Additionally, p-type doping does not seem feasible currently for this material system. On the other hand, GaN, a well-known wide bandgap semiconductor, has a high electron mobility (2050 cm²V⁻¹s⁻¹), high 2D charge (2DEG) density, moderate thermal conductivity (135 W/m-K), and the availability of p-type doping [3]. Therefore, the integration of β-Ga2O3 with GaN can potentially enable the fabrication of novel GaN/Ga2O3 high-frequency and high-power devices combining the merits of both GaN and Ga2O3 in addition to novel optoelectronic devices.

This work integrated single-crystal (0001) N-polar GaN and (-210) UID β-Ga2O3 substrates via wafer bonding using ZnO interlayer deposited by atomic layer deposition (ALD). Both 5×5 mm² GaN and 10×10 mm² Ga2O3 substrates were cleaned in acetone, isopropanol alcohol, and de-ionized water with ultra-sonication, followed by soaking in buffered hydrofluoric acid (BHF) for 10 seconds. The samples were then loaded immediately into the ALD chamber to minimize any surface contamination. The 10 nm-thick ZnO was deposited on both N-polar GaN and (-201) Ga2O3 samples via thermal ALD at 200 °C. Next, the Ga2O3 and GaN samples were placed into contact with each other and transferred to an EVC 510 bonding chamber. The bonding was conducted at 400 °C under the pressure of 4 MPa in vacuum for 3 hours. The surfaces were 100% fully bonded. A thermal bonding, both the front and back sides of the sample were evaporated by Ti/Au 20/200 nm. To investigate the impact of post-annealing temperature on the quality of bonding interfaces, the N-polar GaN/ZnO/Ga2O3 test structure was annealed in N2 for 30 minutes at various temperatures of 600 °C and 900 °C with ramping up and down rates of 2 °C/min. Temperature dependent I-V measurements were performed on the GaN/ZnO/Ga2O3 test structure at temperatures from 300 K to 650 K with step increment of 25 K. A bonded sample without annealing demonstrated Schottky behavior, indicating a conduction band barrier between Ga2O3 and ZnO. As temperature increased, the turn-on voltage decreased because the number of electrons with the required energy to pass over the Schottky barrier increases at higher temperatures. The Schottky barrier of around 0.56 eV was extracted from a linear fit to the Richardson plot. The test structure showed a deviation of I-V curves before and after temperature dependent measurement (up to 650 K) and the I-V characteristics recovered after 48 hrs. This could be explained by the existence of slow traps at the bonded interfaces. After annealing at 600 °C, the I-V curves showed almost linear behaviors, indicating that the test structure could be modeled by a series resistor. The maximum current density of 0.02 A/cm² at V_DSS = 6 V and the resistance of 1714 Ω were measured at room temperature. Additionally, increasing the annealing temperature to 900 °C caused a substantial change in the I-V-T characteristics, exhibiting a significant conduction band barrier occurring at the GaN/ZnO interface. This is probably associated with the recrystallization of amorphous ZnO interlayer during high temperature annealing [4]. This work reported the heterogeneous integration of single-crystal GaN and β-Ga2O3 substrates with ALD ZnO interlayer which shows promises for the development of novel GaN/Ga2O3 high-frequency and high-power devices beyond 5G applications.

11:40 AM D06
(Student, Late News) Heterogeneous Integration of Single-Crystal β-Ga2O3 and N-Polar GaN Substrates with ZnO Interlayer Deposited by Atomic Layer Deposition Zhe Ashley Jian1, Christopher Clymore2, Daphne A gapolu3, Umesh M Ishra3 and Elaheh Ahamdi1; 1University of Michigan–Ann Arbor, United States; 2University of California, Santa Barbara, United States; 3INRS, Canada

This work integrated single-crystal (0001) N-polar GaN and (-201) Ga2O3 substrates via wafer bonding using ZnO interlayer deposited by atomic layer deposition (ALD). Both 5×5 mm² GaN and 10×10 mm² Ga2O3 substrates were cleaned in acetone, isopropanol alcohol, and de-ionized water with ultra-sonication, followed by soaking in buffered hydrofluoric acid (BHF) for 10 seconds. The samples were then loaded immediately into the ALD chamber to minimize any surface contamination. The 10 nm-thick ZnO was deposited on both N-polar GaN and (-201) Ga2O3 samples via thermal ALD at 200 °C. Next, the Ga2O3 and GaN samples were placed into contact with each other and transferred to an EVC 510 bonding chamber. The bonding was conducted at 400 °C under the pressure of 4 MPa in vacuum for 3 hours. The surfaces were 100% fully bonded. A thermal bonding, both the front and back sides of the sample were evaporated by Ti/Au 20/200 nm. To investigate the impact of post-annealing temperature on the quality of bonding interfaces, the N-polar GaN/ZnO/Ga2O3 test structure was annealed in N2 for 30 minutes at various temperatures of 600 °C and 900 °C with ramping up and down rates of 2 °C/min. Temperature dependent I-V measurements were performed on the GaN/ZnO/Ga2O3 test structure at temperatures from 300 K to 650 K with step increment of 25 K. A bonded sample without annealing demonstrated Schottky behavior, indicating a conduction band barrier between Ga2O3 and ZnO. As temperature increased, the turn-on voltage decreased because the number of electrons with the required energy to pass over the Schottky barrier increases at higher temperatures. The Schottky barrier of around 0.56 eV was extracted from a linear fit to the Richardson plot. The test structure showed a deviation of I-V curves before and after temperature dependent measurement (up to 650 K) and the I-V characteristics recovered after 48 hrs. This could be explained by the existence of slow traps at the bonded interfaces. After annealing at 600 °C, the I-V curves showed almost linear behaviors, indicating that the test structure could be modeled by a series resistor. The maximum current density of 0.02 A/cm² at V_DSS = 6 V and the resistance of 1714 Ω were measured at room temperature. Additionally, increasing the annealing temperature to 900 °C caused a substantial change in the I-V-T characteristics, exhibiting a significant conduction band barrier occurring at the GaN/ZnO interface. This is probably associated with the recrystallization of amorphous ZnO interlayer during high temperature annealing [4]. This work reported the heterogeneous integration of single-crystal GaN and β-Ga2O3 substrates with ALD ZnO interlayer which shows promises for the development of novel GaN/Ga2O3 high-frequency and high-power devices beyond 5G applications.

Reference:

SESSION E: Dielectrics and Multifunctional Oxides
Session Chairs: Doug Hall and Patrick Leman
Wednesday Morning, June 29, 2022
Senate Chamber
Transparent conducting oxides (TCO) are critical components in display and photovoltaic technologies requiring simultaneously high visible light transmission and low electrical resistance. SrVO₃ has recently emerged as a promising TCO material that can be incorporated into heterostructures as an epitaxial thin film with high optical transparency and electrical conductivity. Epitaxial SrVO₃ films were formed by crystallizing amorphous layers deposited on SrTiO₃(001) using solid-phase epitaxy (SPE). Thermodynamic calculations predicting the temperature and oxygen partial pressure conditions required to produce the SrVO₃ phase match the experimental conditions. The lattice parameters and mosaic angular width of x-ray reflections from crystallized films exhibit a strain that depends on the film thickness, with 16 and 60 nm films being fully and partially strained, respectively. SrVO₃ layers with 16 nm thickness exhibited a room temperature resistivity of 5.2 × 10⁻⁵ Ω cm and visible light transmission of 99%. Increasing the film thickness resulted in lower room temperature resistivity and a significant reduction in optical transparency. Temperature-dependent resistivity measurements between 5 K and 300 K reveal residual resistivity ratios of 3.8 and 2 for 16 and 60 nm SrVO₃ layers, respectively, suggesting that defect scattering dominates low temperature transport but has a limited effect on room temperature transport properties.

High Transparent Conductor Figure-of-Merit for SrVO₃ Grown by Solid-Phase Epitaxy

Samuel Marks¹, Lin Lin¹, Peng Zuo², Patrick Strohbehn¹, Dongrue Du¹, Jason Waldvogel¹, Ryan Jacobs¹, Donald Savage¹, Susan Babcock¹, John Booske¹, Jason Kawai² and Paul E. Vans¹; ¹University of Wisconsin-Madison, United States; ²University of Wisconsin, United States

10:20 AM E02

The authors gratefully acknowledge support from NSF grant DM R-18-00130.


11:00 AM E04

(Staff) Controlling Charge Distributions near Complex Oxide Interfaces via Defect Engineering

Brenton A. Noesges¹, Daeu Lee¹, Hongwei Wang¹, Thaddeus J. Ase³, Jinbo Pan¹, Jungwoo Lee¹, Qimin Yan¹, Xi Fan Wu¹, Chang-Beom Eom¹ and Leonard J. Brillson¹; ¹The Ohio State University, United States; ²University of Wisconsin-Madison, United States; ³Temple University, United States

Complex oxide electronics are attractive for next generation devices because high mobility conducting interfaces can be achieved between ultrathin layers of otherwise insulating materials. SrTiO₃ is at the center of these applications but defects impacting the properties of SrTiO₃ films can also play a significant role in heterointerfaces involving SrTiO₃ or at junctions between SrTiO₃ and non-stoichiometric SrTiO₃. Defect formation impacts electron performance at interfaces and within ultra-thin layers. The conducting interface between LaAlO₃ & SrTiO₃ is one key example of the impact of defects where the interfacial 2D hole gas (2DHG) wasn’t observed until O vacancies (Vₒ) were sufficiently decreased near the interface. Vₒ donate at least one e⁻ per site which compensates free holes near the interface. Consequently, the interplay of cation defects can be used to control the balance of acceptor-type defects alongside Vₒ which tune n-type carrier density. Using depth-resolved cathodoluminescence spectroscopy (DRCLS), we determined how reducing Sr content in SrₓTiO₃ (0.98 ≤ x ≤ 1.00) films grown on SrTiO₃ impacted defects and electronic structure extending from the Sr-deficient eplayer to tens of nanometers below the interface. DRCLS allowed us to simultaneously measure multiple defect states with optical transitions corresponding to Vₒ, Sr vacancies (Vₛr), Ti on Sr antisites (TiSr) and Ti³⁺. As expected, [Vₒ] increased with decreasing Sr content. At the same time, [TISr] also increased with increasing [Vₛr] indicating Ti filled in Sr vacancy sites. The increase in the acceptor-type [Vₛr] anticolorates with [TISr] as excess electrons which could reduce Ti³⁺ to Ti²⁺ are instead compensated by extra holes from Vₒ. The anti-correlation suggests Vₒ and other acceptor-type defects could balance Vₒ and improve control over free carrier densities. Differential DRCLS (DDRCLS) showed how
the interplay of defects within the epilayer created depth- & Sr-dependent changes in defect densities extending tens of nanometers beneath the interface. DDRCLS is an extension of DRCLS that removes the luminescence contribution of epilayers when studying buried regions. Increasing accumulation of V in the Sr-deficient epilayers suppressed Ti+ within the epilayer but also impacted the distribution of Ti+ extending into the substrate. Control over nanoscale defect-induced charge distributions can advance new device features such as 2DHGs and the performance of existing devices such as ferroelectric tunnel junctions. This study shows how DDRCLS directly measures the relative densities and spatial distributions of multiple native defects within and extending away from nanoscale SrTiO3/SrTiO3 junctions and how their interplay varies with controlled epitaxial growth. These growth-dependent defect variations can help guide SrTiO3 epitaxial growth with other complex oxides. Controlling the interplay of these defects can improve mobility at 2D electron gases (2DEGs) formed between LaO0.65Sr0.35TiO3 and TiO2 sites can be created by increasing the inlet pressure of metal-organic Ti precursor gas which suppresses the amount of V & O, in turn leading to mobility improvements at the interface. Controlled growth to directly observe, introduce, and manipulate both cation and anion-related native point defects on a nanometer scale provides a new avenue to improve the interfaces of SrTiO3 with other complex oxides. This control extends to the defects themselves acting as scattering centers that degrade conductivity or alternatively, wave function overlaps between, e.g., lattice sites for quantum communication. The authors gratefully acknowledge support from NSF grant DM R-18-00130.

11:20 AM E05
(Student, Late News) Mechanothermal Synthesis and Characterization of Ti-Doped Bismuth Ferrite Using Nano-Agitator Milling Process
Lyndon E. Smith, Vijaya Rangari and Shaik Jeelani; Tuskegee University, United States

Using a novel milling process, Ti-doped bismuth ferrite was synthesized with a nominal composition of BiFe0.95Ti0.05O3. Precursor powders were milled for different durations and analyzed using X-ray diffraction and SEM/EDAX before and after calcination. XRD revealed the formation of Bi5(Fe4Ti3)O15 during milling. The powders were calcined at 600°C for 5 hours in air, and the XRD pattern after calcination matched well with the reported JCPDS file for Bi5(Fe4Ti3)O15. The powder was then characterized using XRD, XPS, TEM, and photoluminescence (PL) techniques. Contrary to this, the Pr ions appeared in the HfO2 phase only. This latter was transformed into cubic one upon annealing at 1050°C, while at higher annealing temperature, the formation of monoclinic HfO2 phase was detected. The shape of RE-related PL spectra followed the structural transformation. Narrow RE-related PL peaks were detected in the samples annealed at 1000-1100°C that confirms the location of RE ions in the phase with a high crystal field. The peculiarities of PL spectra and the mechanism of phase separation for different films are discussed.

11:40 AM E06
On the Impact of Impurities’ Nature and Annealing Conditions on Structural and Optical Properties of Hafnia-Based Thin Films
Tetyana V. Torchynska1, Leonardo V. Vega2, M. acosta2, Georgiy Polupan3, Manuel Alejandro Garcia Andrade3, Nadia Korsunska2, Xavier Porter4, Fabrice Gourbilleau2 and Larysa Khomenkova1; 1Macotela1, 2V. Lashkaryov Institute of Semiconductor Physics (Kyiv, Ukraine), Ukraine; 3CIMAP/ENSICAEN, France; 4National University “Kyiv-Mohyla academy”, Ukraine

A mong transition metal oxides, hafnia (HfO2) is mainly considered as the dielectric alternative to silicon dioxide owing to their high dielectric constant. However, HfO2 based materials offer a high refractive index in visible and near infrared range that are promising for photonic applications. For this purpose, the stabilization of the amorphous HfO2 structure is required to minimize the optical losses in the HfO2 based optical components. Since HfO2 is an ionic material, for the stabilization of its amorphous structure the use of silicon is preferable due to the flexibility of covalent Si-O bonds. Earlier, we have reported on the effect of Si content on the formation of Hf silicate host. It turned out that increase of Si content from about 3 at% to 6 at% favours the formation of amorphous HfO2 phase stable upon annealing at ~600°C, whereas the further increase of Si content up to 12 at % stimulates the formation of Hf silicate with amorphous structure stable up to 900°C. It is known that the tetragonal and cubic structure of HfO2 can be stabilized by the introduction of trivalent elements. In this case, electrical neutrality is achieved via the formation of oxygen vacancies, i.e. one vacancy for two dopant elements. At the same time, the interaction between different ions and their redistribution upon high-temperature annealing were not well addressed.

In this report structural transformation of HfO2 thin films doped with silicon and lanthanides (RE) is considered in terms of the evolution of optical and light-emitting properties of these materials. The films were grown on Si substrates by radio frequency magnetron sputtering in argon plasma and annealed at T = 600-1100°C for t = 15-60 min in an inert atmosphere. The transformation of film properties was studied by means of XRD, XPS, TEM and photoluminescence (PL) techniques. For HfO2 films doped with RE ions, the stabilization of the tetragonal HfO2 phase in annealed films was observed contrary to the monoclinic structure of pure HfO2 films. The main reason responsible for this phenomenon is the formation of oxygen vacancies. For RE-doped HfSiOx films, phase separation between SiOx and HfO2 occurs upon annealing. For Nd or Er-doped films, the presence of RE ions was detected in SiOx and HfO2 phases. Contrary to this, the Pr ions appeared in the HfO2 phase only. This latter was transformed into cubic one upon annealing at 1050°C, while at higher annealing temperature, the formation of monoclinic HfO2 phase was detected. The shape of RE-related PL spectra followed the structural transformation. Narrow RE-related PL peaks were detected in the samples annealed at 1000-1100°C that confirms the location of RE ions in the phase with a high crystal field. The peculiarities of PL spectra and the mechanism of phase separation for different films are discussed.
Giant photo-plasticity has been understood for decades, but giant photo-elasticity has remained a mystery. We find that the giant photo-elastic effect arises from strong immunity at point defects. Our results are supported by density functional theory (DFT) and finite element analysis (FEA) simulations. We also find that deep traps can be engineered as functional elements for two-terminal resistive switches. Point defects that feature giant Stark effects exhibit bistable behavior, and can switch between deep and shallow configurations (DX centers are a well-known example), a phenomenon we call defect level switching (DLS). We demonstrate a DLS device based on CdS that switches from high- to low-conductivity at a small forward bias of <0.5 V; this normally-on behavior is qualitatively unlike most resistive devices such as Gunn diodes. We further show how bistable, DLS behavior can be incorporated into a semiconductor device simulation to enable predictive design of nonlinear, hysteretic devices with qualitatively new behavior. We will conclude with discussions of how these opto-mechanical and resistive switching effects may be useful for applications.

**10:20 AM F02**

(Stadent) **Dislocations Altering the Microstructure and Luminescence of InAs Quantum Dots on Silicon**

Eamonn T. Hughes1, Gunnar Kusch2, Jennifer Selvidge1, Bastien Bonet1, Justin Norman1, John Bowers1, Rachel A. Oliver2, and Kunal Mukherjee3; 1University of California, Santa Barbara, United States; 2University of Cambridge, United Kingdom; 3Stanford University, United States

Dislocations strongly impact the degradation behavior of direct epitaxial III-V on silicon lasers. While much attention has been placed on the density of threading dislocations to improve performance and reliability, there has been less focus on how dislocations can alter the structure of the active region itself to negatively impact parameters such as carrier confinement, gain, and linewidth enhancement factor. Here, we study the impact of dislocations on luminescence in a model system consisting of a GaAs buffer on silicon with a single InAs quantum dot (QD) layer near the surface, looking particularly at how dislocations, both local and distant alter the emission intensity and wavelength both by their immediate physical presence but also through secondary effects like structural alterations induced during growth.

In this model structure, we observe the presence and growth of local misfit dislocations (MDs) just below the QD layer in situ by cathodoluminescence (CL). These MDs are not the result of relaxation of the QD layer during growth; instead, they form during cooldown after growth as the structure develops tensile strain due to a mismatch in thermal expansion between the silicon substrate and GaAs-based film. This enables existing threading dislocations (TDs) to glide, aided by energy injected by the scanning electron beam, but the TD segment passing through the QD layer is pinned, so only the lower segment can glide, forming a MD at the base of the QD layer. Continuous-wave (CW) CL shows these MDs as dark line defects. With time-resolved cathodoluminescence (TRCL) mapping using a pulsed electron source, we measure the carrier lifetime across this same region and find that reduced lifetimes associated with non-radiative recombination at MDs are closely correlated with reduced emission intensity.

Looking more broadly at CW CL intensity maps, we see that in addition to the sharp dark lines caused by MDs next to the QD layer, there is an additional diffuse crosshatch pattern of dimmed emission. A map of the peak emission wavelength shows that the crosshatch is blue shifted 15-30 meV. Importantly however, the sharper dark lines caused by local MDs are not measurably blue shifted. We hypothesize that these crosshatch features are caused by extended strain fields from the MD network at a defect filter layer that lies about 700 nm below the QD layer. This strain does not directly impact the emission wavelength but rather alters the growth of the QDs, perhaps making them smaller or modifying their composition. The local MDs, by contrast, form after growth during cooldown and therefore do not impact QD growth.

In addition to growth alterations due to the strain from distant misfit dislocation networks, clusters of sessile threading dislocations with a screw component form hillocks during growth that also impact emission properties. These hillocks are associated with strongly reduced CW CL emission and also a blue-shift in emission wavelength, which may be explained by an increased surface step density surrounding the hillock providing additional nucleation sites for QDs, leading to a higher density of smaller QDs forming here. We further examine these regions by atom probe tomography (APT), but due to the small volume analyzed, we do not capture any QDs and therefore cannot comment on changes in QD size or composition. We do find, however, that the encasing QW is about 25% wider in the hillock region, although the hillock and defect-free regions have similar morphological profiles. The ground state energy level of this thicker QW should be lower and therefore closer to the QD energy states, which could allow for easier thermalization of carriers out of the QDs, thus dimming the region. By combining multiple characterization techniques, we reveal multiple understudied impacts of dislocations on QD emission properties and, in doing so, identify potential avenues to enhancing device performance and reliability.

**10:40 AM F03**

(Stadent) **Defects with Mg Segregation in Mg-Implanted GaN**

Kenny Huynh1, Michael E. Liao2, James Tweedie2, Pramod Reddy2, Matthew H. Breckengridge1, Ramon Collazo3, Zlatko Sitar4, Michael Bockowski5, and Mark Goorsky1; 1University of California, Los Angeles, United States; 2Drexel Materials, United States; 3North Carolina State University, United States; 4Institute of High Pressure Physics of the Polish Academy of Sciences, Poland

In this work, high resolution x-ray scattering and transmission electron microscopy are used to understand the implant-induced strain recovery process and to mitigate the formation of extended defects that cause a degradation in dopant activation efficiency in Mg implanted GaN. Mg ions with a box profile at a total dose level of 1 x 10^{15} cm^{-2} were implanted in homoepitaxial GaN grown on high quality ammonothermal GaN substrates. Post-implantation annealing was performed at 1300 °C, 1400 °C, and 1500 °C for a duration of either 10 minutes or 100 minutes. An ultra-high N pressure of 1 GPa was applied to prevent GaN from decomposition without using a dielectric cap. Ongoing electrical measurements show that annealing at 1400 °C leads to higher dopant activation (~3% at room temperature, ~70% at 500 °C) compared to annealing at 1300 °C (~0.1% at room temperature, ~10% at 500 °C). The triple axis x-ray ω/2θ scans near GaN (0004) peak shows that the implant-induced strain is fully relieved after annealing at 1300 °C for 10 min. Annealing at higher temperatures and longer times, however, does not have any further impact on the strain state. Two beam condition STEM bright field images show residual defects, after annealing at 1300 °C for 10 min, which consist of inversion domains. The inversion domains appear in two morphologies, pyramidal and trapezoidal. High resolution TEM images show that the pyramidal inversion domains (PID) have their base along GaN (0001) plane with facets along the (1123) planes. Energy Dispersive X-Ray Spectroscopy maps and line scans at the PID show an increase in Mg signal close to the base of the PID, where an extra layer of atoms is located, with a decrease in the Ga signal at the same position. The trapezoidal inversion domains (TID) also show base and facets that are similar to the PID. EDX maps and line scans at the TID also revealed Mg segregation near the base. The center part of a TID consists of a series of parallel-aligned pyramids. We speculate that the TIDs are the initial stages of development and will eventually evolve into the PIDs. Thus, both the PIDs and TIDs trap and make inactive Mg atoms and cause a
degradation in Mg activation efficiency. Similar defects have been observed in highly Mg-doped epitaxial layers [1-3]. However, in those structures, it is difficult to remove or suppress the formation of the PIDs unless low growth temperatures are used, such as for metal-modulated epitaxy [4].

However, the PIDs and TIDs are not observed in any of the samples annealed at and above 1400 °C. This suggests that the PIDs and TIDs are thermodynamically unstable and are formed at lower temperatures or would not form at such high temperatures (≥ 1400 °C). This provides insight for improving dopant activation efficiency with annealing temperature ≥ 1400 °C. The prominent residual defects after annealing at and above 1400 °C are dislocation loops. EDX at the dislocation loops shows no sign of Mg segregation. Meanwhile, an overall decreasing trend in the dislocation loop density is observed after annealing at a higher temperature or for a longer time. The loop density measured decreased from 3.8 x 10^9 cm^-2 for 1400 °C 10 min, to 1.5 x 10^9 cm^-2 for 1400 °C 100 min, and further to 1.1 x 10^9 cm^-2 for 1500 °C 10 min. Results from this work are expected to help understand the key steps to achieve high activation efficiency p-type doping for planar, vertical device structures in a scalable framework. This research was supported through the ARA-P-E PNDIODES program under contract DE-AR0001116 at UCLA.

References:

11:00 AM F04

(Student) Growth of High Indium Percentage InGaSb on InP Substrates Using the Interfacial Misfit Dislocation Array Growth Mode

Fatih F. Ince1, Alexander T. Newell1,2, Kevin J. Reilly1, Subhashree Sethi1, Thomas J. Rotter1, Ahmad M ansoroi2, Sadhvikas Addamane1, Darryl Simha1, Leonid Miroshnik1, Brian Rummel1, Andrew Li2, Talid Sinnen2, Sange M. Han2 and Ganesh Balakrishnan1; 1The University of New Mexico, United States; 2Air Force Research Laboratory, United States; 3Sanda National Laboratories, United States; 4University of Pennsylvania, United States

The ability to access lattice constants around 6.3 Å using antimonide alloys such as InAsSb, can result in M WIR and L WIR detectors, which can be used for remote sensing, medical devices or material sciences. Fully relaxed lattice constants between 6.09 Å and 6.47 Å cannot be achieved due to the lack of substrates with these lattice parameters. An approach that has been used in the past is to grow metamorphic buffers, such as those based on InGaSb or AlInSb, through single-step or step-graded approaches to realize lattice constants around 6.17 Å. In this presentation, we make use of the interfacial misfit (IM F) dislocation array-based growth mode to grow In0.53Ga0.47Sb directly on In0.53Ga0.47As/InP. The IMF growth mode is based on the replacement of the As layer with Sb under highly controlled growth conditions. In the case of other systems, such as GaSb on GaAs, this growth mode results in 108 dislocations/cm², with instantaneous relaxation, and reduces to 108 dislocations/cm² by using defect filter layers. This is achieved by the formation of a highly periodic misfit dislocation array between the GaSb and GaAs layers that almost fully accommodates the mismatch. Several publications by various authors have shown cross-section transmission electron micrograph (X-TEM) analysis and selective area diffraction analysis of the growth, showing complete and spontaneous relaxation of the GaSb epitaxial film. Similar to GaSb/GaAs, the objective in this work is to realize high-quality In0.53Ga0.47Sb directly on In0.53Ga0.47As/InP. Successful validation of such a growth mode facilitates the growth of detectors and lasers at this lattice constant.

The MBE growth on undoped InP substrates starts with thermal oxide removal at 540 °C and subsequent growth of a 500 nm thick lattice-matched In0.53Ga0.47As layer on which the In0.53Ga0.47Sb layer is grown. The antimony for arsenic exchange happens similarly to the growth mode on GaSb. Once the InGaSb layer is completed, the arsenic supply is closed for 30 seconds, and the wafer is maintained at 490 °C to allow for the complete desorption of excess arsenic. In the case of GaSb on GaAs, after the introduction of antimony, RHEED characterization shows a distinct 2x8 reconstruction, which is an excellent visual guide to indicate that the IMF has been formed. In the case of In0.53Ga0.47Sb/In0.53Ga0.47As, the lower growth temperatures result in an unclear 2x8 transition, therefore, we cannot rely on RHEED to guide this process. This could mean arsenic is not completely desorbing, such that the interfacial layer is some composition of InGaAsSb.

We present the analysis of such samples grown at various growth temperatures. The baseline structure is grown with the InGaSb at 400 °C, followed by two subsequent growths at 360 °C and 460 °C. In all of these samples, surface morphology, cross-section TEM, HR-XRD, and photoluminescence studies are performed. The presence of the IMF layers is seen very clearly in several samples; however, the expected spacing of 6.2 nm cannot be verified. This could be due to the non-ideal desorption of the arsenic layer in these structures. The XRD analysis of all three samples indicates a fully relaxed In0.53Ga0.47Sb, however, there is a significant peak broadening. TEM analysis of the 400 °C growth shows a periodic misfit dislocation array along the interface. However, for higher atomic-resolution TEM images, we see several different crystal orientations, which indicates the possibility of compositional segregation driven by miscibility gap issues. This presentation provides an in-depth analysis of TEM and photoluminescence characterization of IMF grown InGaSb on InP structures. In addition, we show how phase segregation due to miscibility gap issues associated with high-indium content impacts crystallographic morphology. We will also present results from our recent efforts to suppress segregation due to miscibility gaps.

11:20 AM F05

(Student) Remote Si Doping of InGaAs Nanowires for Topological Quantum Computing

Chunyi Huang1, Didem Dedê2, Martin Friedl1, Anna Fontcuberta i Morral1 and Lincoln Lauthon1; 1Northwestern University, United States; 2EPFL, Switzerland

The manipulation of Majorana zero modes in networks of semiconductor nanowires is a promising route to quantum computing. We have previously demonstrated wafer-scale growth of branched InGaAs nanowires supported on GaAs nanomembranes. However, Si dopants segregated at the nanowire/membrane interface, which contributes to alloy scattering. Moreover, the nanowire morphology was not well controlled. In the present work, we addressed the challenge of simultaneously controlling nanowire morphology and dopant distribution and developed a process to precisely position dopants beneath a well-defined InGaAs channel. InGaAs nanowires were again grown on GaAs membranes, but Al marker layers were used to visualize the growth interface post-growth and infer the growth process. Prior to Si doping, the growth temperature was lowered to suppress Si diffusion, and then a dilute AlGaAs layer was grown immediately after doping to trap excess Si on the growth interface. Following growth of a GaAs spacer to separate the dopants from the channel, the temperature was increased to grow the In0.53Ga0.47As nanowire. In-plane atom probe tomography (APT) analysis found that Si doping during nanowire formation leads to Si segregation on the (111) growth surface, pushing dopants to the top of the nanowire. In follow-up work, enhanced carrier mobilities were realized in nanowires by remote doping of the supporting GaAs nanomembranes. Moreover, Si dopants segregated at the nanowire/membrane interface, which contributes to alloy scattering. Moreover, the nanowire morphology was not well controlled. In the present work, we addressed the challenge of simultaneously controlling nanowire morphology and dopant distribution and developed a process to precisely position dopants beneath a well-defined InGaAs channel. InGaAs nanowires were again grown on GaAs membranes, but Al marker layers were used to visualize the growth interface post-growth and infer the growth process. Prior to Si doping, the growth temperature was lowered to suppress Si diffusion, and then a dilute AlGaAs layer was grown immediately after doping to trap excess Si on the growth interface. Following growth of a GaAs spacer to separate the dopants from the channel, the temperature was increased to grow the In0.53Ga0.47As nanowire. In-plane atom probe tomography (APT) analysis found that Si doping during nanowire formation leads to Si segregation on the (111) growth surface, pushing dopants to the top of the nanowire. In follow-up work, enhanced carrier mobilities were realized in nanowires by remote doping of the supporting GaAs nanomembranes. However, the expected spacing of 6.2 nm cannot be verified. This could be due to the non-ideal desorption of the arsenic layer in these structures. The XRD analysis of all three samples indicates a fully relaxed In0.53Ga0.47Sb, however, there is a significant peak broadening. TEM analysis of the 400 °C growth shows a periodic misfit dislocation array along the interface. However, for higher atomic-resolution TEM images, we see several different crystal orientations, which indicates the possibility of compositional segregation driven by miscibility gap issues. This presentation provides an in-depth analysis of TEM and photoluminescence characterization of IMF grown InGaSb on InP structures. In addition, we show how phase segregation due to miscibility gap issues associated with high-indium content impacts crystallographic morphology. We will also present results from our recent efforts to suppress segregation due to miscibility gaps.
A GaAs trapping layer as intended, forming a narrow doping band several nanometers below the nanowire. By assuming that the Si incorporation rate increases linearly with Al concentration, an empirical model was able to reproduce the Si doping profile, validating the principle of dopant trapping for controlled modulation doping of nanowires grown on faceted supports. Intriguingly, dilute indium bands were observed beneath the nanowire in the atom probe reconstruction, motivating additional structural and chemical analysis. ABF-STEM cross-sectional imaging revealed a region with planar defects in the same region as the indium bands. The disordered region contains twin boundaries and stacking faults confirmed by high-resolution HAADF-STEM imaging. The planar defects nucleated at the intersection between (111) facet and the oblique facets, presumably when Si was introduced. These defects led to a lateral diffusion of indium during the growth of InGaAs NWs. The relative influence of low growth temperature and Si doping on stacking fault generation is under investigation.

References:

11:40 AM F06 Irradiation Effects on Phonon Mediated Thermal Transport and Defect Evolution in GaAs
Joshua Ferrigno and Marat Khafizov; The Ohio State University, United States

Gallium Arsenide (GaAs) is a common semiconductor material found in many integrated circuits and possess a modest thermal conductivity at room temperature. Thermal management of electronic devices is critical to their optimal performance and therefore understanding heat transport has been an active area of research. GaAs thermal conductivity is susceptible to reduction in radiation environments as defects decrease phonon scattering times. For successful space exploration, it is critical to quantify change in thermal conductivity of the semiconductor material. A fast, highly ionizing radiation leads to displacement damage characterized by Frenkel pairs (one interstitial and vacancy). Defect evolution under irradiation governed by production and diffusion of self-interstitials and vacancies within the lattice of solid crystalline material can be conveniently modeled using Rate Theory (RT) equations. Defect concentrations found from RT can be coupled to the Klemens-Calaway model to determine lattice conductivity reduction under irradiation. This coupled model allows for the calculation of the impact of radiation defect accumulation and degradation of GaAs properties, including thermal conductivity.

SESSION G: 2D Material Devices and Sensors
Session Chairs: Kevin Daniels and Daniel Pennachio
Wednesday Afternoon, June 29, 2022
Great Hall Meeting Room 1 & 2

1:30 PM G01 (Student) Multifunctional MoTe2 Transistors for Analog, Digital, Neuromorphic and Modulation Primitives
Sarbashis Das and Saptarshi Das; The Pennsylvania State University, United States

Stagnation in the thickness scaling of silicon (Si) for the complementary metal oxide semiconductor (CMOS) technology has invoked interest in atomically thin two-dimensional (2D) semiconducting materials for next generations of ultra-short-channel devices. However, the vast majority of emerging 2D materials exhibit unipolar transport with either dominant electron or hole currents making their adoption difficult in CMOS technology. Furthermore, Si replacement must be accompanied by a change in traditional von Neumann architecture that keeps the compute and memory separated. In this work, we accomplish both by integrating ambipolar molybdenum ditelluride (MoTe2) based field effect transistors (FETs) with a floating-gate stack, which can program the threshold voltage of the device in an arbitrary and non-volatile manner. Using this property, a pair of MoTe2 FETs have been used to exhibit reconfigurable CMOS inverters, neuromorphic computing primitives such as sigmoid, hyperbolic tangent, and Gaussian neurons and synapses, and multi-bit analog encoding and modulation primitives such as frequency quadrupler, frequency shift keying, and phase shift keying. While some of these computing primitives have been demonstrated in the past, they all use heterostructures with separate p- and n-type materials, and none integrates programmable and non-volatile memory. This is the first demonstration where a single semiconducting material has been used to achieve in-memory 2D CMOS capabilities for a wide range of computing paradigms.

1:50 PM G02 (Student) Near Sensor Security Based on Multifunctional Monolayer MoS2 FETs
Akhil Dodda, Nicholas Trainor, Joan M. Redwing and Saptarshi Das; The Pennsylvania State University, United States

With the emergence of the internet of things (IoT) and its critical role in our day-to-day lives, the risk of information loss or security threats has become a raging concern than ever before. Although conventional software crypto modules are powerful, they consume an enormous amount of energy in ciphering the information, necessitating the need for novel hardware cryptographic primitive. While hardware-based cryptographic modules exist, with the aging silicon technology and von Neumann bottleneck, innovation in materials, devices, and architectures is required in designing next-generation secure electronics. Acknowledging this need and deriving inspiration from nature, we here propose and experimentally demonstrate a low-power, bioinspired, crypto engine based on atomically thin and multifunctional MoS2 field-effect transistors (FETs). We have fabricated an 8 x 8 crossbar array of a fully integrated crypto engine to encode 8 x 8-pixel images where each crypto engine comprises five monolithically integrated MoS2 FETs (5T cell). Each transistor cell is locally back-gated using a gate-dielectric stack comprising of atomic layer deposition (ALD) grown 50 nm Al2O3 on sputter-deposited 50/20 nm Pt/TiN to accomplish sensing and encoding functionalities. All the back-gate islands were placed on a commercially purchased SiO2 "++"-si substrate. Our entire hardware platform utilizes a total of 320 MoS2 FETs to encode the 8 x 8-pixel images. We exploit the unique optoelectronic properties such as the photogating effect to sense the information from an external light source and combine it with a non-volatile programmable gate dielectric stack to encode...
or encrypt the sensed information by adding different amounts of noise. The number of brute force trials required to decrypt the information was found to be significant, in the range of a few hundreds of picoseconds. Finally, to decipher the encrypted information we adopt a population voting-based algorithm, a phenomenon widely observed in biological species.

2:10 PM G03 Are Two-Dimensional Interfaces Really Flat? Zhihui Cheng\textsuperscript{1,2}, Huiaru Zhang\textsuperscript{2}, Son T. Le\textsuperscript{1}, Hattan A. A. Badawi\textsuperscript{1}, Guangyi Li\textsuperscript{1} Linyou Cao\textsuperscript{2}, Albert Davydov\textsuperscript{2}, Aaron D. Franklin\textsuperscript{3,3} and Curt A. Richter\textsuperscript{1}; \textsuperscript{1}Purdue University, United States; \textsuperscript{2}National Institute of Standards and Technology, United States; \textsuperscript{3}Duke University, United States; \textsuperscript{4}North Carolina State University, United States

Two-dimensional (2D) van der Waals materials are subject to mechanical deformation and thus form bubbles and wrinkles during exfoliation and transfer. A lack of interfacial "flatness" has implications for interface properties, such as those formed by metal contacts or insulating layers. Therefore, an understanding of the detailed properties of 2D interfaces, especially their flatness under different conditions, is of high importance. Here we use cross-sectional scanning transmission electron microscopy (STEM) to investigate various 2D interfaces (2D-2D and 3D-2D), and we characterize and compare the flatness of the hBN-2D and metal-2D interfaces down to angstrom resolution. It is observed that the dry mechanical deformation and thus forming bubbles and wrinkles during exfoliation and transfer. A lack of interfacial "flatness" has implications for interface properties, such as those formed by metal contacts or insulating layers. Therefore, an understanding of the detailed properties of 2D interfaces, especially their flatness under different conditions, is of high importance. Here we use cross-sectional scanning transmission electron microscopy (STEM) to investigate various 2D interfaces (2D-2D and 3D-2D), and we characterize and compare the flatness of the hBN-2D and metal-2D interfaces down to angstrom resolution. It is observed that the dry transfer of hexagonal boron nitride (hBN) can dramatically alter the interface structure. When characterizing 3D metal-2D interfaces, we found that Ni-MO\textsubscript{S}\textsubscript{2} interfaces are more uneven and have larger nanocavities compared to other metal-2D interfaces. The electrical properties of an Mo\textsubscript{S}\textsubscript{2}-based field-effect transistor (FET) are correlated directly with the interfacial transformation in the contact and channel regions. The device conductance is improved by 40\% after the hBN encapsulation, likely due to the interface interactions at both the channel and contacts. Overall, these observations reveal the intrinsic of 2D interfaces and their significant dependence on the processes used in their fabrication.

2:30 PM G04 The (Mostly) Unwelcome Guest in Transition Metal Chalcogenides—Native Oxidation and the Effects of Oxygen During Processing Mo\textsubscript{S}\textsubscript{2}, Ti\textsubscript{S}\textsubscript{2}, and Zr(S,Se)\textsubscript{2} Rafael Jaramillo; Massachusetts Institute of Technology, United States

Being a very hard anion, oxygen bonds very differently to transition metals than do the chalcogen elements. The race oxygen in a transition metal chalcogenide (TM D) has a substantial impact on material processing and properties, much more so than for instance the race selenium in a sulfide. Since oxygen is all around us, even in our high-vacuum chambers, it’s essential to understand and control the effects of oxygen on processing 2D materials. We report the results of several studies of the effect of oxygen on synthesizing TM Ds. We find that lowering trace oxygen concentration in the reactor makes it possible to lower the processing temperature for large-area Ti\textsubscript{S}\textsubscript{2} films, made by reacting Ti thin films with H\textsubscript{2}S gas [1]. We quantify how lowering oxygen concentration enables faster metal sulfurization at lower temperatures (down to 500 °C), leading to thin films that are smooth and homogeneous. In contrast, we find the opposite trend for Mo\textsubscript{S}\textsubscript{2}: adding trace oxygen enables lower processing temperatures (down to 375 °C) for large-area Mo\textsubscript{S}\textsubscript{2} films, made by sulfurizing Mo thin films [2]. We understand these contrasting effects in the light of particular transition metal-O and O-O bonds, including molecular dynamics (MD) simulations that suggest that oxygen is a catalyst for M-O bond formation. We also report studies of oxidation rates and mechanisms on freshly-cleaved surfaces of Mo\textsubscript{S}\textsubscript{2} and Zr(S,Se)\textsubscript{2} [3]. Mo\textsubscript{S}\textsubscript{2} surfaces remain pristine for over a year in laboratory ambient conditions, without a trace of oxide formation. Thermal oxidation of Mo\textsubscript{S}\textsubscript{2} results in the formation of crystalline blocks of MoO\textsubscript{3}, due to the high volatility of Mo oxides. We find that non-thermal methods of O\textsubscript{2} plasma processing are required to produce a conformal, amorphous native oxide on Mo\textsubscript{S}\textsubscript{2}. We report on advanced characterization of Mo\textsubscript{S}\textsubscript{2} native oxides formed by thermal and plasma oxidation, including transmission electron microscopy (TEM) studies of structure and composition, and electrical properties measured by atomic force microscopy (AFM). In contrast to Mo\textsubscript{S}\textsubscript{2}, Zr(S,Se)\textsubscript{2} alloys oxidize rapidly, with the native oxide growing at a rate up to 0.5 Å/min in ambient conditions. MD simulations reveal the kinetic mechanisms that limit native oxide growth for Mo\textsubscript{S}\textsubscript{2} and promote it for Zr(S,Se)\textsubscript{2}, despite oxide formation in ambient conditions being thermodynamically-favorable in all cases.

SARS-CoV-2 spike antibodies and epitaxial graphene (EG) on 6H silicon carbide (SiC) substrate for SARS-CoV-2 detection. We have combined the advantages of high sensitivity and fast response time of graphene with the high selectivity of antibodies to develop an ultrasensitive SARS-CoV-2 screening platform. A diagram of the fabrication procedure is shown in Fig. 1. Bilayer EG is grown by the thermal sublimation of silicon from silicon carbide, and subsequent hydrogen intercalation as previously demonstrated [4]. Reactive ion etching (CF$_3$O) was used to pattern the EG, and by e-beam evaporation, metal electrodes (Ti/Au = 30/220 nm) were deposited. To functionalize the EG for the selective detection of SARS-CoV-2, a crosslinker (Poly-L-lysine) and SARS-CoV-2 S1 spike antibodies were immobilized on the EG surface. Samples were characterized by atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS), and Raman spectroscopy to confirm EG substrate and heterostructure integrity. The electrical response of the sensor was measured using the Gamry 3000 Source/M丈ure Unit to investigate the sensor performance with SARS-CoV-2 samples. AFM images of the heterostructure on SiC are shown in Fig. 2. The heterostructure was found to immobilize well on the EG/SiC and withstand repeated cycles of characterization measurements. Figure 3 presents the (a-c) XPS and (d) Raman results of the heterostructure immobilized EG/SiC. These results indicate that the synthesized structures are indeed EG-based heterostructure with antibody/crosslinker. Furthermore, we investigated the sensor with Raman spectroscopy to see a shift in the graphene G-peak position in the heterostructure with antigen (1 ng/mL) as shown in Fig. 4. The G-peak was redshifted after binding of antigen-antibody in the heterostructure, which resulted from strain induced by the antigen-antibody interaction. The prepared sensor was tested with SARS-CoV-2 S1 spike protein and clinical samples and clearly distinguished between blank and SARS-CoV-2 at room temperature as shown in Fig 5. The sensor detected the SARS-CoV-2 spike protein antigen in a concentration as low as 1 ng/mL and infected patients' samples (exhaled breath aerosol) in concentrations as low as 60 copies/mL in seconds. In addition, the sensor demonstrated as a practical application of the portable sensor to detect the SARS-CoV-2 virus as shown in Fig. 6. The portable unit clearly distinguished variant positive saliva samples in 0.6 s at room temperature. Hence, this sensor has great potential as an ultrasensitive SARS-CoV-2 screening platform.
In this study, we report the heterogeneous integration of GaAsSb nanowires (NWs) on graphene by utilizing the advantages of bandgap tunability of GaAsSb NWs and flexibility of graphene substrate for next-generation flexible near-infrared optoelectronic devices. We demonstrate the successful growth of high-quality, good density, and vertical GaAsSb NWs on monolayer-graphene/SiO₂/Si (111) using molecular beam epitaxy. The surface-functionalized graphene using mild O₂ plasma treatment improves the reactivity of semiconductor adatoms on the graphene surface. The increase in defect peak of the Raman mode, reduced surface conductivity, and formation of additional O₂ groups of surface-treated graphene compared to pristine graphene confirms the functionalization of graphene. The vertical yield of NWs on the graphene surface was enhanced by using the optimized plasma power and duration to increase the nucleation centers. In addition, the growth of higher Sb composition GaAsSb (x=0.4) stem helps to improve the vertical density further by chasing the Ga droplets on the graphene surface via the surfactant effect of Sb and provides a better lattice matching. An ensemble photodetector device in the near-infrared region has been demonstrated exhibiting an optical responsivity of 110 A/W with detectivity of 1.1×10^14 Jones. These findings highlight the potential of GaAsSb NWs growth on graphene for flexible NIR PD devices that operate at room temperature, along with the performance metrics required for next-generation optoelectronic device applications.

A dvancements in synthesis techniques allow for electronic-grade 2D materials to be produced at the wafer scale, enabling the fabrication of hundreds of 2D material-based devices in a single batch. Successful incorporation of new materials into large-scale manufacturing environments demands an understanding of the material structure and defects that can lead to device degradation, and sometimes failure, during operation. Device reliability is rooted in material reliability, which fundamentally refers to the stability of the atoms making up a material. Factors affecting material reliability include geometry, microstructure, chemistry, dimensional scale, proximity to other materials, and exposure to external stressors. In this talk, we show how defects in chemical vapor deposited (CVD) M o₂ flakes can be precursors to material damage sustained during subsequent electrical stressing. Here, monolayer M o₂ flakes were transferred to pre-patterned electrodes and subjected to a constant DC voltage for defined times. We observed that pre-existing defects oriented normal to the current flow were susceptible to growth in the direction of current flow, increasing in size with stressing time and magnitude of the electric field. Certain conditions yielded complete material failure in the form of open circuits. Our results demonstrate the importance of understanding how synthesis and processing can lead to material defects, and how such defects can compromise the performance and reliability of 2D material-based electronic devices.
1:50 PM H01
(Student) Defect Characteristics Under Devices and Reverse Leakage Current Investigated Using X-Ray Topography Yekan Wang1, Michael E. Liao1, Kenny Huynh1, William Olsen1, James C. Gallagher2, Travis Andersson2, Xianrong Huang3, Michael Wojcik4 and Mark Goorsky1; 1University of California, Los Angeles, United States; 2U.S. Naval Research Laboratory, United States; 3Argonne National Laboratory, United States

In this work, we investigate defect characteristics, such as defect density and distribution in the substrate and epilayer directly underneath vertical GaN Schottky diodes using x-ray topography and show their impact on the reverse leakage current. GaN Schottky diodes are fabricated using homoepitaxial GaN on HVPE substrate with dot-cores. The core positions, with a spacing of approximately 1 mm, are fixed by intentionally growing periodically patterned inversion domains prior to the bulk growth [1]. During HVPE growth, threading dislocations congregate at the cores and concentrate at the centers of cores while reducing dislocations in regions between the cores. The unique non-uniform but predictable defect distribution makes the dot-core wafer ideal for studying the impact of defects density on the performance of devices with otherwise identical structures.

Our method involves imaging the whole wafer after device fabrication by exposing separate pieces of film to different points along the x-ray rocking curve for the (1120) GaN reflection (“single exposure images” [2]). Globally, the radius of curvature of the wafer is determined to be 34 m. Locally, periodic non-diffracting regions were observed around the core centers, where the defect density is high (up to 10^10 cm^-2). These highly tilted regions are misoriented more than 72 arcsec away from the diffracting regions. Both the global radius of curvature and the amount of local lattice distortion are consistent with what we observed earlier in bare dot-core substrates [3]. In comparison, the regions in between cores, where the defect density is low (as low as 10^8 cm^-2), show uniform contract with no lattice distortion. On the other hand, topography images show distinctive contrast from the metalization pattern and capture the outline of each individual device. Therefore, the distance of each device from the nearest core-center can be determined. Current-voltage (I-V) measurements performed on devices at different distances from the core-centers show that devices located far away (> 300 μm) from the core-centers have low leakage current, on the order of 10^-1 A/cm^2 at a reverse bias of -10 V. However, as the device gets closer to the core-centers (< 150 μm), an increase in the reverse bias leakage by 2-4 orders of magnitude at -10 V is observed. The results from this study show that the substrate defect density and distribution directly affect the device leakage current and x-ray topography is an effective method for studying defect characteristics in the substrate and epilayer underneath individual vertical GaN devices. If necessary, the non-destructive nature of x-ray would make it possible to screen the wafer prior to device fabrication and guide devices to regions with low defect density to achieve high performance.

This research was supported through the ARP.A-E PNDIODES program under contract DE-AR0001116 at UCLA.

References:

2:10 PM H02
(Students) Investigation of the Nature and Origins of Area Defects in Gallium Nitride Substrate Wafers Yafei Liu, Hongyu Peng, Qianyu Cheng, Shanshan Hu, Zeyu Chen, Balaji Raghothamachar and Michael Dudley; Stony Brook University, The State University of New York, United States

Gallium Nitride (GaN) is one of the most promising wide band gap semiconductor materials that are replacing silicon (Si) in power electronic applications. However, the quality of the material is limiting its application in high performance power electronic materials. A part from the threading dislocations reported in our previous studies [1-3], some area defects are observed in both ammonothermal GaN substrates and patterned hydride vapor phase epitaxy (HVPE) GaN substrate by synchrotron X-ray topography (XRT) (Figure 1). Information on the nature of these defects is important to prevent the formation of such defects and improve the crystal quality. Since the growth process of patterned HVPE GaN material involves the use of patterns of inverted GaN polarity on the growth template [4], the area defects are likely to be related to the formation of inversion domains. Ammonothermal GaN substrate wafers also show similar area contrast in XRT images. Therefore, it is possible that inversion domain likely formed during the ammonothermal growth process of GaN.

In this study, Nomarski optical microscopy (NOM), scanning electron microscopy (SEM), and high-resolution transmission electron microscopy (HRTEM) are adopted to investigate the nature of the area defects. A part from XRT images, these domain features are visible in the NOM images (Figure 2). SEM images (Figure 3) show that the area defects are observed as a diffraction contrast instead of the orientation contrast. To investigate the atomic configuration of these domains, HRTEM of specimens sliced from the domains are being compared with those from outside the domains. The characterization results from TEM analysis in conjunction with observations from other techniques will be used to determine the nature of the area defects and their formation mechanisms will be deduced.


2:10 PM H03
Effects of Surface Defects on Vertical GaN Diode Performance James C. Gallagher1, Michael E. Mastro1, Mona E. Bristohl, Alan G. Jacobs1, Brendan Gunning1, Robert Kapoor1, Karl Hobart1 and Travis Anderson1; 1U.S. Naval Research Laboratory, United States; 2National Research Council, United States; 3Sandia National Laboratories, United States

GaN is one of the most promising wide band gap semiconductors for high power applications due to its wide band gap, critical electric field and electron mobility giving it the potential to surpass Si and SiC technology. However, to unlock the full potential of GaN would require perfecting its manufacturing process. Such a process would require a quick, non-destructive technique capable of full wafer mapping.

Since GaN wafer and epitaxial growth technology has not been perfected, most wafers come with localized defects that alter the electrical properties. Many of them can be detected using surface topography techniques such as a wafer scale optical profilometry.
measurement. An advantage of this technique is that it can be performed at micron resolution across full wafers in less than a few hours. However, the presence of benign defects with minimal effect on the diode properties presents a significant challenge. This talk will focus on using data analysis techniques for estimating the yield of vertical GaN diodes with comparison to experimental results.

Though qualitative results can be used to predict which surface defects cause failure (for example, pits in the samples that are several microns deep), it is difficult to develop a computer algorithm which accurately evaluates the whole sample. One method involves identifying defects using a generalized extreme studentized deviate test for outliers. The yield can be estimated by calculating the probability of a randomly placed devices being on a defect, and has shown to be 70% accurate at predicting the failure rate. Another method involves intentionally avoiding the defective areas by using lithography to isolate the defects from the rest of the sample, which has been found to make wafer scale diodes. The third method involves training a machine learning model using the optical profilometry as the input data and the current-voltage sweep of the diodes as the output parameter. This method was found to be 91% accurate at predicting forward bias behavior, though a larger training set is needed to predict reverse bias behavior accurately.

This work is supported by the Office of Naval Research.

2:50 PM H04
(Student) Correlating Optical Characteristics and Electrical Performance of Vertical GaN-on-GaN PN Diodes Yuxuan Zhang1, V Ishank Talesara2, A Mathias A. Daumen2, Zhaoying Chen1, Jae Hyuck Yoo2, Qinghui Shao2, Ted Laurence2, Wu Lu1 and Hongping Zhao1; 1:The Ohio State University, United States; 2:Lawrence Livermore National Laboratory, United States

GaN is advantageous for high power electronic applications because of its large bandgap (3.4 eV), high critical electric field (3.4 MV/cm) and high electron mobility (~1200 cm/s). Vertical GaN PN diode with 5kV breakdown voltage has been demonstrated [1]. The material quality and doping of the thick n-GaN drift layer represent the key parameters that determine the device performance. Therefore, it is critical to probe and understand the fundamental correlation between material properties and device performance including on-resistance (Ron), reverse leakage current (Ir), and breakdown voltage (VBR).

In this work, systematic studies were performed on free-standing HVPE GaN substrates, MOCVD GaN epifilms, and vertical GaN PN diodes, to correlate material properties with device performance. The cathodoluminescence (CL) imaging on GaN substrate revealed three representative regions: (i) dislocation cores originated from the HVPE lateral overgrowth; (ii) coalescent regions, and (iii) inadequate coalescent regions (voids). The threading dislocation densities (TDD) in adequate coalescent regions are estimated as 2x10^6 cm^-2 while that of the dislocation cores can be higher than 10^8 cm^-2.

Room temperature CL spectra showed the highest near band-edge emission (NBE) at the coalescent regions (P1), and much lower NBE with a prominent 520 nm defect peak at the dislocation cores (P3). CL imaging performed on the MOCVD n-GaN epifilm showed that most threading dislocations propagate from the substrate into the epilayer. The coalescence density in the dislocations cores reduces after n-GaN epitaxy. Moreover, new defects with extended dimension were generated after n-GaN epitaxy. Room temperature photoluminescence (PL) with 405 nm laser excitation was utilized to perform the PL mapping. The region in dislocation cores showed low PL intensity, indicating the dominant non-radiative recombination. High PL intensities were observed around the voids regions and the coalescent boundaries, indicating strong radiative recombination in these regions.

To correlate the GaN material properties with vertical PN diodes device performance, a diode structure was grown on a 2° HVPE GaN substrate with 8 µm n-drift layer (Si: 2x10^14 cm^-3), 500 nm p-GaN layer and 20 nm p+GaN layer. Forward and reverse bias measurements indicate that devices located in the coalescent regions have relatively lower leakage currents and higher breakdown voltages. Specifically, devices with 500 µm diameter located in the coalescent regions have an average VBR of (8.1±0.8) × 10^6 V/cm², while the VBR of devices on dislocation clusters are 1014 ± 120 V and (2±0.4) × 10^6 V/cm². Devices with diameter of 100 µm exhibit more prominent location dependence: VBR of 1282 ± 40 V and Ir of (1.13±0.1) × 10^-6 A/cm² (coalescent region); 1037 ± 27 V and (1.49 ± 0.4) × 10^-6 A/cm² (dislocation clusters).

In summary, systematic studies were performed to correlate the fundamental GaN-on-GaN material properties with the vertical GaN PN diodes device performance. Optical characterization (PL and CL) and electrical measurements (I-V) reveal higher reverse leakage current and lower breakdown voltage for devices fabricated on dislocation clusters.

Acknowledgment: This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344, and DOE ARPA-E (DE-AR0001036).

References:

3:10 PM H05
(Student) Interface Trap Density Characterization of ALD Gate Dielectrics for GaN Power MOSFETs Caleb Glaser1,2, Andrew Binder1, Luke Yates1, Andrew Allerman1, Daniel Feezell2 and Robert Kapa1; 1:Sanda National Laboratories, United States; 2:University of New Mexico, United States

This study analyzes the changes in the density of interface traps (DIT) for various atomic layer deposition (ALD) gate dielectric films on gallium nitride (GaN) devices fabricated on bulk GaN substrates. Each film type has been chosen with an optimized insulator/semiconductor interface obtained through chemical cleans or post deposition annealing (PDA). Reduction in dielectric leakage and interface traps in MOSCAP devices may be used in order to understand how these mechanisms affect more complex devices such as vertical GaN MOSESFTs. GaN MOSFET and MOSCAP devices are often investigated and implemented in power systems with applications ranging from electric vehicles (EVs) to smart power grids. The unique material properties of GaN such as wide bandgap, high breakdown voltage, and high electron mobility create unique advantages over traditional silicon FETS. Vertical GaN MOSFETs are better suited for higher voltage applications due to current flow and voltage drop perpendicular to the surface while also reducing required chip area for high operating voltages. Although there are many advantages of vertical GaN devices, such an architecture presents unique challenges that must be addressed before such devices may be implemented in high power applications, such as the requirement for a native substrate and the need to improve the gate dielectric interface. The interface between the gate dielectric and the semiconductor is crucial in order to reduce threshold voltage shift, leakage current, and the density charge traps. Previous work has shown the importance of DIT reduction with chemical cleans and PDAs. Accurate calculations of the density of interface traps (DIT) are vital to fully realize device operation and reliability. The choice between surface cleans and dielectric annealing as a leakage reduction technique is dependent on the material and available processing capabilities. While PDAs may reduce the dielectric breakdown strength, they have been found to reduce gate leakage...
current and improve device performance for most gate dielectrics. Several methods have been proposed for DIT characterization, including the voltage dependencies of low- and high-frequency capacitance (CV), conductance (GV), and surface potential (ΨsV). DIT may be calculated from the surface potential of the dielectric using the quasi-static capacitance and the capacitance of the chosen gate dielectric. This work uses quasi-static CV and surface potential electrical characterization of GaN MOSCAPs to determine DIT of various gate dielectric materials treated with PDA’s and chemical cleans. Optimization of such films on MOSCAPs will allow for implementation into vertical GaN MOSFET architectures. Interface trap density may be reduced by decreasing the capacitance associated with defects and surface contamination or by selection of a dielectric material with a lower dielectric constant. Fixed charges at the dielectric/semiconductor interface are manifested in hysteresis between forward and reverse voltage sweeps and may be the result of contamination prior to ALD or point defects in the material. Al2O3 is an attractive gate dielectric material due to its dielectric constant, which may improve breakdown strength (Fig. 1), but it may suffer from higher memory charge between continuous bias sweeps. SiO2 ALD films have lower breakdown and significantly lower leakage currents but show the lowest density of remaining fixed charges between sweeps. Al2O3 has the lowest DIT of the tested dielectrics (Fig. 2) with the addition of PDA. Results were verified by altering bias conditions during testing in order to accumulate and deplete interface charges. Minor plateaus in capacitance in forward bias indicate the presence of negative fixed interface charges. Additional characterization may be necessary to determine the optimal conditions for DIT reduction for HfO2 films, including reduction in PDA temperatures in combination with improved substrate chemical cleans.

3:50 PM H06
(Student) Thermodynamic and Band Structure Study of ScxAl1-xN
Mahlet Moilia and Emmanouil Kipouropoulos; University of Michigan–Ann Arbor, United States

III-nitrides like AlN have light-emitting and charge carrying abilities that have led to applications in short-wavelength light emitters and high electron mobility transistors (HEMTs). Issues with lattice constant as well as polarization mismatch between III-nitride heterostructures however, have led to the need to alloy AlN with ScN[1,2]. Recent work has found that ScxAl1-xN alloys at certain compositions have enhanced piezoelectric response which allows the coercive electric field for ferroelectric polarization switching to be below its dielectric breakdown limit[3,4,5]. Therefore, the strain and polarization tunability of ScxAl1-xN would grant further applications in electronic and optoelectronic devices that would not be possible with AlN.

ScN exists in the rocksalt structure while AlN exists in the wurtzite structure, so the ScxAl1-xN alloy has shown to be stabilized in several crystal structures depending on the Sc composition. Understanding the phase and thermodynamic stability of ScxAl1-xN alloy is critical to obtain a good baseline for studying its electronic and multiferroic properties. In this work, we performed first-principles calculations based on hybrid density functional theory (DFT) and special quasi-random structure (SQS) methodology to study the ground-state thermodynamic and electronic properties of ScxAl1-xN as a function of Sc composition. We utilized DFT calculations to obtain the formation energy of ScxAl1-xN alloy in cubic, hexagonal, and wurtzite structures for multiple different Sc compositions. The most stable crystal structure for each composition was determined and the corresponding electronic band structure was calculated. This work provides a holistic view of the thermodynamic stability of ScxAl1-xN and its effect on the ferroelectric polarization switching mechanism, and the impact of Sc on the electronic band structure.


4:10 PM H07
(Student) Fabrication of Flexible AIGaN/GaN HEMTs Using Laser Lift off M. Didarul Alam, Kamal Hussain, Grigory Simin, MVS Chandrashekhar and A. Si Khan; University of South Carolina, United States

We report on the first demonstration of flexible AIGaN/GaN high electron mobility transistors (HEMTs) by successful transfer from sapphire substrate to copper tape on flexible polyethylene terephthalate (PET) using excimer laser-based liftoff (LLO). The structural integrity of the heterojunction was preserved during LLO as supported by the marginal decrease in electron mobility (μe) from 1670 to 1630 cm2/Vs as well as the unchanged sheet carrier concentration (n0) of ~9.8×1012 cm−2 before and after transfer. The devices exhibit maximum drain current density (ID, max) of 332 and 332 mA/mm before and after transfer, respectively. This ~21% degradation in maximum current density after transfer, primarily due to the thermal effect because of the large difference in thermal conductivities between sapphire (34.6 W/mK) and adhesive on copper tape (0.2 W/mK), is lower than that of other reported transfer techniques on similar substrates without heat spreaders. Under external applied strain, the maximum reduction in DIT of the tested dielectrics was also investigated. DITs of flexible HEMT increased from 332 to 384 mA/mm under tensile stress with a radius of curvature 0.5 cm, and the threshold voltage (Vth) shifted negatively by ~0.2 V. This new transfer technique demonstrates the capability of large-scale, low-damage flexible GaN HEMT. This proposed approach is also expected to pave the way for the realization of ultrawide bandgap (UWBG) AIGaN-channel flexible HEMT for electronics needing high-temperature, high-frequency, and high-power applications.

The AIGaN/GaN heterostructures used in this study were grown on a c-plane double side polished (DSP) sapphire substrate by metal-organic chemical vapor deposition (MOCVD). The epilayer structure consists of a 30 nm GaN nucleation layer, a 1.8 μm unintentionally doped GaN buffer layer, a 1 nm AlN spacer, and a 20 nm Al0.33Ga0.67N barrier layer. This buffer layer also serves as the channel layer for the device eplayers. After fabrication, the epilayer side of the sample was bonded to a UV tape and a 193 nm excimer laser was used to remove the DSP sapphire followed by the cleaning of the exposed GaN surface with 1:1 dilute HCl. The GaN surface was bonded to a copper tape on PET substrate and the UV tape was removed after curing it in a UV chamber. Involvement of any harsh chemicals or processing is not needed in this technique resulting in intact and low-damage transfer.

Material and electrical characterizations were done before and after transfer onto copper tape. The full width at half maximum (FWHM) values on sapphire and copper tape are 302 and 345 arcsec, respectively suggesting low-damage transfer process. The n0 were measured from frequency-dependent capacitance-voltage (C-V) characteristics. From the transmission line model (TLM) measurements before and after transfer, the contact resistances (Rc) are found to be 0.59 and 0.64 Ω-mm, respectively while the sheet resistance (Rsh) increased slightly from 380 to 390 Ω/μm. The μe was extracted from the values of Rsh and Rc before and after transfer. A ~20% shift was observed from 332 to 332 mA/mm before and after transfer. The ε values of devices on sapphire and copper tape are 0.11 and 0.08 S/mm, respectively. Moreover, the change in 2DEG density under bending based on the
change in current density in the saturation region is in good agreement with the measurement results.

In this paper, we will present the details of our LLO process and characterization of the fabricated flexible AlGaN/GaN HEMT structures.

**4:30 PM H08**

*Efficient N-Type Ion Implantation Activation in GaN with High Mobility*

Alan G. Jacobs¹, Boris N. Feigelson², Jennifer K. Hite¹, Joseph Spencer²,³, Marko Tadjer¹, Karl Hobart¹, and Travis Anderson¹; U.S. Navy Research Lab, United States; Virginia Tech, United States

Gallium nitride (GaN) is the leading material for next generation high power devices owing to its superior figures of merit over current state of the art materials as well as increasing market share in RF applications generating economies of scale. Among the challenges persisting for ease of commercialization include the efficient ion implant activation for n-type, p-type, and durable semi-insulating materials while maintaining the quality and low unintentional doping of unimplanted material. This remains difficult due to instability of GaN at ambient pressures for temperatures high enough to remove ion implant damage and activate dopants, often leading to material degradation and excess unintentional carriers. Here we demonstrate efficient activation of ion implanted silicon in GaN while maintaining film quality and low carrier density of unimplanted material.

Unintentionally doped Ga-polar GaN templates were grown on sapphire 2.2 microns thick by MOCVD. Ion implants were made approximating a 300nm deep, ~1e19 cm⁻³ box profile, with a localized surface concentration of 5e19 cm⁻³ to facilitate contacts, for a total dose of 5e19 cm⁻². Implants were performed at ambient and high temperature (500°C) as well as with an additional matching nitrogen implant to maintain stoichiometry and reduce vacancy formation. Annealing was done via Symmetrical Multicycle Rapid Thermal Annealing (SM RTA) at temperatures up to 1550°C at moderate pressures (~30 bar) where GaN is thermodynamically stabilized to ~1000°C. Successful stabilization of the metastable GaN material up to 1550°C was achieved with a combination of the moderate pressure, a protective PECVD SiN x cap, and rapid heating and cooling at rates up to 300 K/s during SM RTA. Contacts were made using typical Ti/Al/Ni/Au and measured as deposited with a typical measured specific contact resistance of order 10⁻⁴ ohm-cm² by TLM.

Contrary to initial expectations, high temperature silicon implants did not prove advantageous and produced poor mobility with a greater sheet carrier concentration than the implanted dose indicating significant damage generation and retention after annealing. Compensation with room temperature co-implanted nitrogen after the high temperature silicon proved beneficial but still inferior to the ambient temperature silicon implant alone. Implantation of silicon at room temperature yielded a maximum mobility of 160 cm²/Vs, beyond 90% activation efficiency, while maintaining the unimplanted UID material quality with consistent mobility to the as-grown material and electron concentrations from 10²⁰ to 10²¹ cm⁻³. Sequential co-implantation with both silicon and nitrogen at room temperature exhibited slightly reduced mobility compared to silicon alone while the activation efficiency was comparable indicating that the additional defects generated from the nitrogen implant proved equally or more deleterious than any benefit from maintaining material stoichiometry. The high mobility achieved and low UID carrier concentrations show both the ability to maintain undoped crystal quality and produce low compensation high quality implanted and doped films for high power devices enabling new device topologies and freeing device designers from the difficulties and drawbacks of regrowth.

**4:50 PM H09**

*Studying N-Polar GaN/AlGaN High Electron Mobility Transistor Structures on Single-Crystal AlN Substrates*

Zeixuan Zhang¹, Ji-Myong Encomendero², Yeong-In Cho³, Jashan Singh², Kazuki Nomoto¹, Masato Toita¹, Hululu Shigeru Xing² and Debleep Jena¹; Cornell University, United States; Ahsa Kasei Corporation, Japan

High electron mobility transistors (HEMTs) built on wide-bandgap semiconductor platforms are leading contenders in high-power mm-wave electronics [1-3] with current state-of-the-art performance achieved using N-polar GaN/AlGaN HEMTs with output powers above 8 W/mm at up to 94 GHz.[2] The performance of N-polar III-N HEMTs could be further improved by increasing the Al content in AlGaN barrier. Because of the large bandgap (~6 eV) and high thermal conductivity (~340 W/mK) of AlN, incorporating Al-rich AlGaN buffer layer has the advantages of enhanced thermal management and a maximized conduction band offset to reduce buffer leakage and short channel effects.[1] Due to smaller lattice mismatch to Al-rich AlGaN compared with GaN substrates, single-crystal AlN substrates are ideal platform for the realization of GaN/AlGaN HEMTs with Al-rich AlGaN barriers thanks to the low dislocation densities (<10¹⁰/cm²) and the absence of undesired thermal boundary resistance (TBR) unlike AlN templates. We report the epitaxy of undoped pseudomorphic N-polar GaN/AlGaN heterostructures on single-crystal N-polar AlN substrates by plasma-assisted molecular beam epitaxy (MBE). A schematic layer structure is shown in Fig. 1(a). Three samples with GaN channel thickness varied from 5 nm to 10 nm are studied. A band-diagram simulation suggests the presence of a high-density two-dimensional electron gas (2DEG) at GaN/AlGaN interface [Fig. 1(b)]. A further parallel channel with lower electron density could also exist at the bottom AlGaN/AlN interface (not shown).

Fig. 1(c-d) shows the 10x10 and 2x2 um² atomic force microscopy (AFM) images on the as-grown surface of the sample with 8 nm GaN. The presence of atomic steps suggests the step-flow growth mode. Similar surface morphology is observed for the other two samples. Fig. 1(e) shows the measured X-ray diffraction (XRD) pattern. The clearly visible interference fringes suggest the abrupt hetero-interface. The reciprocal space maps (RSM) further suggest that the GaN and AlGaN layers are fully strained to the underlying AlN (not shown).

Temperature dependent Hall-effect measurements were conducted in van der Pauw geometry on as-grown heterostructures with indium dots as the contacts. The red circles in Fig. 2 (a) show the 300 K electron density as a function of GaN channel thickness. The electron densities show almost no change while cooling down to 77 K, as expected for polarization-induced 2DEG. The measured electron densities match well with the calculated values at GaN/AlGaN interface [gray dashed line in Fig. 2(a)] with the surface Fermi level at ~0.4 eV below GaN conduction band.[4] Fig. 2 (b) shows the dependence of 300 (red circles) and 77 K (blue circles) electron mobility on channel thickness. A sharp drop (~50%) in electron mobility is observed when the GaN channel thickness decreases to 5 nm. Similar behavior reported in N-polar GaN/AlGaN HEMTs on GaN platform [5-6] is attributed to a stronger interface scattering when channel thickness scales down. The measured electron densities with AlN buffer layers in this work (red triangles) are higher than those with GaN buffer layers [5-10] (blue circles) due to a higher Al-content in the AlGaN barrier [Fig. 2(c)]. Meanwhile, comparable sheet resistances of ~400-600 Ω/sq at room temperature are achieved. We believe this is the first experimental demonstration of high mobility 2DEG in N-polar AlGaN structures on AlN platform.

Remote epitaxy is a promising new technique for epitaxial film removal and substrate reuse that utilizes monolayer graphene as a release layer [1]. Epitaxial graphene (EG) natively grown on SiC(0001) substrates were used to produce different SiC surface morphologies and EG layer numbers. Ar:H2 process gas flow ratio, growth precursor C/Si ratio, and growth temperature were optimized during hot-wall CVD remote epitaxy to promote smooth film morphology. Nomarski optical microscopy, scanning electron microscopy, and atomic force microscopy found growths at 1620°C with Ar/H2 ratios <20/5 slm, indicating high-quality EG growth and processing, negating the requirement of transferring the EG to another substrate. In addition, EG has reduced defect generation at C/Si ratios > 1.0. Such prismatic slip was also observed to generate BPDs and SFs along ‘a’ directions originating from micropipes [3]. Since the defect has a smaller highly defective core, its influence on devices was mostly observed in a limited region. However, expansion of defects from the core and the sixspoked DA’s have not been investigated. This could cause reliability issues over a significantly larger region of the wafer. In this work, we investigate the expansion of SFs emanating from the star-shaped defect and its six DA’s as well as secondary DAs using ultraviolet photoluminescence (UVPL) and x-ray topography (XRT).

For this work, 150 mm diameter SiC wafers with 10 mm thick n-type epitaxial layers were commercially obtained. Whole wafer UVPL imaging was performed to observe extended defects using a custom system equipped with a 355 nm quasi-continuous excitation laser, automated XYZ sample stage, and a LN2 cooled camera connected to microscope setup with 660 nm long pass filter. XRT imaging was performed using Rigaku XRTM icon system with 70 mm microfocus CuMo rotating anode, collimating mirror, reflection/transmission sample stage and a high resolution x-ray camera. High resolution UVPL imaging with higher UV excitation was performed at the star-defect to expand SFs from BPDs in both the substrate as well as epitaxial layer. Five star defects were observed in UVPL wafer map. As previously reported [1], they appear as having a center core of dislocations and six DAs emanating from it. However, we also observed secondary DAs from some of the primary DAs, which also lie in one of the ‘a’ directions making an angle of 60° with the primary DA. Some of the core regions appeared bright and were dark. Upon further UV excitation, the bright core star defects generated SFs which expanded throughout the epitaxial layer. The dark core star defects did not generate SFs until a higher intensity UV power of ~1000 W/cm² was used. This indicates that the bright core star defects had generated BPDs inside the epitaxial layer, whereas the dark core ones had BPDs inside the substrate only. The high intensity UV causes faulting of BPDs inside the substrate and the SFs enter the epitaxial layer and expand up to the surface. Furthermore, high intensity UV excitation also resulted in SF generation at the intersection of primary and secondary DAs. Details of the expansion behavior as well as depth resolved section x-ray topography will be presented.


Silicon Carbide (SiC) power devices are being widely used for electric vehicles, traction control and other high power applications due to its superior breakdown field and thermal conductivity compared to silicon, which results in lower losses, compact system, and low system cost. For wider SiC adoption, long term device reliability must be addressed and related issues need to be investigated. Basal plane dislocations (BPDs) in SiC generate stacking faults (SF), which leads to forward voltage degradation in bipolar devices. SFs also cause increased reverse bias leakage and higher on-state resistance in all SiC devices. Recently a star-shaped defect was reported to cause device degradation in SiC gate turn-off thyristors (GTO) [1]. This defect was reported by Lee et. al. [2] to originate from a core region with high threading dislocations and extending with six arms of dislocation arrays (DA) along the ‘a’ directions. The six DAs are consistent with a prismatic slip: a/3(11-20)<1-100>. Such prismatic slip was also observed to generate BPDs and SFs along ‘a’ directions originating from micropipes [3]. Since the defect has a smaller highly defective core, its influence on devices was mostly observed in a limited region. However, expansion of defects from the core and the sixspoked DA’s have not been investigated. This could cause reliability issues over a significantly larger region of the wafer. In this work, we investigate the expansion of SFs emanating from the star-shaped defect and its six DA’s as well as secondary DAs using ultraviolet photoluminescence (UVPL) and x-ray topography (XRT).
Silicon Carbide (SiC) is a wide bandgap semiconductor, which has been widely applied to power electronics due to its excellent properties of wide band gap, high breakdown voltage and thermal stability. High voltage superjunction devices are necessary for realization of hybrid aircraft and intelligent power systems. Ghandi and coworkers have demonstrated 2 kV superjunction PIN diode with single 12um epilayer by novel high energy implantation system at Brookhaven National Laboratory (BNL) [1, 2].

Implantation employing high energy Al ions, can create lattice strain in the wafer by displacing the Si and C atoms. To characterize the nature of lattice strains in 4H-SiC wafer implanted with Al ions at energy range of 13 M eV to 65 M eV, synchrotron X-ray rocking curve topography (SXRT) [3] has been employed. With utilization of Si(331) beam conditioner in tandem with Si(111) double-crystal monochromator, the angular resolution of synchrotron X-ray topography (XRT) is increased by an order of magnitude. Using this setup, the recorded rocking curves reveal multiple diffraction peaks with an angular separation of only 2 arcseconds are observed on the topographs, indicating inhomogeneous strain distribution across the implanted layer. Using Rocking-curve Analysis by Dynamical Simulation (RADS), the strain profile of the implanted layer is obtained, showing a relatively lower strain near the surface and bottom of the implanted layer, while center of the layer has relatively uniform strain. This arcsecond are observed on the topographs, indicating inhomogeneous strain distribution across the implanted layer. Using Rocking-curve Analysis by Dynamical Simulation (RADS), the strain profile of the implanted layer is obtained, showing a relatively lower strain near the surface and bottom of the implanted layer, while center of the layer has relatively uniform strain. This result shows a strong correlation with the results from SIMS analysis of the doping profile. Reference:
more simplified factor based on an approximate expression for the misorientation is also introduced in this study as an alternative to the full ray-tracing simulation approach. The effective penetration depth determination method presented in this study enables three-dimensional dislocation configuration analysis and accurate density calculations.

Reference:

3:10 PM Refreshment Break

SESSION J: Nanoscale Characterization
Session Chairs: Lincoln Launon and Luis M Iaja Avila
Wednesday Afternoon, J June 29, 2022
Archie M. Griffin West Ballroom

3:30 PM J01
EUV Pulsed Atom Probe Tomography of β-Ga2O3 Semiconductor Materials
Luis M Iaja Avila1, Benjamin Caplin2, A.nn Chiaramonti3, Ming- Sun Lee4, Kris Bertness4, Rebecca L. Peterson5 and Norman Sanford6; 1National Institute of Standards and Technology, United States; 2University of Michigan, United States

β-Ga2O3 is an attractive ultra-wide bandgap semiconductor material due to its applications in optoelectronics and high-power devices [1]. Accurate measurements of the composition, dopants, and impurities in Ga2O3-based devices is of critical importance. Atom probe tomography (APT) is one of the analytical tools used to measure the composition of materials; however, recent APT measurements of III-nitride semiconductor materials have revealed compositional biases on such systems [2,3].

In this work we perform compositional APT studies of unintentionally doped β-Ga2O3 using a commercial APT instrument and a custom-built extreme ultraviolet (EUV) APT. While the commercial near-UV (NUV) APT system utilizes a 355-nm laser to induce field ion evaporation, in the custom system we replaced the near-ultraviolet laser in a straight flight-path atom probe tomograph with a coherent EUV light source and a vacuum beamline. With these modifications, we were able to illuminate the specimen’s tip with 30-45 eV energy photons [4].

In our EUV APT measurements we maintain a constant ion detection rate while varying the EUV pulse energy by approximately two orders of magnitude (x120) and sample standing voltage. Our results show an underestimation of the oxygen composition when performing APT experiments under high EUV pulse energy or low E-field conditions. Compositional values closer to stoichiometric are obtained when performing experiments under high E-field conditions. These results are similar to recently published results with a NUV APT instrument [5]. These NUV experiments were performed at 100 kHz laser repetition rate, for this reason we performed additional studies with a commercial NUV APT instrument at 25 kHz. A careful compositional analysis comparison between the NUV and EUV systems will be discussed.

Our EUV APT data also shows the existence of unintentionally doped Si in the β-Ga2O3 sample. This is of importance as technologically-relevant devices with Si implantation are under development [6]. Further studies will focus on EUV APT reconstructions of Si-implanted β-Ga2O3.

References

3:50 PM J02
(Student) STM Simulation of High Aspect Ratio Tunneling Behavior on the Example of In Situ Harvested GaAs Nanowire
M. Ortiz Hanesmann, Dorothee S. Rosenzweig and Holger Eiseler; Technische Universität Berlin, Germany

In general, for scanning tunneling microscopy (STM) investigations the actual tip shape is negligible beyond the assumption of being reasonable sharp and the investigated topological differences are small in comparison with the tip. This assumption does no longer hold true, as soon as the size of the investigated structures get into the regime of the tip apex diameter. In this presentation, we show how through simulation of the physics of the tip-sample-system, we can explain the non trivial influence of the tip shape on a STM single scan line. Thus, we were able to reproduce STM measurements taken on GaAs nanowires (NW) with a diameter of 90 nm using this simulation. The simulation uses Monte-Carlo integration to approximate the tunneling current and simulates the resulting scanning process accordingly. The code is written in Python 3.8 using the numpy library. The program is not tailored to this explicit example, but rather simulates a specific tip geometry scanning a defined surface. It accepts the tip geometry and surface topology as a list of points respectively. Each point is then treated as an individual atom. An additional parameter can be added to each atom, which is used in the tunneling current calculation. Thus it is possible to create electrical differences for specific atoms, which could be used to represent chemical contrast. Although there is no individual calculation of an actual tunnel current. The calculated tunnel current is simply based on a precalculated function, which only depends on the distance between a tip atom and a surface atom and the respective chemical parameters. This is sufficient for a first order approximation for the scanning behavior, although a sophisticated poison-solver could be added at this step, to increase the accuracy of the simulation in specific situations. One major insight gained by the simulation is that in cases, in which the tip diameter exceeds the NW diameter, the resulting scan line images the tip geometry in the sidewall regions of the NW instead of the NW topology. This results in an image, in which the NW appears to be much broader than its actual size/width, but with the height roughly in the right size. This
Copper oxide based catalysts have the promising capability to selectively reduce CO$_2$ into useful products, however the details of the mechanism are not well understood. Scanning tunneling microscopy (STM) studies performed on oxidized Cu(100) single crystal surfaces allow for the investigation of the fundamentals of this process on an atomic scale. The well understood Cu(100)-O (2√2×2)R45° missing row reconstruction is an initial oxidation step and acts as a starting point for our investigation of more highly oxidized surfaces. These surfaces were prepared by annealing a Cu(100) single crystal in 10$^{-6}$ mbar O$_2$ between 80-275 °C, and then further UHV annealing at 150 °C. In addition to flat terraces, the surface also became more highly faceted, with grains 10s to 100s of nm high. Atomic-resolution STM imaging revealed a new hexagonal surface lattice, qualitatively consistent with Cu$_2$O(111). With significant uniaxial strain, Tunneling spectroscopy of the new oxide surface indicates a gap-like feature of roughly 1.5 eV, somewhat less than the bulk Cu$_2$O gap of ~2.2 eV. These studies emphasize the sensitivity of copper oxidation to initial conditions and sample history. After STM structural and electronic characterization of the surfaces, CO$_2$ was dosed in situ under cryogenic (77 K) conditions. Individual CO$_2$ molecules were not observed, however scratchiness in the imaging following deposition indicates physisorbed CO$_2$, likely being perturbed by the apex of the tip during scanning.

---

Zero-Field Magnetoresistance (NZFMR) spectroscopy, as well as how this measurement can be generalized to other scanning probe techniques by exchanging the electron tunneling with the actual interaction of the respective technique.

---

Scanning tunneling microscopy studies performed on oxidized Cu(100) single crystal surfaces allow for the investigation of the fundamentals of this process on an atomic scale. The well understood Cu(100)-O (2√2×2)R45° missing row reconstruction is an initial oxidation step and acts as a starting point for our investigation of more highly oxidized surfaces. These surfaces were prepared by annealing a Cu(100) single crystal in 10$^{-6}$ mbar O$_2$ between 80-275 °C, and then further UHV annealing at 150 °C. In addition to flat terraces, the surface also became more highly faceted, with grains 10s to 100s of nm high. Atomic-resolution STM imaging revealed a new hexagonal surface lattice, qualitatively consistent with Cu$_2$O(111). With significant uniaxial strain, Tunneling spectroscopy of the new oxide surface indicates a gap-like feature of roughly 1.5 eV, somewhat less than the bulk Cu$_2$O gap of ~2.2 eV. These studies emphasize the sensitivity of copper oxidation to initial conditions and sample history. After STM structural and electronic characterization of the surfaces, CO$_2$ was dosed in situ under cryogenic (77 K) conditions. Individual CO$_2$ molecules were not observed, however scratchiness in the imaging following deposition indicates physisorbed CO$_2$, likely being perturbed by the apex of the tip during scanning.

---

Therefore, we studied the GaAs(110) surface and modifications by adsorption of hydrogen at room temperature and above. For the nanoscopic analysis of such facets, hydrogen cleaning is a common procedure to achieve examineable surfaces. While this is reported to be destruction free [2] and achieving clean, atomically flat surfaces, as they are present directly after MBE growth, the actual process and dynamics during the cleaning procedure are rarely examined. From surface investigations without real space resolution in the 1980es [3] it is well known, that the introduction of hydrogen to such surfaces is rather destructive.

Therefore, we studied the GaAs(110) surface and its modifications as model system introduced by hydrogen at room temperature and under commonly used cleaning conditions by STM and STS. For depiction and measurement at the atomic scale, we used scanning tunneling microscopy and spectroscopy under UHV conditions. Using these methods we study the geometric arrangement of the adsorbed atoms as well as adsorption induced additional electronic states, band bending, defect states and Fermi level pinning. For the experiments, we used n-type and p-type highly doped GaAs single crystals with carrier concentration of 2×10$^{18}$ cm$^{-3}$ and 1.6×10$^{18}$ cm$^{-3}$, respectively.

A tomically resolved STM images of both clean surfaces are presented. Both cleavage surfaces are planar without noticeable steps. Defects on the n-type surface are identified as As vacancies. At room temperature, the n-type surface, Ga vacancies develop from the replacing of one Ga atom from the surface lattice to an adatom on top of the surface. Both defects are negatively charged, therefore they cannot recombine. At higher temperatures, defect formation rate is increased. Hydrogen annealing treatment at 400°C leads to etching off the surfaces; especially adatoms are removed rapidly. Only thermally stable defects remain. As a result, there are only the Ga vacancies left on the n-type surfaces. p-type surfaces form As vacancies with increasing density over time. Therefore, the removed A$_2$S atoms desorb quickly. Hydrogen exposure of 1 L (langmuir) at room temperature to both surfaces introduce an increase of defect density as well as a diversity of defect appearances. At cleaning temperatures, we find the surface of n-type GaAs with a distinctly different appearance: The defect density is severely reduced, some monoatomic steps are left to the surface and the defects have a much more uniform appearance.

---

Therefore, the state can only be related to the defects shown in the images. For the p-type material there is no accumulation current shown in the spectra of the clean surface. While additional hydrogen does not change the fundamental band gap or the onset of the bands in general, there is an additional state visible on the conduction band side reaching into the band gap. These findings have severe consequences on the hydrogen cleaning procedure of III/V semiconductor surfaces.

---

References:
measurement frequency. We present X-band data showing NARS EDMR spectra on a-Si:H capacitors and 4H-SiC/SiO₂ MOSFETs that are undistorted and identical to both spin-dependent recombination (SDR) [3] and spin-dependent trap-assisted tunneling (SDTAT) [4] continuous wave (CW) EDMR spectra that are less sensitive to noise. This experimental set-up preserves the CW-EDMR line shape and chemical information, while providing the potential for a boost in sensitivity and time-resolution, with few changes to the experimental apparatus.

We utilize essentially the same data acquisition system to detect NZFMR. In our NZFMR measurements, we utilize the mixing of singlet and triplet states at near-zero fields. NZFMR utilizes the mixing of states at near-zero fields due to local magnetic field interactions. NZFMR has been modeled using Wageman’s two-site hopping model [5] and the stochastic quantum Liouville equation in the past define a steady-state solution for traditional slow-sweep NZFMR experiments. This approach has been used to identify important chemical devices in semiconductor devices, such as nuclear hyperfine constants and kinetic rates [2,6]. We demonstrate a comparison of both continuous-wave and NARS NZFMR measurements in a-Si:H capacitors.

A great advantage of NZFMR is that there is no radio-frequency mixing of states at near-zero fields required. The NZFMR response can be interpreted to provide much of the analytical power present and far more expensive and complex EDMR and conventional EPR measurements in systems in which such measurements would be essentially impossible. In combination, NARS and NZFMR could be used as a tool to observe changes in defect concentrations of packaged device systems at high time resolution, such as integrated circuits.

Citations
lateral spacing controls the dispersion of a propagating surface mode. The separation in longitudinal direction of the ridges, which controls coupling between the meta-atoms, is varied from 30 nm to 2.5 μm.

To determine the range of the coupling between meta-atoms, we measure the far-field diffraction pattern of the fabricated metasurfaces using continuous-wave lasers that emit at 473, 532, and 633 nm, a curved projection screen, and a camera, Fig. 1(b). For l = 532 and 633 nm, bright far-field peaks corresponding to primary order diffraction peaks (i.e., m = ±1, 0, -1) are observed at angles predicted by diffraction theory. In addition to these primary peaks, we also observe dimmer secondary diffraction peaks for all three wavelengths. The number and angular position of these secondary diffraction peaks is related to long-range coupling between meta-atoms, and the number of coupled meta-atoms can be determined using Laue diffraction theory for a finite crystal. The recovered coupling range is shown by the blue diamonds in Fig. 1(c). To further understand the observed phenomena, we develop an analytical model that incorporates a decaying propagating surface mode that couples the meta-atoms, solid line in Fig. 1(c). The model incorporates loss in the propagating mode due to absorption and non-unity coupling between meta-atoms, Fig. 1(d). We incorporate realistic parameters into the model obtained using COMSOL Multiphysics (there are no free parameters) and observe good agreement with our measurements. This approach to long-range coupling in metasurfaces could be leveraged as an additional degree of freedom in metasurface design, enabling applications in ultra-flat beam steering, structured illumination imaging, and topological photonics. Additionally, our approach to determining the coupling range offers a new approach to metasurface characterization.

2:10 PM K03
Electromagnetics and Photonics in the Age of Digital Manufacturing Raymond C. Rumpf; The University of Texas at El Paso, United States

Digital manufacturing is revolutionizing the manufacturing industry. Recent breakthroughs in hybrid 3D printing by the EM Lab at the University of Texas at El Paso have made it possible to build three-dimensional parts composed of any distribution of metals, dielectrics, and other materials. This talk will cover some of the new and exciting applications in circuits, electromagnetics, photonics, and metamaterials that are being enabled by digital fabrication. Electrical circuits can be made three-dimensional where components are placed at any position xyz and oriented at any angle theta-phi. Interconnects can meaner along smooth paths throughout all three dimensions. This creates new degrees of freedom for layout and routing that can make circuits more compact, smaller, and lighter. Shorter trace lengths reduce parasitic impedance to improve power efficiency and increase bandwidth. 3D circuits can be manufactured using unconventional form factors and exploit physics, such as dielectric anisotropy, not easily accessed by planar circuits.

A nether breakthrough by the EM Lab allows periodic structures to be bent, twisted, deformed, and otherwise spatially varied without deforming the size, shape and spacing of unit cells. Such deformations would weaken or erase the electromagnetic and optical properties of the lattice. The technology was first applied to photonic crystals where discoveries were made that led to the twelfth bend of unguided optical beam, refractionless lenses, and photon funneling. The technology was next applied to metamaterials to develop a tool to generate metamaterial lattices for devices designed by transformation optics. The technology is now being used to generate periodic structures across doubly-curved surfaces.

2:30 PM K04
Electroplating of Helical Slow-Wave Structures for Millimeter-Through-Terahertz Vacuum Electronic Devices Anjali Chaudhary1, Divya J. Prakash7, R B Jacobson1, Donald Savage1, Shiva Hajitabarmarznik1, David Weide1, Max L. Lagally2, and Francesca Cavallo2; 1University of Wisconsin-Madison, United States; 2The University of New Mexico, United States

We report our recent results on scalable fabrication of helical slow wave structures (SWSs) applicable in millimeter-through-THz traveling wave tube amplifiers (TWTA) [1]. The structure is unique in that it has microscale diameter dimensions, a helical geometry, and potentially higher electrical/thermal conductivity than other previously reported self-assembled helices. We fabricate the SWSs by self-assembly of a metal nanomembrane (NM) and electroplating of the helical film, thereby overcoming the inherent trade-off between NM thickness and helix diameter/pitch. Here we focus on our recent efforts on understanding and controlling electrodeposition on freestanding and curved NMs. In particular, we investigate the effect of varying current and temperature on the thickness of the deposited film and its uniformity. In addition, we characterize and justify any changes occurring in the geometry of the helix due to electrodeposition. Fabrication of microscale SWSs started with defining NM strips by optical lithography, metal evaporation, and lift-off. In our work we used Cr/Au/Cr NMs that have an inherent stress gradient across their thickness. We defined the metal strips onto a bulk Si substrate coated with a sacrificial or release layer such as Ge or GeOx. The released NM self-assembled into helices with a diameter between 100 and 200 nm upon selective etching of the sacrificial layer by a XeF2 plasma. Helix diameter and pitch are controlled by varying the thickness, the elastic modulus, the residual stress, and the in-plane geometry of the NM s. The electroplating procedure employs a two-electrode electrochemical setup with the self-assembled helix and a platinized mesh serving as cathode and anode, respectively. A sulphate-based gold solution is used for the process. We use pulsed current source with variable frequencies to obtain uniform electrodeposition of an Au film with a thickness of 1-2 μm depending on the electrodeposition parameters. In all investigated electroplating conditions, we observed uniformly deposited gold with lower roughness than the skin depth of the metal at THz frequencies, which are crucial attributes to minimize losses and heating in a TWTA based on the helical SWS.

Reference

Work supported by U.S. AFOSR-Award No. FA9550-19-1-0086

SESSION L: Gallium Oxide Growth
Session Chairs: Lisa Porter and Hongping Zhao
Wednesday Afternoon, June 29, 2022
Ohio States Inc. Traditions Room

1:30 PM L01
Epitaxial Growth on β-Ga2O3 (110) Substrate by Plasma-Assisted Molecular Beam Epitaxy Takeki Itoh, Akhil Mauze, Yawei Zhang and James S. Speck; University of California, Santa Barbara, United States

Epitaxial growth of β-Ga2O3 with outstanding crystal quality has been performed on different crystal orientations such as (100),
(010), and (-201) via plasma-assisted molecular beam epitaxy (PAMBE) [1]. So far, most of the research on crystal growth and device fabrication has been performed on (010) substrates. However, investigation of surface morphologies on (010) substrates has revealed that (110) facets are revealed the chevron consistent features in reflection high-energy electron diffraction (RHEED) studies, which indicates (110) is a natural plane in β-Ga2O3 [2]. Figure 1 shows atomic models of (110) and (010) planes with RMS roughness around 1.0 nm. Additionally, elongated features oriented along the [001] direction are exhibited in the plateau regime on both (110) and (010) substrates; while this feature is not expected on the β-Ga2O3 epitaxial films grown on the (110) substrates due to the absence of clear faceting. Despite the appearance of (110) facets in growth of (010) β-Ga2O3, the (110) plane does not have tendency to show a well-defined step-terrace structure. This may be attributed to the absence of step features on the as-received (110) substrates potentially due to the negligible miscut.

were measured by energy-dispersive X-ray (EDX) spectroscopy. The samples were characterized by a scanning electron microscope (SEM), showing the surface becomes rougher in samples with higher Mg contents. Three typical monoclinic structure diffraction peaks located at 19.12°, 38.50°, and 59.14°, which correspond to the β phases of (-201), (-402), and (-603) were investigated by X-ray diffraction (XRD), and all these diffractions peaks exhibit an obvious blue shift compared with that of reference β-Ga2O3. Raman spectra were investigated by a confocal Raman microscope equipped with a high-resolution laser centered at 532 nm with a power of 60 mW. Four out of ten A1g and four out of five B2g Raman-active optical phonon modes were observed. The reduced peak intensity of A1g (2), A1g (3), B2g (2), and B2g (3) indicates that Mg2+ atoms have displaced the position of Ga3+ ions in both octahedral and tetrahedral chains. The ultra-wide bandgap absorption and transmission spectra were measured using a UV-VIS-NIR spectrophotometer. Ultra-wide bandgaps of 4.98, 5.05, 5.20, and 5.30 eV were measured for pure Ga2O3, sample A, B, and C, respectively with all transmittances of light over 80% in the visible spectrum region. Temperature-dependent photoluminescence (PL) spectra were investigated by a 325-nm laser with temperatures ranging from 13 to 300 K, revealing only intermediate level transitions, which decrease with the increase of temperature. A solar-blind ultraviolet photodetector (PD) fabricated based on MgGa2O3 films with Pt/Au electrodes. Photoresponse has been studied by typical dark and irradiated wavelength dependent I-V curves.

2:30 PM L 04

(Student) MOCVD Growth of Si Doped (010) β-AlGaO3 Films—Structural and Electrical Properties A. F. M. Anhar Uddin Bhuiyan, Zixuan Feng, Lingyu Meng, Andreas Fiedler, Hsien-Lien Huang, Adam T. Neal, Erich Steinbrunner, Shin M o j, Jinwoo Hwang, Siddharth R aja n, and Hongping Zhao. 1The Ohio State University, United States; 2Air Force Research Laboratory, United States

β-(Al,Ga)2O3 alloy with its tunable bandgap energy (4.87-7.51 eV) and high predicted breakdown field (~16 MV/cm) with e for (010) β-AlGaO film with Al = 0.06, 0.18, and 0.33 grown on MgGa2O3 substrate than the theoretically predicted critical thickness, indicating strong influence of MOCVD growth conditions on film relaxation. The cross-sectional STEM and optical macroscopic surface images reveal the formation of cracks along [001] direction for higher Al compositions due to the increased lattice mismatch. The (100) cleavage plane with the lowest surface energy is identified as the major cracking plane, which leads to highly anisotropic and inhomogeneous resistivity in high-Al β-AlGaO films (Figure 2). In summary, MOCVD growth and fundamental characteristics of Si doped (010) β-AlGaO films were systematically investigated. Results from this study will provide fundamental understanding of Si doping in β-AlGaO, critical for future device designs and fabrications.

Acknowledgment: AFOSR (FA9550-18-1-0479) and NSF (1810041, 2019753).

References:

2:50 PM L 05

(Staff) MOCVD Epitaxy of β-Ga2O3 Thin Films on (100) β-Ga2O3 Substrate Lingyu Meng, Zixuan Feng, A. F. M. Anhar Uddin Bhuiyan, Hsien-Lien Huang, Jinwoo Hwang, and Hongping Zhao. The Ohio State University, United States

Ultrawide bandgap (UWBG) gallium oxide (Ga2O3) represents an emerging semiconductor material promising for high power high frequency electronics, considering its associated advantages of wide energy bandgap (~4.8 eV), high predicted breakdown field strength (~8 MV/cm), and the availability of high quality native substrate. For the most thermally stable monoclinic β-Ga2O3 crystal, the available surface planes of native substrates include (-201), (010), (100) and (001). Epitaxial high crystalline quality β-Ga2O3 thin films with high purity and high mobilities on (010) crystal orientation have been demonstrated via metalorganic chemical vapor deposition (MOCVD) [1, 2]. However, understanding of growth mechanisms and material properties on other orientations are still limited.

Previously, MOCVD growth of β-Ga2O3 on (100) Ga2O3 substrates revealed the importance of using miscut angles towards [001] to promote step-flow growth mode and improve crystalline quality of the (100) epi-films [3]. However, a systematic mapping of the MOCVD growth on (100) β-Ga2O3 is still lacking. In this work, we studied the correlation between the MOCVD growth parameters and the (100) β-Ga2O3 thin films properties. Specifically, key growth parameters including growth temperature, growth pressure, V/I/III molar flow rate ratio and carrier gas (shroud gas) flow rate were tuned. Comprehensive material characterization was performed on the grown materials to probe the surface morphology (AFM, SEM), charge transport (Hall measurement), and growth rate (cross-sectional SEM).

Experimental results showed that decrease of shroud gas flow rate leads to the increase of surface smoothness of the epi-films. As
the VI/III molar flow rate ratio increases, the growth rate of the film decreases but with an enhancement of the electron Hall mobility. Although there is no significant correlation of electron mobility with the surface morphology under different growth temperature, the general trend shows that the electron Hall mobility increases as growth temperature increases. A higher chamber pressure leads to a decrease of growth rate, mainly due to the more severe gas phase reaction. The carrier concentration of (100) β-Ga2O3 thin films was tuned between low-1017 cm-2 to low-1019 cm-2 via the control of silane flow rate. Under an optimized growth condition, a (100) β-Ga2O3 thin film with RMS roughness value of 1.64 nm was achieved. However, its room temperature mobility is still limited at 24 cm2/Vs with a carrier concentration of 7.0×1017 cm-3. High resolution STEM imaging is performed to investigate the defects in the epi-films.

In summary, MOCVD growth of on-axis (100) β-Ga2O3 thin films was systematically investigated. Results indicate that the MOCVD growth condition has a significant impact on the film surface morphology, growth rate and electron transport. However, the electron Hall mobility is limited below 25 cm2/Vs mainly due to the formation of twin lamellae and stacking faults for films grown along-on-axis (100) crystal orientation.

Acknowledgment: AFOSR (FA9550-18-1-0479) and NSF (1810049, 2019753).

References


3:10 PM Refreshment Break

3:30 PM L06

(Student) Phase Composition and Microstructure of κ-Ga2O3 Heteroepitaxial Films Grown by MOCVD Kunyao Jiang, Jingyu Tang, Matthew Cabral, Anna Park, Liuxin Gu, Robert Davis and Lisa Porter; Carnegie Mellon University, United States

Gallium oxide (Ga2O3) is an ultra-wide bandgap semiconductor (4.85-5.3 eV) with emerging applications in power electronics because of its high thermal stability, large breakdown voltage and high dielectric constant. Ga2O3 occurs in the α, β, γ and κ polymorphs having trigonal, monoclinic, cubic normal spinel and orthorhombic structures, respectively. β-Ga2O3 is thermodynamically stable and produced in melt-grown substrates. Recently, κ-Ga2O3 has accrued increased interest because it has demonstrated stability at temperatures ≥ 700 °C2 and its large spontaneous polarization could be exploited in heterostructures3 for high electron mobility transistors. In this study, metal organic chemical vapor deposition (MOCVD) was used to grow epitaxial Ga2O3 films under different growth conditions including temperature, growth rate, and diluent gas flow rate. The growth experiments were conducted in a vertical, low-pressure, cold-wall MOCVD reactor using triethylgallium (TEGa) and O2 precursors and commercially available 0.15 off-axis (toward m-plane) c-plane sapphire.4 N2 was used as both the carrier gas for TEGa and the diluent gas. The chamber pressure was held at 20 Torr. The growth rate was controlled by the TEGa flow rate which ranged from 0.29 sccm to 2.1 sccm. The diluent gas flow rate was varied from 4 sccm to 8 sccm. The O2 flow rate was maintained at 500 sccm. The temperature was constant for each growth but varied from 470 °C to 570 °C. Phase composition and microstructure of the films were investigated using different analytical tools including the X-ray diffraction (XRD), scanning electron microscopy (SEM), high-resolution transmission electron microscopy (HRTEM) and scanning transmission electron microscopy (STEM). XRD and SEM revealed that the top layer varied in phase composition between ~100% κ-Ga2O3, and the bottom layer of β-Ga2O3; the surface microstructure ranged from poorly coalesced to completely coalesced grains as a function of growth temperature, growth rate, or diluent gas flow rate. In general, it was found that the κ-phase tends to grow at lower temperatures and higher growth rates (higher TEGa flow rates). The growth of nominally single-phase κ-Ga2O3 within the top layer was observed in a temperature range between 500 °C and 530 °C. Below ~470 °C, only amorphous Ga2O3 was obtained; above ~570 °C only the β-phase was deposited. HRTEM and STEM of a film grown at ~530 °C revealed the initial pseudomorphic growth of 3-4 monolayers of α-Ga2O3, a 20-60 nm transition layer that contained both β- and γ-Ga2O3, and a top ~700 nm thick layer of phase-pure κ-Ga2O3.


3:50 PM L07

(Student) Inhomogeneous Aluminum Incorporation in (-201) β-(AlxGa1-x)2O3 Films Grown on c-Plane and Miscut Sapphire Substrates Kenny Huynh1, Ye kan Wang2, Michael E. Liao2, Megan Klein3, Praneeth Ranga2, Sriram Krishnamoorthy3 and Mark Goorsky1; 1University of California, Los Angeles, United States; 2The University of Utah, United States; 3University of California - Santa Barbara, United States

High aluminum content striations were observed in (-201) β-(AlxGa1-x)2O3 thin films (~500 nm) grown on (0001) and 6° miscut (0001) sapphire substrates. A modulated Al composition structure was observed whose orientation depended on the substrate miscut. High resolution x-ray diffraction (XRD) and transmission electron microscopy (TEM) were used to investigate the structural and chemical properties of the β-(AlxGa1-x)2O3 films (with 0 < x < 0.1) and the in-plane relationship with the underlying sapphire substrate. (-201) β-(AlxGa1-x)2O3 films were grown by metalorganic vapor phase epitaxy and the Al composition was controlled by tuning the ratio of trimethylaluminum to triethylgallium flow. The growth was carried out at a substrate temperature of 810 °C and a reduced growth pressure of 15 Torr to minimize Al precursor prereaction.

Scanning transmission electron microscopy measurements (sensitive to Z-contrast) reveal alternating layers of high and low contrast features throughout the β-(AlxGa1-x)2O3 film. In conjunction with energy dispersive spectroscopy, the striations are identified as regions of high Al content. In the films that were grown on c-plane sapphire, the high Al content striations ran parallel to the (-201) surface. However, in the case of the 6° miscut sapphire substrates, the high Al content striations are oriented about 8°-10° from the surface. Recent studies of β-(AlxGa1-x)2O3 film growth on common orientations including (010), (001), (-201) found that a lower surface energy found in (-201) surface planes. Recent studies of β-(AlxGa1-x)2O3 film growth on common orientations including (010), (001), (-201) found that a lower surface energy found in (-201) surface planes. Recent studies of β-(AlxGa1-x)2O3 film growth on common orientations including (010), (001), (-201) found that a lower surface energy found in (-201) surface planes. Recent studies of β-(AlxGa1-x)2O3 film growth on common orientations including (010), (001), (-201) found that a lower surface energy found in (-201) surface planes. Recent studies of β-(AlxGa1-x)2O3 film growth on common orientations including (010), (001), (-201) found that a lower surface energy found in (-201) surface planes.
X-ray phi scans revealed six-fold symmetry of the (-201) β-(Al,Ga)2O3 films, which corresponds to three sets of twinning and an in-plane orientation where β-(Al,Ga)2O3 reflection were taken to estimate the aluminum composition in the deposited films. In general, the (-603) peak shifts towards higher angles for higher Al concentration as expected, although the broadness and asymmetry of the peaks suggest non-uniform or concentration gradients of the Al content that exist in the samples, which supports the observations made under TEM. In addition, the β-Ga2O3 layers as well as all of the β-(Al,Ga)2O3 layers exhibited a different strain state (different a, b, c, and β lattice parameters) than bulk material as determined through multiple reflection reciprocal space maps.

References

4:10 PM L08
(Student) MOCVD Development and Bandoffsets of ε-Ga2O3 on GaN, AlN, YSZ and c-sapphire Substrates A. F. M. Anhar Uddin Bhuiyan, Zixuan Feng, Hsien-Lien Huang, Lingyu Meng, Jinwoo Hwang and Hongping Zhao; The Ohio State University, United States

Ga2O3 represents an ultrawide bandgap (4.5-5.3 eV) transparent semiconductor oxides promising for next generation high power electronics. Among the five different polymorphs (α, β, γ, δ and ε) of Ga2O3, monoclinic β-Ga2O3 is the thermodynamically most stable structure. Only recently, orthorhombic c-phase Ga2O3 (also referred to as ε-Ga2O3) with a bandgap energy similar to β-Ga2O3 has attracted substantial interests owing to its existence of strong spontaneous polarization (0.31 Cm^-2) as compared to those of polar semiconductors such as GaN (-0.034 Cm^-2) and AlN (-0.09 Cm^-2) [1]. The spontaneous polarization of ε-Ga2O3 is predicted to generate two orders of magnitude higher 2DEGs density (10^14 cm^-2) at ε-Ga2O3/AlN (GAN) interfaces than the traditional AlGaN/GaN heterojunctions, potentially allowing the fabrication of high-electron-mobility transistors for high-power and radio frequency electronic applications. Although ε-Ga2O3 growths have been demonstrated by different growth techniques, investigation on the phase stabilization of ε-Ga2O3 on various substrates is still limited. In this work, a systematic growth mapping of ε-Ga2O3 films is performed via MOCVD on different substrates including c-sapphire, GaN-on-sapphire, AlN-on-sapphire, and yttria stabilized zirconia (YSZ). Moreover, the band offsets at the heterointerfaces of ε-Ga2O3/AlN (GAN), /Sapphire, and /YSZ) are measured via XPS for the first time.

ε-Ga2O3 thin films were grown in an AICTN/Agiliis MOCVD reactor using TEGa and pure O2 as Ga and O precursors, respectively. The growth temperature and pressure were varied between 510-650 °C and 4-15 Torr, respectively. The growth of phase pure ε-Ga2O3 films is achieved on YSZ, GaN and AlN-on-sapphire substrates as shown in the XRD θ-2θ scans in Figure 1, whereas Ga2O3 film grown on sapphire substrate is found to be composed of both β- and ε-phases. Both lower pressure (3-5 Torr) and temperature (620-650 °C) facilitate the growth of pure ε-Ga2O3 films. Owing to its large lattice mismatch with the substrates, ε-Ga2O3 films exhibit in-plane rotational domain structures viewed from XRD ϕ-scans and STEM nano diffractions. The compositional homogeneity and abrupt interfaces between ε-Ga2O3 and different substrates are observed from atomic resolution STEM imaging. The asymmetrical reciprocal space mapping (RSM) indicates the growth of fully relaxed ε-Ga2O3 films on all investigated substrates. While relatively smooth surface morphologies with RMS roughness of ~1.6-3 nm are measured for the films grown on sapphire, GaN and YSZ substrates, ε-Ga2O3 films grown on AlN-on-sapphire show rougher surface morphologies which can be attributed to the strong oxidation of Al adatoms on the growth surface. The chemical compositions, surface stoichiometry, band gaps and the band offsets at ε-Ga2O3/substrate interfaces are evaluated by XPS measurements. The O:Ga ratios are determined to range between 1.47-1.51, indicating that the surface stoichiometries of the films are well maintained. The bandgaps of ε-Ga2O3 films vary between 5.06-5.10 eV on different substrates. A type-II (staggered) band alignment is observed at ε-Ga2O3/c-sapphire (AlN and YSZ) interfaces, whereas ε-Ga2O3/AlN interface exhibits a type-I (straddling) band offset (Figure 2).

Larger conduction band offsets of 5.92, 2.6, 1.40 and 1.07 eV are determined at the ε-Ga2O3/c-sapphire (GAN, AlN and YSZ) interfaces, respectively, indicating great potential for excellent carrier confinement at the heterointerfaces between ε-Ga2O3 and various investigated substrates. In summary, MOCVD growths of ε-Ga2O3 films on various substrates were systematically investigated. Results from this study will provide guidance for future epitaxial growths, device design and fabrication based on ε-Ga2O3 films.

Acknowledgment: AFOSR (FA9550-18-1-0479) and NSF (1810041, 2019753).


4:30 PM L09
(Student) Electronic and Optical Properties of Rare-Earth Doped β-Ga2O3 Crystals Jani Lesenovec, Benjamin L. Dutton, Brooke Downing and John S. McCloy; Washington State University, United States

β-Ga2O3 is an emerging ultrawide bandgap material which can be alloyed with Al2O3 to increase the electronic bandgap. In this work, we explore analogous Sc2O3 alloying, producing bulk Czochralski single crystals of 10 mol.% Sc2O3 (β-(Sc0.1Ga0.9)2O3), i.e., monoclinic 10 mol.% SGO). These materials show a +0.15 eV increase in the bandgap compared to β-Ga2O3, 10 mol.% SGO was characterized for structure (X-ray diffraction, rocking curve, Raman microscopy), purity (glow discharge mass spectroscopy, X-ray fluorescence), optical transmission (200 nm - 20 μm wavelengths), resistivity, and rare earth luminescence (laser induced fluorescence microscopy). Structural measurements indicate successful incorporation of Sc, although overall lower quality than β-Ga2O3 and β-(Al0.1Ga0.9)2O3 crystals. Bulk crystals of β-(Sc0.1Ga0.9)2O3 demonstrate intense Stark luminescence characteristic of Nd3+, which are concentrated in certain areas of the crystal. SGO is not the best candidate substrate for thin film growth due to lower quality single crystals and numerous microscopic defects related to ubiquitous rare earth impurities.

4:50 PM L10
(Student, Late News) Si-Doping in MBE-Grown Beta-Ga2O3 with Room Temperature Mobility > 125 cm²/Vs J. Jonathan McCandless1, Vladimir Protasenko1, Brad Murrell1, Erin Steinbrunner2, Adam T. Neal2, YongJin Cho1, Nick Tanen1, Huili Grace Xing3 and Debdeep Jena1; 1Cornell University, United States; 2Air Force Research Laboratory, United States

Since 2012, the semiconductor β-Ga2O3 has gained significant attention due its large bandgap (~4.7 eV), corresponding large critical electric field strength, and the availability of large-area, semi-insulating substrates. [1, 2] To make high-power diodes and high-frequency switches, devices that take advantage of these properties, it is critical that reliable doping control and low doping
densities be achieved [3]. Epitaxial layers of this material have been grown by many techniques such as halide vapor phase epitaxy, [3] pulsed laser deposition, [5] metalorganic vapor phase epitaxy, [6] and molecular beam epitaxy (MBE). [7, 8]

While MBE is a useful growth technique for forming atomically sharp interfaces, to-date, low doping of Ga2O3 by MBE has been challenging due to the n-type doping sources (e.g., silicon) oxidizing during the growth. As a result, doping densities tend to be high and uncontrolled, and the mobilities tend to be low due to ionized impurity scattering.


SESSION M: Solar Cell Materials and Devices
Session Chairs: Deidra Hodges and Mark Wisely
Wednesday Afternoon, June 29, 2022
Senate Chamber

1:30 PM M01
(Student, Late News) GaAs Laser Power Converters for Cryogenic Applications
Bora Kim, Minjoo L. Lee, Mijung Kim and Brian Li; University of Illinois at Urbana-Champaign, United States

In power-over-fiber (PoF) technology, a continuous-wave laser mode is guided through optical fiber to a photovoltaic cell to provide power in applications where electrical isolation is critical. PoF is widely deployed for electronics and sensors in demanding environments that are sensitive to electromagnetic noise from wires or that are prone to failures by electrical arcing. An emerging application for PoF is in cryogenic environments, e.g. quantum computers, particle physics experiments, deep-space satellite missions. In this project, we are investigating the use of GaAs laser power converters (LPCs) to provide power for both analog and digital electronics in cryogenic neutrino sensors. We are using a deep n-type p-n junction in the forward mode.

We show that majority carrier blocking at heterojunctions can severely hamper fill factor FF at -100°C, leading to lower power conversion efficiencies under moderate laser power densities (e.g., < 1 W/cm²); in contrast, homojunction GaAs LPCs where majority carrier blocking is negligible give high FF values across all temperatures. We have recently grown new GaAs LPCs with redesigned heterojunctions that cause minimal majority carrier blocking at cryogenic temperatures, opening the potential for efficiency exceeding 60%.

All samples were grown by solid-source molecular beam epitaxy (SSMBE) and processed using standard photolithography, e-beam deposition, and wet etching methods. Cells were tested under illumination from an 808 nm laser over a range of temperatures. Sample A was conventional cell design consisting of a 2 μm GaAs absorber surrounded by a lattice-matched n-InGaP window on the front and a lattice-matched p-InGaP back surface field (BSF) layer on the back. While these cells exhibit good characteristics at room-temperature, we noticed anomalously high series resistance values as temperature decreased to -190°C, accompanied by low FFs of 60-70%. Some degree of carrier freezeout was found to occur in layers used in the cells by Hall effect measurements of calibration samples, but all samples remained conductive. In contrast, a GaAs homojunction solar cell (sample B) that only uses n-GaAs as the window and p+GaAs as the BSF showed higher FF values > 80% at all temperature values tested, confirming the role of heterojunctions in increased series resistance. Heterojunctions are still important for cryogenic LPCs, however, for ensuring high open-circuit voltage and external quantum efficiency (EQE), and we therefore designed and grew a new cell (sample C) with an n+InGaP window and p+GaAs BSF.

While testing is still in progress, this cell shows very high FF of 88-89% at -100°C at laser power densities up to 7W/cm². Despite the differences in FF, cells A and B showed high open-circuit voltage values (~1.37-1.41 V) at -190°C, thanks to the excitation power reductions in dark current at such low temperatures. All cells show a reduction in EQE at 808 nm at cryogenic temperature, which may result from the combined effects of reduced optical absorption coefficient and reduced carrier diffusion length at low temperature. Overall, this work shows that GaAs solar cells cannot be simply repurposed for use as LPCs at cryogenic temperatures. Despite the benefit of strongly reduced dark current, GaAs LPCs must be carefully designed to minimize majority carrier blocking to ensure efficient operation at cryogenic temperatures.

1:50 PM M02
(Student) Time-Resolved Photoluminescence Studies of Perovskite Chalcogenides
K. Diroll1, J. C. Ravichandran2 and R. Jaramillo1; 1Massachusetts Institute of Technology, United States; 2University of Southern California, United States; 3Argonne National Laboratory, United States

Chalcogenides in the perovskite and related crystal structures may be useful for future optoelectronic and energy conversion technologies in as much as they have good excited-state, ambipolar transport properties [1]. In recent years, several studies have suggested that semiconductors in the Ba-Zr-S system have slow non-radiative recombination rates [2,3]. Here we present a more detailed time-resolved photoluminescence (TRPL) study of excited-state carrier mobility and recombination rates in the perovskite-structured material Ba2ZrS3 and the related Ruddlesden-Popper phase Ba2ZrS5. Ba2ZrS5 is a semiconductor with direct band gap of energy E_g = 1.8 eV. Ba2ZrS5 is an indirect-gap semiconductor with fundamental gap E_g = 1.25 eV, and has strong near-infrared absorption due to a direct transition near 1.3 eV. We measure state-of-the-art single crystal and epitaxial film samples, to identify intrinsic properties free from the influence of secondary phases and random grain boundaries [4,5]. We model and fit the data using a semiconductor physics simulation, to enable more direct determination of the material parameters k and is possible with empirical data modeling. We model the data using a simulation of generation-diffusion-drift-recombination processes, implemented using software PC-1D [6]. We perform nonlinear
least-squares model refinement using a MATLAB script that runs using PC-1D as the kernel and can perform global refinement of few parameters. We find that both materials have Shockley-Read-Hall recombination lifetime on the order of 100 ns and excited-state diffusion lengths on the order of 5 μm, which bode well for ambipolar device performance in optoelectronic technologies including thin-film solar cells.

1. R. Jaramillo and J. Ravichandran, "In praise and in search of superior CdTe solar cells. The record efficiency of CdTe solar cells of 22.1% is still far below the theoretical limit of 29% mainly due to the low open-circuit voltage. Further improvement can be obtained by increasing the p-type carrier concentration in CdTe absorbers. Group-V impurities, P, As and Sb were shown to be promising for p-type doping in CdTe as seen in a recent Hall measurements where high p-type doping efficiencies were reported. However, early theoretical studies indicate rather high ionization energy for Sb and the formation of self-compensation AX centers, limiting the hole concentrations. From these calculated results, high p-type doping efficiency could not be achieved using group-V doping. To understand this contradiction between experiment and DFT calculations, we revisited the behavior of group-V acceptors and their AX centers in CdTe by using hybrid density functional. We pay special attention to the inclusion of spin-orbit coupling and the finite size effect of supercell to deal with the shallow acceptor levels. We find that the AX center is unstable for P and As, and barely stable in the case of Sb, suggesting that the formation of AX center is unlikely to play important roles as compensation center. The calculated acceptor transition levels of ~100 meV can explain the observed hole concentrations from temperature-dependent Hall measurements when a relatively low level of compensation from yet unknown donor defects is assumed.

2:20 PM M03
(Student) An Optical Response Analysis of Cadmium Telluride-Based Solar Cell Structures Incorporating High Resistivity Transparent Layers of Magnesium-Zinc Oxide
Mohammed Alaani1, Prakash Koirala1, Balaji Ramanujam1, Amlanath Shan1, Adam Phillips1, Michael Heben1, Stephen O’Leary2, Nikolai Podraza1 and Robert Collins1; 1Wright Center for Photovoltaics Innovation & Commercialization and Department of Physics & Astronomy, University of Toledo, United States; 2The University of British Columbia, Canada

Parametric expressions that describe the complex dielectric function of polycrystalline Mg2Zn1–xO thin films as a function of the bandgap Eg have been applied in the metrology of cadmium telluride-based solar cell structures. Valid over the range 3.264 ≤ Eg ≤ 3.826 eV, these parametric expressions are applied to facilitate mapping spectroscopic ellipsometry of device structures consisting of M2Cd1–xO deposited on TEC™-15 glass. Mapping spectroscopic ellipsometry is shown to provide maps for the Mg2Zn1–xO effective thickness, or volume per planar substrate area, and Mg2Zn1–xO bandgap within confidence limits of ±1 nm and ±0.003 eV, respectively. As a second application of the parametric expressions, an as-deposited cadmium telluride-based device structure has been analyzed by through-the-glass spectroscopic ellipsometry. Such an analysis is also shown to provide the Mg2Zn1–xO effective thickness and bandgap. The outcome of the through-the-glass spectroscopic ellipsometry analysis for this device structure enables simulations of the external quantum efficiency spectra of the resulting solar cell assuming different recombination losses within the individual layers of the structure. A comparison of these simulations with corresponding experimental spectra reveals high current collection from the front of the device for the almost complete outcome of the Mg2Zn1–xO/cadmium sulfide components of the M2Cd1–xO/cadmium sulfide/cadmium telluride interface layers of the structure.

2:30 PM M04
(Student) Group-V Acceptors and Their AX Centers in CdTe
Marzieh Savadkoohi1,2, Daniel Gopman2 and Pawan Tyagi1; 1University of the District of Columbia, United States; 2National Institute of Standards and Technology, United States

CdTe solar cells are leading and commercially available thin-film technology. Several factors such as low cost, simple and rapid production, high photo absorption coefficient and a direct band gap of 1.5 eV have been driving the research to improve the efficiency of CdTe solar cells. The electronic charge-based photovoltaic effect is a familiar phenomenon in solar cell technology. Displacement of photon-excited electrons produces a potential difference and electricity. The spin-based photovoltaic effect [1] is a relatively newer phenomenon that is additionally sensitive to the spin of current-carrying electrons and the underlying magnetic properties of their host electrodes. This spin-based effect can similarly be used to generate electricity and perhaps more economically due to the usage of earth-abundant elements such as Nickel (Ni), Cobalt (Co), and Iron (Fe). Identifying systems that demonstrate this behavior is vital to the development of this phenomena as a viable approach for efficient photovoltaic technologies. This research investigates the charge transport properties and spin photovoltaic (P-V) effect in a spintronic device that exhibits a measurable spin P-V effect - a molecular-based spintronic device at room temperature. We observed a photovoltaic effect on a magnetic tunnel junction which was treated with organometallic molecules (OMC) at the exposed edges. Paramagnetic molecules, with a non-vanishing net spin state, can tailor magnetic exchange coupling between the ferromagnetic electrodes (FM Es) in magnetic tunnel junction-based molecular spintronics devices (MTJ) and correspondingly modify the magnetic electrodes transport and optical properties [1-3]. We previously observed spin-photovoltaic effects on M TJs comprising CoNiFe bottom and NiFe top electrodes separated by an AlOx insulator. This study reveals that the photovoltaic effect seen previously is also evident in MgO-based MTJs, which is of much closer technological relevance to MgO-based MTJs used in commercial magnetic tunnel junction sensors and magnetic random-access memories. The MTJs were
Compounds—A2Cd(SCN)2X2

film into photoresponsive material [4].

3:30 PM
3:10 PM Refreshment Break

studies in which OMC transformed a NiFe-based ferromagnetic was observed in the current MTJMSD agrees with our previous exceed 90 °C to keep FME stable. The intriguing P

noteworthy that our sample preparation steps were designed not to temperatures (RT to 120 °C) showed stability until 100 °C. It is

observed photovoltaic phenomenon is due to the MTJMSD’s light

intensities using a solar simulator. Our results showed that the repeated the charge transport study of MTJMSD at different light

effect under regular white light (=400

We also observed an intriguing spin-based photovoltaic (P-V)

electronic properties we performed a Kelvin force probe microscopy (KPFM) scans. Our preliminary results showed a noticeable voltage difference (V =100mV) between the top and bottom electrodes after molecular treatment during KPFM scans. We also observed an intriguing spin-based photovoltaic (P-V)

3:10 PM Refreshment Break

3:30 PM M06
(Student) A New Family of Hybrid Tiocyanate-Halide Compounds— A2Cd(SCN)2X2 A Alexander A. Milder and Patrick Woodward; The Ohio State University, United States

Perovskites, a class of compounds that share the structure type of CaTiO3, are notable for their massive structural and chemical adaptability, making ideal functional materials in a variety of device applications. Perovskite oxides have long been explored for their ferroelectric and magnetic properties and halide perovskites have achieved widespread recognition as solar cell and LED materials. However, to meet the demand for materials in a variety of device applications, the reflective behavior of MTJMSD at a variety of temperatures (RT to 120 °C) showed stability until 100 °C. It is noteworthy that our sample preparation steps were designed not to exceed 90 °C to keep FME stable. The intriguing P-V effect that was observed in the current MTJMSD agrees with our previous studies in which OMC transformed a NiFe-based ferromagnetic film into photoreponsive material [4].

3:50 PM M07
Designing New Sustainable Semiconductor Materials with Cu-Chalcogenide Nanocrystals Soubantika Palchoudhury, Zeyad Al Abri, Madison Jones and Nicholas Saunders; University of Dayton, United States

Transition metal multinary chalcogenides are a unique class of material for photovoltaic (PV) and quantum dot light emitting (QLED) applications. They offer a higher level of flexibility from a materials perspective to achieve tunable band gaps through structural and compositional control. We aim to realize new and more sustainable direct band-gap semiconductor materials from multinary compounds of earth-abundant elements. To this end, detailed ab initio calculations are first performed for the parent binary Cu-chalcogenide composition. A series of new p-doped, n-doped, and degenerate semiconductors based on multinary Cu-chalcogenide nanocrystals are predicted using the theoretical investigations of the band gap and density of states. We experimentally realized the new multinary Cu-chalcogenide compositions via novel solution chemistry approaches. A detailed material characterization based on x-ray diffraction, electron microscopy, and ultraviolet-visible spectroscopy is reported for the new Cu-chalcogenide nanocrystals and thin films. These new results will provide key theoretical and experimental insights for achieving more sustainable absorber layer materials for inorganic solar cells.

4:10 PM M08
(Student, Late News) Solar Cell Effect with Magnetic Metamaterials Produced by Combining Magnetic Tunnel Junction and Magnetic Molecules Samba Gaye, Marzieh Savadkoohi, Eva M utunga, Andrew C. Grizzle, Rodney J. Taylor, Pius Suh and Pawan Tyagi; University of the District of Columbia, United States

A new class of magnetic metamaterials can be produced by placing magnetic molecules between two ferromagnetic electrodes. Magnetic molecules can be designed to create strong exchange coupling between two ferromagnetic electrodes. Magnetic molecule-induced strong exchange coupling that can be harnessed as the means to initiate an automatic spin filtering process to shuffle the spin density of states in the two ferromagnetic electrodes. Our recent preliminary experimental studies showed that iron and nickel atom-based organometallic molecules (FeNi-OM C) produced a strong spin filtering effect between NiFe and CoNiFe ferromagnetic electrodes (Tyagi, P.; Riso, C., Molecul ar spintronics devices exhibiting properties of a solar cell.

A new class of magnetic metamaterials can be produced by placing magnetic molecules between two ferromagnetic electrodes. Magnetic molecules can be designed to create strong exchange coupling between two ferromagnetic electrodes. Magnetic molecule-induced strong exchange coupling that can be harnessed as the means to initiate an automatic spin filtering process to shuffle the spin density of states in the two ferromagnetic electrodes. Our recent preliminary experimental studies showed that iron and nickel atom-based organometallic molecules (FeNi-OM C) produced a strong spin filtering effect between NiFe and CoNiFe ferromagnetic electrodes (Tyagi, P.; Riso, C., Molecul ar spintronics devices exhibiting properties of a solar cell.

A new class of magnetic metamaterials can be produced by placing magnetic molecules between two ferromagnetic electrodes. Magnetic molecules can be designed to create strong exchange coupling between two ferromagnetic electrodes. Magnetic molecule-induced strong exchange coupling that can be harnessed as the means to initiate an automatic spin filtering process to shuffle the spin density of states in the two ferromagnetic electrodes. Our recent preliminary experimental studies showed that iron and nickel atom-based organometallic molecules (FeNi-OM C) produced a strong spin filtering effect between NiFe and CoNiFe ferromagnetic electrodes (Tyagi, P.; Riso, C., Molecul ar spintronics devices exhibiting properties of a solar cell.

A new class of magnetic metamaterials can be produced by placing magnetic molecules between two ferromagnetic electrodes. Magnetic molecules can be designed to create strong exchange coupling between two ferromagnetic electrodes. Magnetic molecule-induced strong exchange coupling that can be harnessed as the means to initiate an automatic spin filtering process to shuffle the spin density of states in the two ferromagnetic electrodes. Our recent preliminary experimental studies showed that iron and nickel atom-based organometallic molecules (FeNi-OM C) produced a strong spin filtering effect between NiFe and CoNiFe ferromagnetic electrodes (Tyagi, P.; Riso, C., Molecul ar spintronics devices exhibiting properties of a solar cell.
Further experimental studies are conducted to design several other forms of novel magnetic metamaterials by combining a wide range of Single-molecule magnetic (SMM) and porphyrin-like magnetic molecules with various permutations of magnetic electrodes. To produce a magnetic tunnel junction testbed that is to be used to test various molecules, we made extensive experimental optimization efforts at each stage of device fabrication to address device fabrication challenges associated with molecule-ferromagnet interactions. In this study, we have systematically optimized several factors using multiple Taguchi Design of Experiment approaches to improve the fabrication of the bottom electrode of the magnetic metamaterial. We systematically varied photolithography parameters and plasma treatment process to yield a bottom ferromagnetic electrode with <0.4 nm Ra roughness and oval-shaped edges. For this optimization work, we mainly focused on the plasma etching duration and the different aspects of the photolithography process, which included: the spin-coating speed, the baking temperature, the soaking time, and the exposure time. After lithography and plasma treatment, RF sputtering was performed to create a seed layer and NiFe ferromagnetic electrode, followed by the lift-off step. Atomic force microscopy was performed to study the roughness of the electrode and edge profile. We observed that only a few parameter combinations in Taguchi Design of experiments were successful in producing oval edge ultrasmooth bottom electrodes for advancing magnetic metamaterial experimental research. This foundation work is critical for making robust tunnel junction testbeds for harnessing magnetic molecule strengths and attributes of producing magnetic metamaterials.
Further experimental studies are conducted to design several other forms of novel magnetic metamaterials by combining a wide range of Single-molecule magnetic (SMM) and porphyrin-like magnetic molecules with various permutations of magnetic electrodes. To produce a magnetic tunnel junction testbed that is to be used to test various molecules, we made extensive experimental optimization efforts at each stage of device fabrication to address device fabrication challenges associated with molecule-ferromagnet interactions. In this study, we have systematically optimized several factors using multiple Taguchi Design of Experiment approaches to improve the fabrication of the bottom electrode of the magnetic metamaterial. We systematically varied photolithography parameters and plasma treatment process to yield a bottom ferromagnetic electrode with <0.4 nm Ra roughness and oval-shaped edges. For this optimization work, we mainly focused on the plasma etching duration and the different aspects of the photolithography process, which included: the spin-coating speed, the baking temperature, the soaking time, and the exposure time. After lithography and plasma treatment, RF sputtering was performed to create a seed layer and NiFe ferromagnetic electrode, followed by the lift-off step. Atomic force microscopy was performed to study the roughness of the electrode and edge profile. We observed that only a few parameter combinations in Taguchi Design of experiments were successful in producing oval edge ultrasmooth bottom electrodes for advancing magnetic metamaterial experimental research. This foundation work is critical for making robust tunnel junction testbeds for harnessing magnetic molecule strengths and attributes of producing magnetic metamaterials.
Commerically available GaN-based electronic and optoelectronic devices are mainly fabricated on Gallium-polar GaN substrates. However, recent research has shown superior performance of the Nitrogen-polar GaN high electron mobility transistors (HEMTs) in the W-band in comparison with the Ga-polar GaN HEMTs. Meanwhile, the research and progress on N-polar films have been limited due to the fact that it is very challenging to grow films of high quality, unlike the metal-polar case.

Although AlGaN has been commonly used as the barrier in GaN HEMTs with scaled channel. In particular, In0.18Al0.82N has been explored as a barrier due to its high band gap, and its lattice constant, which is close to that of GaN. However, growth of N-polar GaN HEMTs has been limited due to the fact that it is very challenging to grow films of high quality, unlike the metal-polar case.

First, the quality and the composition of the InxAl1-xN were explored at various growth temperatures (600 to 800 °C). For this purpose, a Veeco GenXplor MBE system was used for epitaxial growth of the samples. First, a 200 nm-thick GaN layer was grown on top of a solvent-cleaned commercial bulk N-polar GaN substrate at 750 °C to ensure a smooth surface morphology. The growth was then interrupted to change the substrate temperature for the growth of the other (Al,Ga)N layers in the epi-structure.

In this work, we present high temperature growth of InAlN on N-polar GaN substrate using plasma assisted molecular beam epitaxy (PAMBE). Next, we implement our findings in high temperature growth parameters, including the growth temperature of InAlN. The effects of different growth parameters are investigated on the morphology and 2DEG sheet charge density of the N-polar InAlN back barrier, and GaN as the channel. The effects of different growth parameters are investigated on the mobility and 2DEG sheet charge density of the N-polar InAlN back barrier, and GaN as the channel. The effects of different growth parameters are investigated on the mobility and 2DEG sheet charge density of the N-polar InAlN back barrier, and GaN as the channel. The effects of different growth parameters are investigated on the mobility and 2DEG sheet charge density of the N-polar InAlN back barrier, and GaN as the channel.

First, the quality and the composition of the InxAl1-xN were explored at various growth conditions (600 to 800 °C). For this purpose, a Veeco GenXplor MBE system was used for epitaxial growth of the samples. First, a 200 nm-thick GaN layer was grown on top of a solvent-cleaned commercial bulk N-polar GaN substrate at 750 °C to ensure a smooth surface morphology. The growth was then interrupted to change the substrate temperature for the growth of the other (Al,Ga)N layers in the epi-structure.

In this work, we present high temperature growth of InAlN on N-polar GaN substrate using plasma assisted molecular beam epitaxy (PAMBE). Next, we implement our findings in high temperature growth parameters, including the growth temperature of InAlN. The effects of different growth parameters are investigated on the mobility and 2DEG sheet charge density of the N-polar InAlN back barrier, and GaN as the channel. The effects of different growth parameters are investigated on the mobility and 2DEG sheet charge density of the N-polar InAlN back barrier, and GaN as the channel. The effects of different growth parameters are investigated on the mobility and 2DEG sheet charge density of the N-polar InAlN back barrier, and GaN as the channel. The effects of different growth parameters are investigated on the mobility and 2DEG sheet charge density of the N-polar InAlN back barrier, and GaN as the channel.
Studies of the radiation tolerance and electrical behavior of gallium nitride (GaN) based devices are important for the next generation of high-power and high-frequency electronics for use in harsh environments such as nuclear reactors, particle accelerators, and aerospace applications. In this work, we study the behavior of Ga-polar and N-polar GaN n-type Schottky diodes before and after exposure to fast (550 fast:1 thermal) and fast-thermal (1 fast:2 thermal) neutrons. Samples were irradiated to three different Fast Neutron Irradiator (FNI) fluences (10^{15}, 10^{16}, and 10^{17} n/cm^2), and to 10^{17} n/cm^2 thermal neutron in the Dry Tube, which provided a higher ratio of thermal to fast neutrons.

Temperature-dependent current-voltage (I-V) and circular transmission line method (CTLM) measurements were used to study the electrical characteristics. A strong reduction in reverse leakage current and an increase in differential resistance in forward bias were observed after neutron irradiation. A hysteresis effect depending on sweep direction was also observed after neutron irradiation on both Ga-polar and N-polar diodes. Thermionic emission (TE), Frenkel-Poole emission (FP), and Fowler-Nordheim tunneling (FN) models were used to explain the I-V characteristics pre- and post-irradiation. The effective barrier height for electron emission from trap sites extracted from the FP model shows a slight decrease for Ga-polar diodes after fast and fast-thermal neutron irradiation, while for N-polar diodes the effective barrier height increased after fast neutrons and disappeared altogether for the fast-thermal neutron irradiation. The FN tunneling model shows that tunneling at higher reverse bias becomes less dominant after neutron irradiation on Ga-polar diodes, while the effective tunneling barrier height is increased after fast neutron exposure and increased after-thermal neutron irradiation on N-polar diodes. The study shows that Ga-polar and N-polar GaN Schottky diodes exhibit significant and different changes in electrical behavior after fast and thermal neutron irradiation. The reverse bias characteristics of N-polar appear to be more tolerant after both fast and fast-thermal neutron irradiation compared to Ga-polar. On the other hand, for the case of fast neutron irradiation, N-polar diodes show slightly higher degradation in bulk resistivity. For the fast-thermal neutron irradiation, while the Ga-polar shows only degradation in contact properties, the N-polar shows degradation in both bulk resistivity and contact properties, suggesting that fast neutrons have more impact on N-polar diodes even at lower fast to thermal ratios. The Schottky barrier height (SBH) and ideality factor extracted from C-V measurements are also in agreement with the above changes in these diodes. The origin of the different behaviors is attributed to the fundamental differences between the Ga-polar and N-polar orientations, such as their opposite polarization and differences in impurity incorporation, defect types, and surface reactivity.

In this work, we demonstrate the epitaxial growth of FeSe thin films directly on Al_{2}O_{3}(0001) surfaces using molecular beam epitaxy (MBE), and probe their structural and spectroscopic properties via various in situ and ex situ characterization techniques, including reflection high-energy electron diffraction (RHEED), X-ray diffraction (XRD), and Raman spectroscopy. Growth at elevated temperatures with an accompanying annealing step yields well-structured FeSe films with high crystalline quality and atomically flat surface morphologies, as evidenced by the sharp, streaky features seen in RHEED patterns of film surfaces. XRD analysis shows characteristic peaks corresponding to the (0 0 1) family of planes in FeSe, along with those peaks originating from the Al_{2}O_{3} substrate. This confirms the growth to be epitaxial in nature, as no peaks other than the aforementioned (0 0 1) peaks are seen to be present. From the XRD, the c-axis lattice constant was extracted and found to be 5.53 Å, which matches well with that of thin film bulk FeSe [1]. Raman spectroscopy of the films yields two primary peaks at 183.9 cm^{-1} and 193.8 cm^{-1}, each matching well to one of the characteristic vibrational modes of FeSe (the A_{1g} mode of Se and the B_{1g} mode of Fe respectively) [4]. The absence of other peaks, namely those linked to FeSe_{2} (180 cm^{-1}, 217 cm^{-1}, and 254 cm^{-1}) and oxidation (250 cm^{-1} and 300 cm^{-1}) respectively, which further indicates the quality of our films [5].

We hope these results could later prove useful in understanding the role of substrate properties, such as dielectric and lattice constant, in the modulation of the film-substrate interface physics and significantly progress the state of the art in heat flux measurement technologies. We report on the use of single crystal Antimony prismatic structures to demonstrate the efficacy of the Transverse Seebeck Effect in unconventional heat flux sensor arrangements. A prototype heat flux sensor was constructed using a single Antimony sensing element and revealed a linear relationship between the applied temperature gradient and the measured perpendicular voltage. Measurements of the principal Seebeck coefficient tensor components in single crystal Antimony specimens accompanied with computational simulations reinforced the validity of the prototype sensor configuration. Integration of multiple Antimony transducers into a single package demonstrated the scalability of Transverse Seebeck Effect-based devices, as multiple sensing elements can be connected in series to amplify the measured electrical signal for a given heat flux. This work is supported by the Department of Energy Award Number DE-FE0031902.
subsequently lead to discovery of even higher critical temperatures in this material on other yet to be tested substrates.

This work was supported by the Army Research Office (ARO) Grant #W911NF-17-1-0312 (MURI).

References

PS06
(Studnet) A Machine Learning Attack Resilient True Random Number Generator Based on Stochastic Programmability in Two-Dimensional Transistors
Akshay Wali and Saptarshi Das;
The Pennsylvania State University, United States

Information exchange forms the heart of modern-day communications technologies such as the Internet of Things (IoTs) that requires transmission of humongous volumes of data over increasingly complex networks. To guarantee security of encryption and decryption schemes for exchanging sensitive information, high quality random numbers are required. A true random number generator (TRNG) is a critical hardware component that guarantees such protection. Random numbers are widely used for information security, cryptography, stochastic modelling and banking and financing. In this article, we demonstrate a machine learning resilient TRNG by exploiting stochastic nature of carrier trapping and de-trapping phenomenon in a two-dimensional (2D) transistor with layered transition metal dichalcogenides (TM Ds) such as tungsten diselenide (WSe$_2$) and tungsten disulfide (WS$_2$) as the channel material and a programmable gate stack consisting of a 50 nm alumina (Al$_2$O$_3$) as the gate dielectric and a Pt/TiN/O$^x$/Si as the gate electrode. Our TRNG offers advantages in terms of circuit complexity and size since the randomness is derived from a single device. Furthermore, the generated bits pass the specified NIST Sp 800-22 rev. 1a randomness tests without any post-processing highlighting the potential of 2D-based hardware security primitives.

PS07
(Studnet) In Situ Chemical Analysis of Complex Oxide Interfaces via Auger Electron Spectroscopy
Harish Kumarabramanian, Thomas Orvis and Jayakanth Ravichandran;
University of Southern California, United States

Complex Oxides [1-3] have been investigated for their unconventional physical and chemical properties and ensuing broad technological applications, especially in the epitaxial thin film form. The key to controlling the properties of complex oxides is sensitively tied to their structure, composition, and chemical state of the transition metal ions in these materials. For ultra-high vacuum epitaxial growth methods such as molecular beam epitaxy, in situ structural characterization methods such as reflection high energy electron diffraction (RHEED) and low energy electron diffraction (LEED) have revolutionized our ability to control the structure of thin films, heterostructures and superlattices of complex oxides down to a single unit cell. These methods, RHEED in particular, have been adopted to high-pressure epitaxial growth methods such as Pulsed Laser Deposition (PLD). Nevertheless, the studying of the chemical state and composition of the materials in situ, especially in high-pressure environments, remains challenging due to the need to develop facile, accurate and versatile chemical and compositional analysis probes.

Recent developments in probe design for surface sensitive chemical analysis techniques such as Auger Electron Spectroscopy (AES) have expanded their use in harsh oxygen-rich atmosphere required for oxide thin film growth using PLD. This has been achieved by using a differential pumping system that uses a retarding field analyser (RFA), coupled with a collimator lens. This has led to increased sensitivity and much improved signal-to-background and signal-to-noise. This has further enabled us to measure and understand subtle changes in composition of the films in situ. Laser fluence and pressure [4]. Quantitative, real-time measurements of the composition during the growth have also led us to monitor and deliberately switch the surface termination of different oxide films [5].

Oxide heterostructures exhibit novel interfacial phenomena such as two-dimensional electron gases (2-DEGs), emergent ferromagnetism, tunable spin-charge interconversion and topological states. These interfacial phenomena are sensitive to surface reconstructions and charge transfer across the interfaces.

To probe and manipulate these interfacial phenomena, it is imperative to study the chemical state of transition metals and oxygen at the single unit cell level. Considering that Auger electrons are particularly sensitive to chemical state due to their outer-shell origins, real-time, in situ measurements of oxidation during growth would help us understand the interplay of charge transfer with lattice, spin, and orbital ordering. In this work, we simultaneously measure the oxidation state, surface composition and in essence the surface termination of complex oxides by monitoring the relative intensity ratios and shifts of satellite peaks in Auger fine spectra of both the transition metal cations and oxygen. Structural characterization using methods such as in situ RHEED and High-Resolution X-Ray Diffraction have been used to corroborate these findings.

REFERENCES:

PS08
(Studnet) Design and Fabrication of ITO Based Transparent and Flexible Electrode Array for Simultaneous 2-Photon Imaging and Electrophysiology
Vikrant Kumar1, Connor M McCullough2, Caroline Yu1, Emily Gibson3, Diego Restrepo2 and Ioannis Kymissis1;
1Columbia University, United States; 2University of Colorado Denver, United States

Neural electrodes with good electrical conductivity and optical transparency from visible to near-infrared could potentially allow for simultaneous 2-photon imaging and electrophysiology of brain tissues. Additionally, ultra-miniaturization of the microelectrode arrays is needed to achieve a higher spatial resolution of the neural recordings which requires simple fabrication techniques. Here we present a design and fabrication of an ITO-based transparent, flexible electrode array for simultaneous neurophysiological recording and 2-photon imaging. Finding correlation of imaging data and electrical recordings can provide additional insights towards understanding neural circuits. This is often achieved using opaque metal electrodes used for recording electrical signals which don’t allow optogenetic activation of neural cells directly underneath the electrodes. Transparent conductive electrodes from
visible to near-infrared (NIR) spectrum are needed to enable simultaneous 2-photon imaging and electrical recording. Along with transport properties, it is also important to have individual electrode sizes of the same order as the neural cells for improved spatial resolution of the recorded signals while maintaining the signal-to-noise ratio (SNR) of the system. The presented system addresses the above-mentioned issues. The size of the individual electrodes is 12 µm x 12 µm and the array has 34 channels arranged in a circle with a total area of 250 µm x 250 µm to fit at the bottom of a GRIN lens. The ITO electrodes showed optical transmittance of more than 80% in visible to NIR range in spectrophotometry. Electrical characterization (electrochemical impedance spectroscopy) showed an average impedance magnitude of around 325 kΩ for 10 different channels of the array when interfacing with physiological saline as electrolyte. Two-photon imaging with a 920 nm laser light source through the electrode array showed no significant loss in the IR loss signal demonstrating its transparency at the desired wavelength. The electrode array is connected to a custom PCB using a heat seal connector for data acquisition. The integrated array can further be mounted on a head-bar which can be used as a head-mounted device on a freely moving rat for simultaneous 2-photon imaging and electrical recording in the future.

**PS09**  
(Students) Impact of Biquadratic Exchange Coupling via Molecular Spins on Magnetic Tunnel Junction (MTJ) with Competing Molecular Spintronics Devices

Molecular spintronics self-assembled on magnetic tunnel junction (MTJ) testbeds are a promising method to attain functioning nanoscale devices. To fabricate a magnetic tunnel junction molecular spintronics device (MTJ-MSD), the desired geometry is created using photolithography, then the thin film MTJ material is deposited via physical vapor deposition. Molecular magnets self-assemble—under an applied electric potential—across the MTJ dielectric gap and covalently bond to the MTJ ferromagnet creating a complete MTJ-MSD. There is much to comprehend about competing couplings between the ferromagnetic metal electrodes when fabricating MTJ-MSDs. The attachment of molecule allows for Biquadratic exchange coupling (BC) and Heisenberg coupling (HC) between the ferromagnetic electrodes. Prior studies have focused on direct exchange coupling and Heisenberg exchange coupling, whereas this paper will explore the effects of BC with no direct exchange coupling and competing HC. Scaling up production of robust devices requires a detailed understanding of how the interaction between BC and HC affects the magnetic properties of the device, the device’s response to applied magnetic fields, and hence its performance. BC favors the perpendicular orientation, an effect which competes with Heisenberg exchange coupling. In this study, Monte Carlo simulations (MCS) focused on molecule-induced BC are used to understand how this exchange coupling affects overall device behavior. Our MCS utilizes the 3D Heisenberg model to simulate the MTJ-MSD design. This simulation study looks at the effects of increasing BC when molecules spanning 4 edges connect ferromagnetic electrodes of a cross junction MTJ configuration. Simulated devices stabilized after 200 million iterations sampled with a frequency of 25000. Our results showed that BC in the absence of HC had no effect on the magnetic susceptibility of the ferromagnetic electrodes of the device but induced a high and localized magnetic susceptibility at the molecular region. However, in the presence of both BC and HC, the magnetic susceptibility increased in the ferromagnetic electrodes and diminished at the molecular region. Here, we will also discuss how BC and HC exchange couplings influence the heat capacity of MTJ-MSDs to elucidate their response to applied thermal energy. This study provides insights for designing and understanding futuristic molecular spintronic devices. This research is supported by the National Science Foundation-CREST Awar (Contract #HRD-1914751), Department of Energy/ National Nuclear Security Agency (DE-FOA-0003945). [1] P. Tyagi: Multilayer edge molecular electronics devices: a review. Journal of Materials Chemistry B 21, 4733 (2011). [2] P. Tyagi, Nanotechnology, vol. 26 no.30, 305602 (2015). [3] H. Brown, A. Grizzle, C. D’Angelo, B.R. Dalal, and P. Tyagi, AIP Advances 11, 015228 (2021). [4] A. Kartsev, M. Augustin, R.F.L. Evans, K.S. Novoselov, and E.J.G. Santos, Npj Computational Materials 6, (2020)

**PS10**  
(Students) Spin Fluctuations in Molecular-Electrode Magnetic Tunnel Junction-Based Spintronics Devices

Understanding the charge transport of paramagnetic single-molecular magnets (SMM) sandwiched between optimized magnetic tunnel junction (MTJ) electrodes is essential for designing innovative molecular electronics. As a result, magnetic tunnel junction-based molecular spintronic devices (MTJ-MSDs) with increased optical, electrical, and magnetic properties are developed. Previous computational and experimental studies show that when molecules with fluctuating spin states are placed at room temperature between ferromagnetic electrodes, they display substantial antiferromagnetic coupling. On the other hand, quantifying the SMM's spin state when attached to the MTJ-MSD remains challenging. In turn, we conduct a Monte Carlo Simulation (MCS) analysis to investigate the spatial and temporal influence of the SMM spin state and spin fluctuation on the cross junction-shaped MTJ-MSD. Using a Markov process lead MCS and a Heisenberg model of the MTJ-MSD, we investigated the temporal and spatial distribution of the molecular-ferromagnet correlated phases. We also looked at the magnetic moments of the MTJ-MSD as a function of the SMM spin fluctuation, device thermal energy, and molecular coupling strengths. We also looked into the MTJ-MSD’s heat capacity and magnetic susceptibility. To generate highly correlated phases and the overall MTJ-MSD antiparallel state, the normalized molecular spin state must be greater than 0.2. Furthermore, the MTJ-MSD moment varied non-linearly with molecular coupling intensity. Our findings imply that while developing MTJ-MSDs, it is critical to quantify the SMM spin state.

**PS11**  
(Students) A Comparison Between Heisenberg and Biquadratic Exchange Coupling Effects on Magnetic Tunnel Junction Molecular Spintronics Devices (MTJ-MSDs)

The MTJ-MSD nanostructure consists of two adjacent ferromagnetic (FM) electrodes separated by an insulator with molecules bridged across the tunnel barrier. The molecules enable communication via electron flow between the FM electrodes. The Heisenberg Exchange Coupling (HC) and Biquadratic Exchange Coupling (BQC) are present in this phenomenon and affect the device’s magnetic behavior. Strong HC is exhibited between the FM electrodes and the molecules that bridge the two electrodes of the MTJ-MSD. BQC—perpendicular alignment of the spin vectors of the adjacent FM electrodes—also occurs via the insulator or molecular nanostructures. Little is known about the competing effects between these two types of interlayer exchange couplings on MTJ-MSDs. We studied this effect using Monte Carlo simulations (MCS) based on a 3D Heisenberg model. We varied...
the BQC strength for a device with strong parallel and antiparallel molecular HC, and examined the physical and magnetic properties of the MTJMSD. We found that as we increased the BQC strength in an MTJMSD with antiparallel molecular HC, the range of the antiparallel molecular coupling effect increased in both FM electrodes. However, only slight changes in the overall magnetization of the device were observed, and the antiparallel state was maintained. HC still ultimately dominated the magnetization of MTJMSD. We also studied the effect of BQC on the device’s magnetic equilibrium state by examining the temporal evolutions of the device. Here, we will present our results that indicate BQC plays a lesser role in overall device magnetization as it cannot overcome the more substantial magnetization effect produced by the HC. We will also discuss our results from several other HC versus BQC possibilities under which BQC promoted the development of magnetic phases at 90-degree alignment. The presence of BQC provides a plausible explanation for the experimentally observed difference in magnetic phase orientations other than parallel and antiparallel states around MTJMSD.

This research is supported by National Science Foundation-CREST Award (Contract #HRD-1914751), Department of Energy/National Nuclear Security Agency (DE-FOA-0003945).

References


PS12 (Student) A Monte Carlo Study of Paramagnetic Nanostructure Coupled with Two Ferromagnetic Electrodes of a Cross-junction Shaped Spintronics Device at Different Thermal Energies Pranshu Tyagi1, Andrew C. Grizzle2, Christopher D’Angelo1 and Eva M utunga2; 1Springbrook High School, United States; 2University of the District of Columbia, United States

Nanoscale spintronics devices can revolutionize computer logic and memory units. Interestingly, paramagnetic nanostructures strongly exchange coupled with two ferromagnetic electrodes can yield novel forms of magnetic materials. However, there is a knowledge gap about the role of the number of paramagnetic nanostructures on the various properties of whole spintronics devices. To make this study relevant to the experimentally attainable device structure, we focus on the magnetic tunnel junction (MTJ) based spintronics device architecture. Under this approach, paramagnetic nanostructures are placed along the MTJ perimeter. We assume that the tunnel barrier of the MTJ does not allow any leakage current or exchange coupling, and paramagnetic nanostructures dictate the exchange coupling between the ferromagnetic electrodes. Also, the width of the ferromagnetic electrodes is governed by the number of paramagnetic nanostructures. This study systematically varied the number of nanostructures from 1 to 625 (25 x 25). The overall device was represented by a Heisenberg 3D model containing five atomic layer thick ferromagnetic electrodes. The number of paramagnetic nanostructures governed the width of the ferromagnetic electrodes. For instance, the device with a single nanostructure and 5 x 5 nanostructure possessed FM electrodes with one atom and five atom width, respectively. The paramagnetic nanostructures - sandwiched between the two FM electrodes - were placed on the perimeter of the 5 x 5 square with an empty space inside the square. The empty space shows the presence of an insulating layer of 11 being the thickness of the MTJMSD and 5 x 5 x 50 being used in this study is represented by a 11 x 50 x 50 Ising model, crucial to improving the performance of MTJMSD. The MTJMSD enables the utilization of paramagnetic nanostructures to control the spin dynamics of the device. The strength of exchange coupling between the paramagnetic nanostructure and ferromagnetic electrodes was fixed to be antiferromagnetic, consistent with experimental observations with analogous devices. We observed that thermal energy strongly influenced the temporal evolution of the equilibrium state of devices. The device with a single paramagnetic nanostructure struggled to align the left ferromagnet (Left-FM) and right ferromagnetic electrode (Right-FM) at low thermal energy of $kT = 0.01$. At higher thermal energy, devices with a single paramagnetic nanostructure underwent significant fluctuations. The device with a 5 x 5 paramagnetic structure also had difficulty attaining the fully antiparallel state at low thermal energy of $kT = 0.01$. However, at higher thermal energy of $kT = 0.1$, 5 x 5 paramagnetic nanostructure started producing conclusive antiparallel ferromagnetic electrodes. This paper will discuss the full range of paramagnetic nanostructures up to 25 x 25 sizes over the thermal energy range from 0.01 to 0.1. To estimate the spatial impact range of the nanostructures, we also investigated the spatial correlation factor for each case. In addition, we also compute the spatial magnetic susceptibility and heat capacity of the device.

References:

PS13 (Student) Influence of Crystallographic Orientation on the Asymmetric Emission of Calcite Ka’la S. Diaz-Granados1, Weliang Ma2, Guanyu Lu3, Peining Li1 and Joshua Caldwell1, 1Vanderbilt University, United States; 2HuaZhong University of Science and Technology, China

Calcite is a naturally occurring crystal that has a high level of anisotropy, and as such, exhibits thermal properties that are asymmetric. The orientation of the optic (or anisotropy) axis of the crystal with respect to its surface is experimentally shown to modify its thermal emission pattern. As the optic axis is tilted away from the surface, the emissivity peaks associated with the primary IR vibrational modes of calcite are seen to change in both shape and magnitude, indicating that tilting the optic axis effectively changes the contributions of each mode to the measured emissivity. Further varying the optic axis orientation by changing the altitude, azimuth and polarization angle for each tilt angle suggests that the emissivity signature is sensitive to changes in both the in-plane and out-of-plane optic axis orientation, and that, consistent with polarization selection rules, changes in the optic axis alignment with respect to the detector and the polarization orientation modify the sampled vibrational modes. The observed asymmetries suggest that changing the orientation of the optic axis offers a way to tune the material dictated R-estrahlens bands in naturally anisotropic crystals.

PS14 Magnetic Anisotropy Effect on the Magnetic Tunnel Junction Based Molecular Spintronics Devices Bishnu R. Dahal, Marzieh Savadkhoohi, Eva Mutunga, Christopher D’Angelo and Pawan Tyagi; University of the District of Columbia, United States

Molecular spintronics is gaining attraction because molecules possess a weak scattering mechanism. As a result, molecules retain spin information over time. Molecular Spintronics devices (M SD) are also considered crucial for futuristic quantum computing.
technology [1]. However, the fabrication of robust and mass-producible MSDs at the nanoscale is a major concern. To overcome this issue, we have designed a magnetic tunnel junction-based molecular spintronics device (MTJ MSD). The MTJ MSD is fabricated by bridging paramagnetic molecules across the edges of the ferromagnetic electrodes. These molecules form conducting channels over tunneling conduction between two ferromagnetic electrodes of am M T J. The MTJ MSD enables the utilization of ferromagnetic electrodes with a wide range of magnetic anisotropies. Here, we are analyzing the magnetic switching mechanism, hysteresis loop (M-H Curve), and the overall magnetic properties of M T M D as a function of anisotropies along with constant Heisenberg couplings.

In this paper, we report a theoretical Monte Carlo Simulation (MCS) study to explain the impact of anisotropies on the MTJ MSD equilibrium properties. We also investigate theoretically how the nature of magnetic hysteresis changes as we apply the in-plane, out-of-plane, and in-plane and out-of-plane at the same time on the same ferromagnetic electrode. The application of in-plane anisotropy creates multiple magnetic phases of opposite magnetic spins on the same ferromagnetic electrode. The application of out-of-plane anisotropy created a dominant magnetic phase on the electrode. When in-plane and out-of-plane anisotropies are applied on an electrode simultaneously, the magnetic moment of the electrodes possessed its maximum value. The MTJ MSD possessed its maximum value since the competing effect of anisotropies wiped out the multiple magnetic phases.

In this study, we also investigated the effect of anisotropies on the nature of the hysteresis curves generated computationally using MCS. We applied the in-plane and out-of-plane magnetic anisotropies on the same ferromagnetic electrode of an MTJ. The effect of the in-plane anisotropy transformed the regular magnetic hysteresis of M T J MSD into a “wasp-waisted” -like hysteresis curve[2]. The “wasp-waisted” -like hysteresis curve is hypothesized due to the presence of multiple magnetic phases present on the ferromagnetic electrodes caused by strong magnetic anisotropy. The application of equal magnitude of in-plane and out-of-plane anisotropies brings back the M-H curve into a regular hysteresis curve but with nearly zero coercivity. The zero coercive hysteresis closely agrees with the experimentally measured hysteresis under the same situations. In this paper, we will also present the overall properties of MTJ MSD when the spin fluctuations option is incorporated in the MCS code.

This research is supported by National Science Foundation-CREST Award (Contract # HRD-1914751), Department of Energy/National Nuclear Security Agency (DE-FOA-0003945).

References

PS16
Control of the Color Centers in Diamond Through Surface Encapsulation Summayya Kouser and Peter V. Sushko; Pacific Northwest National Laboratory, United States

Color or vacancy centers in the diamond lattice have found applications in novel fields like quantum computation and single spin magnetometry due to the possibility to prepare and read out their corresponding spin state optically and their long spin coherence times [1-2]. For example, Nitrogen vacancy (NV) centers can act as single-photon emitters in the near-infrared with absolute photo stability at room temperature. These vacancy centers occur in several charged states. Behavior of these optically addressable spin defects (OSDs) is affected by surface termination, roughness, proximity of the spin defects to the surface, polar & charged surface adsorbents and interfaces with other materials. Optically favorable NV centers show a mixed coupling state [3] to the surface which can be controlled by tuning the surface. The surface termination of the NV charge state is a crucial point, as defects with reliable spin properties in close vicinity to the surface are required. Surface termination can evolve due to interactions with environmental species, thus affecting properties of the defects [4]. We propose that surface encapsulation with 2D materials can be used to preserve the ordered H-termination and the Fermi level can be tuned by simultaneous adsorption of appropriate electron scavengers on the capping layer by tuning surface dipole. To this end, we use ab initio simulations to examine binding energies of species that saturate dangling bond on diamond surfaces, their interaction with encapsulating 2D materials, and the effect of electron charge redistribution on the band bending in the vicinity of the surface. We also consider the barriers for the diffusion of the adsorbed species across encapsulating layer to identify environmental conditions that allow for surface protection.


PS15
Control of the Color Centers in Diamond Through Surface Encapsulation Summayya Kouser and Peter V. Sushko; Pacific Northwest National Laboratory, United States

Color or vacancy centers in the diamond lattice have found applications in novel fields like quantum computation and single spin magnetometry due to the possibility to prepare and read out their corresponding spin state optically and their long spin coherence times [1-2]. For example, Nitrogen vacancy (NV) centers can act as single-photon emitters in the near-infrared with absolute photo stability at room temperature. These vacancy centers occur in several charged states. Behavior of these optically addressable spin defects (OSDs) is affected by surface termination, roughness, proximity of the spin defects to the surface, polar & charged surface adsorbents and interfaces with other materials. Optically favorable NV centers show a mixed coupling state [3] to the surface which can be controlled by tuning the surface. The surface termination of the NV charge state is a crucial point, as defects with reliable spin properties in close vicinity to the surface are required. Surface termination can evolve due to interactions with environmental species, thus affecting properties of the defects [4]. We propose that surface encapsulation with 2D materials can be used to preserve the ordered H-termination and the Fermi level can be tuned by simultaneous adsorption of appropriate electron scavengers on the capping layer by tuning surface dipole. To this end, we use ab initio simulations to examine binding energies of species that saturate dangling bond on diamond surfaces, their interaction with encapsulating 2D materials, and the effect of electron charge redistribution on the band bending in the vicinity of the surface. We also consider the barriers for the diffusion of the adsorbed species across encapsulating layer to identify environmental conditions that allow for surface protection.


PS16
Student Spatial and Thermal Properties of Magnetic Tunnel Junction Based Molecular Spintronics Device (MTJ MSD) Due To Magnetic Anisotropy Rodmecia Taylor, Bishnu R. Dahal, Eva Mutunga, Andrew C. Grizzle, Christopher D’Angelo and Pawan Tyagi; University of the District of Columbia, United States

Magnetic tunnel junction molecular-based spintronics devices (MTJ MSDs) make the miniaturization of spintronics devices possible. MTJ MSDs are durable and mass-produceable. Here, a Monte Carlo Simulation (MCS) study is designed to study the MTJ MSD properties. The MTJ MSD nanostructure consists of covalently bonded paramagnetic molecules bridged across the edges of ferromagnetic electrodes of a cross-junction magnetic tunnel junction (MTJ)2. We have studied the magnetic and thermal properties of MTJ MSDs based on various parameters such as anisotropy, FM electrodes’ coupling strengths, molecule type, insulator thickness, spin state, device dimension, and thermal energy (kT).

In this paper, we looked at the anisotropy effect of the ferromagnetic electrodes on the MTJ MSD’s properties at various thermal energies. Magnetic anisotropy is important for molecular spintronics because applying the logic of controlled anisotropy is crucial to improving the performance of MTJ MSD. The MTJ MSD used in this study is represented by a 11 x 50 x 50 ising model, with 11 being the thickness of the MTJ MSD and 5 x 50 being the size of each electrode. These two electrodes are connected by 5 molecules on each edge at the cross-junction. We ran the Markov process for 500 million iterations to reach the equilibrium state. Our study shows that the multiple domains of opposite spins start to appear on a FM electrode as the anisotropy strength increases. These domains impact the overall magnetic properties of the device. Symmetric magnetic properties of MTJ MSD were observed in the spatial spin state as the out-of-plane anisotropy was switched across the left and right FM electrodes. In the strong molecular coupling regime, the effect of variation in anisotropy was stable at a relatively high thermal energy. We observed that
anisotropy maintains the higher magnetic moment of the device close to the levels observed at Curie temperature, even when all the coupling effects get nullified due to thermal agitation. These studies are expected to impact the electrical and magnetic-transport properties of M TMjMSD and may help in designing M TMjMSDs for logic and memory operation. Heat capacity and magnetic susceptibility, essential quantities that are commonly used to measure anisotropy, will be part of this discussion.


PS17 (Student) The Design and Synthesis of Lead-Free Layered Hybrid Perovskites as Room-Temperature Ferroelectrics
Joseph T. Race and Patrick Woodward; The Ohio State University, United States

A promising crystal structure type for ferroelectricity is the layered organic-inorganic perovskite (HOIP) due to their tendency for polar structural distortions, a requirement of ferroelectricity. The most prominent layered HOIPs reported to be ferroelectric have the Ruddlesden-Popper (RP) structure consisting of inorganic slabs n-octahedra thick separated by organic cation bilayers and often contain a water-soluble form of toxic lead (Pb2+). We aim to synthesize hybrid RP double perovskite ferroelectrics that replace Pb2+ with non-toxic M+/M3+ cation pairs (i.e. Ag+/Bi3+ or Ag+/In3+) and to better understand the structural distortions that lead to these polar structures.

One of the common structural distortions in hybrid RP perovskites is an octahedral tilt/torsion of the corner-connected octahedra to optimize the hydrogen bonding interactions between inorganic perovskite slabs and organic cations. We aim to understand the octahedral tilting patterns that allow the dipole moments of the polar organic molecules to align, creating a spontaneous electrical polarization within the crystal. We also seek to probe the contribution of the inorganic layer to the electrical polarization and if it aligns cooperatively with the organic layer. X-ray diffraction will be used to study the phase transitions of these compounds.

PS18 (Student) Characterization of Aqueous Lead Sensing Performance of Bismuth Functionalized 3D Inkjet Printed Electrochemical Electrodes
Anamata Arif and Robert C. Roberts; The University of Texas at El Paso, United States

This research represents the design, fabrication, and characterization of bismuth (Bi(I)) functionalized 3D inkjet printed (IP) thin film metal electrodes on shape memory polymer (SMP) towards improved electrochemical sensing performance of lead (Pb(II)). The fabricated Bi(III) coated electrodes are characterized with the sample analyte prepared with 10 µg/L lead (Pb(II)) added to drinking water (El Paso, TX). The electrochemical cell fabricated in this research consists of a three electrodes cell: a counter electrode (CE), a working electrode (WE), and a reference electrode (RE). The WE is modified with Bi(III) by two different procedures: (a) ex situ - under potential deposition (UPD) of Bi(III) with a full cycle of cyclic voltammetry (CV) electrochemical analysis and (b) in situ - addition of 400 µg/L Bi(III) to a sample anlyte of alkaline based drinking water contaminated with Pb(II).

Bi(III) is an environment friendly material. It plays an important role for heavy metal ion detection. The advantages of Bi(III) coated electrodes in case of heavy metal ion detection are less toxicity, high capacity for fused-alloy formation, less interference of the dissolved oxygen in the test medium, and wide negative potential window. One major disadvantage of Bi(III) is that it requires specific test medium such as an alkaline solution to activate its behavior. In this research, the disadvantage is overcome by preparing sample analyte by adding a very small amount of 50% sodium hydroxide (NaOH) directly to Pb(II) contaminated drinking water. The achieved pH of the sample analyte is 14. The electrodes are initially IP (Fujifilm, DMP-P-2831) on SMP substrate using silver (Ag) nanoparticle conductive ink (A.N.P, DGP-40-LT-15-C). The electrochemical cell containing one CE, WE, and RE are cuted, sintered, and shrunk simultaneously at 180 °C for 3 min. The final lateral dimension of the electrochemical cell is 13 x 10 x 1.52 mm² and the lateral working electrode surface area is 4 mm². The CE and WE are then gold (Au) plated with 24K brushed gold solution. The RE is chlorinated with dilute sodium hypochlorite solution for 60 seconds for silver chloride (AgCl) formation. Finally, the Au working electrode is Bi(III) coated by electroplating a film of Bi(III) on the surface of the electrode. This process can be performed in two different ways such as ex situ and in situ. This research has focused on both procedures to understand their effectivity towards improved electrochemical sensing performance.

In the ex situ procedure, the electroplating is conducted prior to the electrochemical sensing analysis. In this research, the ex situ Bi(III) plating is performed in two steps. In the first step, the solution of bismuth (III) chloride (Bi(III)Cl) and water (H2O) was prepared. Bi(III)Cl3 is soluble in HCl and H2O. In the next step, a full cycle of CV analysis is performed on the Au based IP SMP incorporated electrodes to deposit Bi(III) film on the electrodes based on UPD. After Bi(III) coating the electrodes are applied to electrochemical sensing such as Pb(II) detection in the drinking water (alkaline). It is observed from the CV analysis that the Pb(II) stripping is sharper and appeared at more negative potential compared to Au platted electrodes. In the in situ procedure, the electroplating is conducted simultaneously with the electrochemical sensing process. 400 µg/L Bi(III) was added with the sample analyte of Pb(II) contaminated tap drinking water optimized with NaOH. It is observed from the CV analysis that in situ Bi(III) electroplated electrodes perform significantly better in terms of stripping peaks (sharpness and appearance at the potential) for electrochemical sensing performance of Pb(II) detection in the optimized drinking water.

PS19 (Student) Spin Fluctuation Effect on Magnetic Tunnel Junction-Based Molecular Spintronics Devices

Arush Guirani1, M Chiha Tefera2, Patricia Reesen3, Andrew C. Grizzle4, Christopher D’Angelo4, Eva Mutungu4 and Pawan Tyagi5; 1Dublin High School, United States; 2Virginia Tech, United States; 3University of the District of Columbia, United States

When paramagnetic molecules covalently bond to a ferromagnet (FM), they undergo extensive hybridization with the surface and result in a spin-polarized molecule-ferromagnet interface. The resulting ferromagnet-molecule hybridization leads to a wide range of active functionalities, such as energy-level control and spin filtering capabilities. Magnetic tunnel junction-based molecular spintronics devices (M TJ M SDs) are fabricated by bridging monolayers of molecules across the M T J M S D s barrier, where they chemically bond with the FM electrodes. Thus, M TJ M SDs become a highly promising testbed for controlled spintronics at room temperature. M TJ M SD testbed also allows the molecule-ferromagnet interface to become a significant spin pathway enabling new equilibrium density of states over long range. Understanding the role of spin fluctuations in M TJ M SD with various types of metallic electrodes is exceptionally challenging. We conducted theoretical studies to understand the free electrons spin effect on M TJ M SD magnetization using 3D Heisenberg-based Monte Carlo simulations. For this study, we varied the electron spin in 1) ferromagnet-ferromagnet, 2) ferromagnet-paramagnet, and 3) ferromagnet-antiferromagnet electrode pairs. In general, we found that as the magnitude of free electrons spin in the electrodes
and molecules increased, the device magnetization increased when the free electron had parallel coupling with its host atom. Conversely, the total device magnetization decreased for antiparallel electron-atom coupling. Interestingly, long-range ordering in antiferromagnetic electrodes diminished with antiparallel electron-atom coupling and was enhanced with parallel coupling for a free-electron spin of equal magnitude at room temperature. In this study, we also recorded the correlated distribution of the devices’ magnetic moment to elucidate the spatial impact range of molecules as a function of free electron spin. We also explored the electron spin effect on magnetic susceptibility and heat capacity. This research may inform the designing of novel molecular spintronics devices by providing a knowledge base about the impact of free electron spin for varying electrode materials.

This research is supported by National Science Foundation-CREST A ward (Contract # HRD- 1914751), Department of Energy/ National Nuclear Security Agency (DE-FOA-0003945).


PS20
(Student) Phase Equilibria in the Metal-Sc-N Systems and Their Relevance for Contacts to ScN, ScGaN and ScAlN by Li Yao and Suzanne Mohney: The Pennsylvania State University, United States

The properties of neighboring layers in thin-film structures are critical for the reliability and lifetime of electronic devices, and the reactivity of metals on semiconductors can markedly affect contact resistance. Wurtzite alloys of GaN or AlN with ScN are emerging thin-film piezoelectric materials.[1] Some researchers have also suggested that ScN might be used to advantage for in situ ohmic contacts in nitride devices, [2] although there is limited work on contacts to ScN. [3] Little work has been performed to examine the reactivity of ScN with other transition metals. This study calculates ternary phase diagrams for the Sc-M-N systems (M =transition metal) using reported experimental and estimated values of thermodynamic data. The calculated phase diagrams allow the identification of the dominant phase(s) for each Sc-M-N system. Systems are classified as ScN dominant (in which ScN is unreactive with the metal), metal-scandide dominant, metal-nitride dominant, or no phase dominant. It appears that ScN is stable against reaction with more transition metals than is GaN [4] and perhaps even AlN. [5] Among the metal-nitride dominant systems, we predict Ti, Zr, and Hf to be reactive should kinetics permit.

Palladium, Pt, and Au are also predicted to be reactive due to the stability of their metal scandides. Future work will consider the mutual solubility of ScN and other transition metal nitrides, and we will present the results of annealing studies of metals on ScN.

zinc blende crystal structure and are mutually soluble. GaBi has also recently been reported to grow epitaxially 1D or 2D on GaAs nanowires [1]. For the II-VI compounds, ZnSb is a well-known thermoelectric semiconductor [2]. It has the orthorhombic Pbcn #61 structure referred to as ‘electron pool’ [3]. The same structure is reported for ZnAs [4] however it requires growth under high pressure. The compound ZnBi with Pbcn structure has been reported but is also unstable [5]. The compounds ZnP and ZnN don’t exist with the same crystal structure but containing similar short order consisting of polyhedra. The mono pnictogens could hypothetically intermix and stabilize in a common crystal structure stabilized by entropy of mixing, like high entropy alloys. We have made mixtures of these elements and given melting and heat treatments followed by phase characterization and compactation of samples followed by electrical characterization. Mixtures of Zn, As, and Sb, resulted in phase structures with phase separation between arsenide and antimonide dependent upon the mixing ratio. Here we report on some interesting results for a parameter space winding yielding composite of the semiconductors ZnSb and ZnAs from X-ray analysis and analytical electron microscopy inspection. ZnAs is a semiconductor [6]. We doped the composite by Cu. The temperature dependence of the is metallic like or like that of a degenerate semiconductor while the Seebeck coefficient is very high for the undoped material. The Hall coefficient and the sign of the Seebeck coefficient both show p-type behavior. The doping of the composite with Cu lowers the resistivity and the Zebeck coefficient but the latter is still interestingly high and the thermal conductivity low.

References
7. I. G. Statov, N. N. Syrba, V. V. Uzakin, A. V. Dorogan, Optics Communications 285, 3104 (2012)

PS24
(Student) Flexible Electrochemically Reduced Graphene Oxide Sensors for Lead and Cadmium Detection
Rebekah De Penning and Sonal Padalkar, Iowa State University of Science and Technology, United States.

Electrochemically reduced graphene oxide (ERGO) is an excellent sensor material for toxic heavy metal ion detection due to its unique properties. The ERGO combines the conductivity of pristine graphene with oxygen-containing defects that provide active binding sites for ions such as Pb2+ and Cd2+. Sensors can be fabricated directly via electrochemical reduction from graphene oxide (GO) solution. This GO solution can be prepared in bulk by the Hummers method. The ERGO layer thickness can easily be controlled by changing the process parameters during the electrochemical deposition cycle. It can be easily deposited on substrates with varying degree of conductivity including glassy carbon, indium tin oxide on glass, carbon paper, carbon cloth etc. The carbon cloth substrate is particularly interesting in that it is flexible, three-dimensional, conductive and inexpensive. The combination of carbon cloth and ERGO forms a sensitive and disposable solution to the simultaneous electrochemical detection of Pb2+ and Cd2+. By using differential pulse anodic stripping voltammetry, ERGO on glassy carbon can detect down to 50 nM of Pb2+ and 100 nM of Cd2+ and could result in simultaneous oxidation peaks for both ion species. Furthermore, the ERGO-carbon cloth sensor shows vastly improved current response compared to the glassy carbon substrate due to the cloth’s 3D nature and high surface area combined with ERGO’s affinity for heavy metal ions. Therefore, electrochemically reduced graphene oxide and carbon cloth form a promising material combination for heavy metal sensing in water and food products.

PS25
Superconducting Properties of Fe (T, Se) Thin Film on YSZ Substrate Using Pulsed Laser Deposition (PLD) Technique
Himanshu Chauhan and Ghanshyam D. Varma, Indian Institute of Technology Roorkee, India.

More than a decade after the discovery, the Fe-based superconductors (FeSCs) continue to fascinate the material science and condensed matter physics communities, not only due to their high transition temperature, strong irreversibility field, and excellent crystallographic symmetry, but also as a platform to investigate the correlated quantum matter. Recently, topological states have also been reported in the iron-based superconductor which suggests a promising direction to realize topological superconductivity. In recent years, several groups have been trying to understand the origin of topological states in thin films, but so far there is not much experimental agreement on these issues, and further studies are needed. Here, we have studied structural, superconducting, and topological properties of Fe1−xT,Se2 thin films on Y tri-stabilized zirconia (YSZ) single-crystalline substrates using pulsed laser deposition (PLD) technique. The superconductivity in the thin grown film at Tc = 14 K has been affirmed by the temperature-dependent resistivity measurements. Superconducting parameters such as upper critical field Hc2(0) and corresponding coherence lengths λc and activation energy Δ0 have been estimated using magnetotransport measurements. In addition, A non-saturating linear magnetoresistance (LMR) is also observed, suggesting the presence of a possible topological superconducting state in the grown thin film. Furthermore, I-V measurement data has been used to calculate transport Jc (~104 A/cm²) of grown thin film and the high Jc value demonstrates its
potential for high current applications. Our work will be helpful in
developing thin films of Fe (Te, Se) superconductors with good
superconducting properties that are important for various
superconducting electronic devices. The study of the presence of
the topological phase in the grown film is very relevant to the
current focus of developing quantum devices.

PS26
(Student) Phase-Control Enabled Tunable Optical Properties
of Nanostructured GeO2 Wide Band Gap Semiconductor Thin
Films Paul Gaurav G. Nalam, Debabrata Das and Chintalapalle
Rama; The Center for Advanced Materials Research, UTEP, United
States

Germanium dioxide (GeO2), which is an ultra-wide band gap
material, has been explored in detail due to its promising thermal,
optical, and electrical properties. While GeO2 films exhibit quite
interesting electronic properties, such as a high dielectric constant
and refractive index, understanding the process-property
relation is the key to tailor their device performance. In this
work, GeO2 films (100 nm) were deposited onto Si(100) and
sapphire substrates using sputtering in an oxidizing environment.
The post-deposition annealing was performed at 800–1100°C in
order to study the temperature-induced effects on the structure,
morphology, and optical properties of GeO2 films. While the as-
deposited GeO2 films were amorphous, increasing temperature
induces amorphous-to-crystalline transformation. At 800°C, GeO2
films exhibit hexagonal phase and then a clear phase transition
with tetragonal structure at 1000°C. Correspondingly, the optical quality
and band gap variation is noted in annealed GeO2 films. The results
will be presented and discussed to establish the structure-
property correlation.

PS27
(Student) Optimized Light Absorption in GaAsSb(N)
 Nanowires for Photodetector Application Kendall D. Dawkins
and Shanthi Iyer; North Carolina A & T State University, United
States

Nanowires (NWs) offer the ability to fabricate 3rd generation
devices with unique properties such as enhanced optical
absorption, quantum confinement, low footprint, and high surface-
to-volume ratios. The nanowire architecture also allows for a high
tolerance for lattice mismatch, which results in the ability for
nanowires to be grown on a multitude of surfaces. Since the
diameter of nanowires is constrained to usually tens of nanometers
with the length varying up to several micrometers, this confines the
 carriers in two dimensions and allows for free propagation in the
3rd dimension. This correlates to the high density of electronic
states leading to electrical, optical, and magnetic properties that are
different than bulk and thin-film devices. By changing certain
physical features of the nanowires, one can potentially design
nanowires to exhibit distinct features for specific devices. GaAsSb
is an important material system covering the telecom wavelength
range of 870 nm (GaAs) to 1700 nm (GaSb). Incorporation of
small amounts of nitrogen, usually less than 2%, leads to the
reduction in the bandgap as well as lattice constant which is unique
for the dilute nitride system. In this study, Lumerical Finite-
Difference Time-Domain (FDTD) modeling has been used to
simulate the absorption characteristics of GaAsSb(N) nanowires.
The optimal absorbance spectra for GaAsSb(N) nanowires for
arrays were determined by varying nanowire diameter (D), pitch
(P), length (L), and array configuration. From our results, we show
that particular D/P ratios of 0.5 offer optimized light absorption for
GaAsSb(N) nanowires. We show that GaAsSb(N) nanowires are
excellent materials choices for absorption in the telecom
wavelength spectra reaching 1.55 μm in a first-of-its-kind study for
the GaAsSb(N) material system.

Acknowledgment: This material is based upon research supported
by the Air Force Office of Scientific Research (AFOSR) under
grant number W911NF1910002 and National Science Foundation
Award #ECCS-1832117.
limits the resistivity between 44 (Ω cm) (ZnO:0%In) and 0.017 (Ω cm) (ZnO:3.5%In). The radius of In^{3+} ions (0.81Å) larger than the radius of Zn^{2+} ions (0.74Å) that causes the stresses in the doped ZnO:In films, which influence on their structure and optical properties. To minimizing the doping stimulated stresses in ZnO films, the ZnO films with Al and In co- doping are investigated in this work. Note that the radius of Al^{3+} ions (0.53Å) smaller than those of Zn^{2+} ions.

The variation of the optical, structural and electrical parameters of ZnO nanocrystal films co-doped with In and Al atoms has been studied. The ZnO:In:Al films were deposited by spray pyrolysis with constant In content of 1at% in all ZnO films, but the different Al concentrations in the range of 1.0-3.5 at%.

ZnO films have been studied using scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS) and X-ray diffraction (XRD) for the analysis of the composition and structural parameters. Furthermore, the photoluminescence, absorption and transmittance spectra were measured for monitoring optical parameters, as well as electrical resistivity has been controlled for all films. Two doping stages of the measurement of all studied parameters were analysis and discuss. The optimal concentration of In and Al co-doping is estimated.

PS30

(Student) Growth and Characterization of (Ba_{x}Ca_{1-x})TiO_{3} Single Crystals in Ir, Pt and Mo Crucibles Benjamin L. Dutton, Jani J. Jesenovec, Brooke Downing, Matt D. M. Culuskey and John S. McCloy; Washington State University, United States

Selecting a crucible material for crystal growth of high melting temperature oxides is often limited due to atmospheric and chemical conditions. In the case of Barium Titanate (Ba_{x}Ca_{1-x})_{2}TiO_{3} (BCTO), iridium, platinum and molybdenum crucibles were explored for Czochralski (CZ) and Vertical Gradient Freeze (VGF) growths. Compositions of x = 0.185 and x = 0.227 were utilized to avoid the hexagonal-cubic phase transition upon cooling which typically destroys a pulled BCTO crystal and achieve congruent melting in the case of the latter composition. Growth in an Ir crucible was found to produce the largest single crystals (~1 x 1 x 1 cm), although cost of growth in Ir in the current market is prohibitively expensive. Platinum crucibles were found to be difficult for CZ growth due to vertical temperature gradients inherent to induction heating, as well as a melting temperature near that of BCTO. Molybdenum was economic in comparison and was explored with various (Zr,Ti)O_{2} graphite insulation materials in order to minimize oxidation and melt interaction of the crucible at T_{m}.

As-grown and oxygen annealed single crystals were analyzed via Raman microscopy, X-Ray Diffraction and Scanning Electronic Microscopy (SEM), including Energy Dispersive Spectroscopy to determine dopant content, structure and analyze heterogeneous secondary phases. Fourier Transform Infrared Spectroscopy and Ultraviolet-Visible Near Infrared spectroscopy were used to study the optical properties of the crystals.

PS31

Fabrication of a Roll-to-Roll Printed Cantilever Type Touch Sensing and Actuating Device Sang Hoon Lee, Jae Hak Shin and Sangyoon Lee; "University of California, Irvine, United States; "Kookmin University, Korea (the Republic of)

Devices that serve touch sensing and actuating are particularly applicable for Haptic technology. In the MEMS technology, there is an air-gap under the cantilever type capacitive touch sensor, and the cantilever beam is deformed when a touch is applied. The sensor detects the change in capacitance depending on the distance between the electrode above the cantilever beam and at the bottom. In addition, in the case of the MEMS actuator, there is an air-gap under the cantilever, so it is easily actuated by applied external input. Compared to the MEMS technology, printed electronics has significantly high productivity. However, only 2D structures can be fabricated with printed electronics technology, and it is difficult to fabricate 3D structures with air-gaps. In this study, a cantilever type capacitive touch sensor and actuating device was fabricated. An air-gap was made by printing and removing a water-soluble polyvinyl pyrrolidone (PVP). (Figure 1) This method is similar to the wet etching in MEMS fabrication. In particular, productivity was further improved by using a roll-to-roll graving technique (Figure 2) which has a high throughput capability. First, the bottom electrode was made on a flexible polyethylene terephthalate (PET) substrate by roll-to-roll graving and printing a silver paste, and the dielectric layer was made by roll-to-roll graving printing a barium sulfate (BaSO_{4}). Then, a water-soluble PVP was roll-to-roll graving printed to make the sacrificial layer. And the top electrode was made by spin-coating a stretchable silver paste. On the top electrode, magnetic actuating layer having the same shape and size with the top electrode was made by spin coating an iron oxide (Fe_{3}O_{4}) and SU-8 mixture. Finally, the sacrificial layer was removed with water to make an air-gap. As a result of actuating and sensing tests, the magnetic actuating layer of the device was deformed up to 2 mm by the applied electromagnetic fields, and touch sensing sensitivity was 0.153 %/kPa.

PS32

Force Spun PVDF-TPU/Au Nanofiber Based TENG for Flexible Energy Harvesting and Bio Mechanical Motion Sensor Sk Shamim Hasan Abir and M. Jasim Uddin; University of Texas Rio Grande Valley, United States

Over the last few years, nanofiber based triboelectric nanogenerator (TENG) has caught great attention to the researchers all over the world for its inherent capability of converting mechanical energy to usable electrical energy. In this study, poly(vinylidene fluoride) (PVDF) and thermoplastic polyurethane (TPU) nanofiber prepared by Force spinning (FS) technique were used to fabricate TENG for self-charging energy storage and bio mechanical body motion sensor. The surface of the TENG was modified by uniform deposition of thin gold film to enhance the frictional properties; yielded 254 V open circuit voltage (Voc) and 86 μA short circuit current (isc), an increase of 112% Voc and 87% isc in contrast to bare PVDF-TENG. Moreover, the fabricated PVDF-TENG was tested against variable capacitors and resistive load and showed that with a 3.2 x 2.5 cm² active contact area, it can charge quick up to 7.64 V within 30s using a 1.0 μF capacitor and generate significant 2.54 mW power enough to light 75 commercial LEDs (1.5 V each) by the each tapping motion at 4 Hz (240 beats per minutes (bpm)) load frequency. Furthermore, the TENG was attached to different body parts to capture distinctive electrical signals for various body movement elucidated the prospective usefulness of our prepared nanofiber based TENG in self-powered flexible body motion sensor application.

PS33

Effect of Radical on Morphology and Charge Generation in Polymer Non-Fullerene Solar Cells Benjamin Gautam1, Sheenamalia Jones2, Tiawright3, Daria Thomas2, Shubo Han4 and Evgeny Danilov2; 1Fayetteville State University, United States; 2North Carolina State University, United States

Conjugated polymers and small molecules have been intensively studied due to their unique electronic and optical properties, and studies have shown the potential for optoelectronic applications including solar cells. Here, we studied the effect of galvinoxyl radical on the morphology and charge generation dynamics in polymer non fullerenes blends. We employed photoluminescence and transient absorption spectroscopy, and atomic force microscopy to study the charge carrier dynamics in morphology of polymer in these systems. With galvinoxyl, the morphology changed and 3% radical is added to PDDB-T:T1TC blend. The changes include the increased surface roughness and the aggregation. The change in aggregation is also reflected in photoluminescence spectra of these
blends. Transient absorption dynamics indicates that the ITIC exciton splitting is more efficient in radical added FDBB-T:ITIC blend compared to the pristine blend. Our results provide important guidelines for the design of efficient polymer non fullerene solar cells.

**PS34**

*(Student) Micro-sized Si-based Anodes Characterization and Optimization Using In situ Atomic Force Microscopy* Jian Li, Hanna Cho and Jung Hyun Kim; The Ohio State University, United States

Recently, extensive research efforts have been devoted to developing high-energy anodes for lithium-ion batteries (LIBs) by using Si-based materials due to their superior energy densities compared with conventional graphite anodes. Compared to Si nano powders, micro-sized Si-based anodes have unique advantages of high tap-density, low manufacturing cost, and good manufacturing safety. However, the practical implementation of the micro-Si anode requires understanding its electro-chemo-mechanical behaviors and its optimal operational conditions at the cell level. Otherwise, the large volume expansion of Si (c.a., 310 %) will lead to the mechanical pulverization of particles and consequent loss of electrical contact. In addition, the cracking of Si particles will produce new SEI layers, which not only consume active Li-ions but increase cell impedance.

To optimize the electrochemical performance of micro-Si anode, we developed approaches to mitigate the Si mechanical degradation during battery cycling. We characterized the real-time morphological changes using in-situ Atomic Force Microscopy (AFM) and a designed AFM unit cell. We successfully tracked the volumetric variations of a micro-Si particle with respect to the cell state-of-charge (SOC) change and revealed its morphology-performance relationship.

From the in-situ AFM measurement, we successfully characterized multiple important electro-chemo-mechanical behaviors of the micro-Si such as volume-expansion behavior, particle crack generation, and SEI growth. We found these mechanical behaviors were closed related to electrochemical voltage windows and would directly affect the cycling performance of micro-Si anodes. Micro-Si particles underwent initial particle pulverization and subsequent large volume expansion (180%) during lithiation, then Si surface fractures were generated when excessively removing Li from Si. The Si surface fracture and resultant SEI growth significantly increased the cell impedance and degraded the cell performance. Our observations provide direct evidence that micro-Si degradation was triggered by reaching critical electrochemical cycling conditions. Then, we demonstrate a proof-of-concept that micro-Si anode can deliver an improved cycle life and lower cell resistance by applying the optimal cell cycling conditions. The results propose that micro-Si anode can offer a stable performance after further optimization of the cell materials and systems for next-generation high-energy Li-ion batteries.

**PS35**

*(Student) Magnetic Modification of Boron Nitride Nanotubes for Alignment in Thermal Interface Composite* A desewa O. Mgebulu and Jeffrey Aiston; North Carolina A&T State University, United States

Boron nitride (BN) nanotube is an anisotropic nanomaterial that possesses unique intrinsic properties like high thermal conductivity, electrically insulating, high oxidation resistance, superior mechanical strength, and piezoelectric property. The incorporation of the BN nanotubes in polymer has created opportunities to produce composites with a wide range of possible applications like aerospace applications, thermal interface material. However, the improved properties of these composite like thermal transport ability are still far from expected and theoretical stipulations due to the random orientation of these nanotubes with excellent in-plane properties and poor out-of-plane properties. Therefore, controlling the orientation of the nanotubes in the composite is important for optimizing its performance. This paper focused on the magnetic modification of boron nitride nanotubes for their alignment in polymer composite.

The magnetic modification of the BN nanotube is carried out by functionalizing nanotubes with iron oxide nanoparticles (magnetite) which produces paramagnetic BN nanotubes. These functionalized BN nanotubes exhibit magnetic responses that can enable control over their orientation and position under low external magnetic fields in low viscous fluids. The BN nanotubes are modified through electrostatic interaction with the iron oxide nanoparticles, therefore, preserving their intrinsic properties and structure. The paramagnetic nanotubes are to be dispersed in polymer fluid, controlled with magnets, and cured to maintain nanotubes’ position and alignment. The magnetic functionalization of BN nanotubes can provide the ability to spatially manipulate these nanotubes into more complex networks crucial for applications in nanoelectronics, sensors, spintronics, and thermoelectric devices. It can also enable the fabrication of anisotropic composite materials with improved directional property and high thermal transport ability.

**PS36**

*A Universal Expression for Transport in Nanostructured Materials and Devices* Andrés V. Cerón; University of São Paulo, Brazil

The Space-Charge-Limited-Current (SCLC) spectroscopy technique in solids is an extension of the one-dimensional Child-Langmuir law for vacuum gaps leading to the well-known Mott-Gurney law. Beyond that, the trap filling process leads to the Mark-Huffrich law. More recently, quantum and relativistic effects, as well as higher dimensions were incorporated. All these models can be expressed as a single scaling law, relating the current, \( J_{SCLC} \), with voltage, \( V \), and gap or sample thickness, \( D \), as \( J_{SCLC} \propto V^{2/3} D^{-1/3} \), with different values for the exponents. Other mechanisms are expected to occur in nanoscale solids and devices, such as field emission (FE) and Fowler-Nordheim (FN) tunnelling, which might lead to different dependencies of the current on voltage. However, some aspects of this technique remain obscure, especially when dealing with very thin (sub-10nm) gaps and solids. Beyond, the abrupt transitions between regimes, unusual SCLC characteristics, such as the transition from collisional to quantum tunneling regimes expected in out of 2D plane of 2D-material-based heterostructures, still remain unexplored. Therefore, there is a need for a universal model to describe SCL currents to include different conduction mechanisms as well as smooth transitions between them. This goal, pursued for decades without substantial success, might be not achievable based on the mentioned simple scaling laws, requiring a new approach. In this work we present a proposal for such universal model by writing the scaling laws in a slightly different way, with the same underlying physics, except for the treatment of transport through localized states, such as traps. A function \( h(V) \) which contains the relevant information for transport accounts for most of the fingerprints observed in experimental I-V curves of the most diverse set of physical systems, form materials to devices, is proposed. This approach leads to the usual scaling laws for constant values of \( h(V) \), whereas it is abandoned for the trap filling regime, although the same familiar higher slopes can be recovered. In contrast to the usual interpretation, the proposed model relates slopes of the log I - log V plot to trap (or localized states) density instead of trap energy. In order to show its applicability and accuracy, the proposed model is used to fit the I-V curves of different materials and device, namely, nanostructure organic composites, ultra-thin Metal-Oxide-Semiconductor devices and GaAs/AlGaAs/ double barrier resonant tunneling diodes.
With a net spin state, paramagnetic molecules can cause magnetic exchange coupling between two ferromagnetic (FM) electrodes in the magnetic tunnel junction-based molecular spintronic devices (MTJ/M). Magnetic coupling between paramagnetic molecules and two FM electrodes in MTJ-based devices is dependent on a net molecular spin state. However, there exists a missing piece of information regarding the role of the coupling between molecule to molecule on the magnetic properties of the MTJ/M. In this research, we tested the hypothesis that variation in the strength and nature of intra-molecular coupling among multiple segments of a molecule can produce a novel testbed to observe the novel phenomenon.

This paper investigates the effect of intra-molecular coupling (Jm) on the MTJ/M SD magnetic properties using Monte Carlo Simulation (MCS). The strength of Jm was varied from different molecular orientations, and its subsequent impact on the MTJ/M SD magnetic properties at different thermal energies studied. The total device magnetization was recorded as a function of time for various simulation counts to achieve device stabilization and to capture its temporal evolution. Our M CS results showed that low Jm yielded an impact localized around the junction area. These studies, creates a platform and serve as an appetizer for subsequent investigations on the effect of intra-molecular coupling on the magnetic properties of the MTJ/M.

**PS38**

**Modifed ZnSnO3 Structure in the Smart Helmet as a Promising Human Motion Sensor**

Sk M Md All Zaker Shawon and M. J asimuddin; University of Texas Rio Grande Valley, United States

Lead-free perovskite oxides in Piezoelectric nanogenerators (PENGs) as a prospective sustainable energy source have drawn the attention of the scientific community owing to their non-toxic nature of intra-molecular coupling among multiple segments of a molecule. In this work, we have grown gallium oxynitride on sapphire substrates using magnetron sputtering. Nitrogen incorporation was controlled by tailoring the percentage of nitrogen plasma during deposition. Substrate temperature was kept at a preoptimized value to demonstrate crystalline gallium oxynitride thin film with lowest possible defect density. Optical transmission measurement showed a gradual band gap shifting, which is because of nitrogen incorporated elevation of valence band maxima. The structure-chemistry-property correlation will be discussed to optimize the gallium oxynitride thin films for optoelectronic applications.

**PS40**

(Student) **A Numerical Study of Perovskite Solar Cells by Bandgap Tuning of Active Materials and Operating Temperature Variance**

Ahir Abrar, Srabanti Datta, Matty Sey and Deidra Hodges; Florida International University, United States

Perovskite solar cells have shown potential for high performance and low production costs and are considered as one of the most emerging solar cells technologies. In single-junction topologies, the solar cell efficiency of laboratory-scale devices using these materials improved from 3.8% in 2009 to 25.7% in 2021. Compositional differences in perovskites (ABX3) can produce a wide variety of crystal formations, phases, and structures. In this work, the mixed halide perovskite configuration of ABX3 (A = CH3NH3+, HC(NH2)2+, Cs+; B = Pb+2; X = I-1, Br-1) integrated with Spiro MO ETAD as the HTL layer, SnO2 as the ETL, FTO as the transparent front contact on a glass substrate, and Ag as the back contact studied theoretically. The solar cell simulation program wxAMPs has been used, which was an improvement of the prominent solar cell simulation platform AMPs. The research provided a thorough understanding of the effects of each layer throughout the solar cell as well as its impact on the overall photovoltaic parameters. The bandgap of the active materials and operating temperature of the simulated solar cell were found to have a strong impact on solar cell performance. Furthermore, the simulation results show that photovoltaic parameters are strongly dependent on the thickness and defect density of the light-absorbing layers.

**PS41**

(Student) **Towards a High-Modulation Reconfigurable Filter for Photodetectors via an Electrochromic Device**

Mauricio C. Victorio, Vladimir Pozdin and Pulak Bhushan; Florida International University, United States

Portable systems have received significant attention owing to widespread applicability in personal health monitoring and environmental sensing applications. Among the various sensing modalities implemented in a flexible and small form factor, optical detection remains the most attractive method. However, flexible implementation of optical sensing is limited to fixed wavelength due to hardware limitation and optical filtering for low power operation. Detection of multi analytes with multimodal sensing allows one to obtain more fine-grained and personalized understanding of an individual’s health condition or environmental changes. Multimodal sensing in portable systems requires duplicate hardware, which increase system footprint and cost. Thus, taking advantage of materials with tunable wavelengths to measure multiple signals can benefit multimodal optical biosensing applications. This work demonstrates a flexible reconfigurable filter via an electrochromic mechanism. An electrochromic longpass filter based on Prussian Blue electrodeposited on indium tin oxide/polyethylene naphthalate (ITO/PEN) electrodes is presented here. The multi-color electrochromism of the deposited film is achieved through tuning of the electrolyte composition and the film structure. In addition, functionalization of multi-walled carbon nanotubes (MWNTs) on the electrode surface are utilized to further enhance the electrochromic performance of the device.
The presented device structure serves as a proof-of-concept to achieve reconfigurable filters for multiwavelength optical detection in wearable and environmental applications.

PS42
Simulation and Modeling of Perovskite Solar Cells for Renewable Energy Application Luis F. Hernandez Camas; The University of the District of Columbia, United States

The importance of renewable energy in our current time merits for further research. Solar energy has the capability to harness the energy required to power space satellites, homes, cars, etc. The conversion of sunlight into electricity thereby has become essential and promising. Perovskite Solar Cells (PSCs) are low cost, environmentally friendly and a new emerging technology that provides a solution. We have studied inorganic n-i-p planar structure to achieve a higher efficient solar cell. With the use of SCAPS simulation we simulate the deficient conditions of each layer of the PSCS such as thickness, defects, metal work function, shallow uniform acceptor density and the impact of different elements within the structure. In our model, we have different layers that consist of TiO2, SnO2, perovskite and a HTM layer. The highest efficiency is 23.09% and is found within CuSCN. The reason is high bandgap and high mobility which reduce back contact barrier and increase hole collection. The thickness of the perovskite also plays a role since it impacts photocurrent but slightly impacts open circuit voltage.

PS43
2D Material Based Ag₂ZnO₃:CeO2 Heterostructure for Solar-Driven CO₂ Reduction Mohammed Al-Ghobari1,2; King Abdulrahman University of Science and Technology, Saudi Arabia; 1Alba University, Saudi Arabia

CO₂ emission is the main contributor to global warming that severely affects life on the earth. Thus, there is an urgent need to reduce atmospheric CO₂ concentration. Solar-driven photocatalytic CO₂ reduction to produce useful fuels is a promising green approach to address the CO₂ emission and energy crisis simultaneously. An efficient photocatalyst should have full solar spectrum harvesting ability, negligible charge recombination rate, efficient charge transfer and separation, high concentration of photocatalytic active sites, and enough redox potential. Due to their ultrathin morphology, 2D semiconductor materials exhibit high surface area, more catalytic exposed active sites, and high capacity of light absorption which made them promising materials for photocatalytic CO₂ reduction. Photocatalyst designing with negligible electron-hole recombination, and maximized redox potential is an essential prerequisite for achieving commercial-scale photocatalytic CO₂ reduction. This contribution combines surface plasmon resonance and Z-scheme charge transport in a single photocatalyst (Ag₂ZnO₃:CeO₂ heterostructure) aiming to improve its performance for photocatalytic CO₂ reduction. The Ag₂ZnO₃:CeO₂ heterostructure is fabricated via sunlight-driven combustion and deposition approaches. Ag plays dual rules as an electron mediator to facilitate the Z-scheme charge transport and plasmonic material to maximize the light absorption in the visible region. The designed photocatalyst exhibits significantly enhanced photocatalytic activity for CO₂ reduction under simulated sunlight irradiation. This work offers the opportunity of constructing an efficient Z-scheme photocatalyst from wide bandgap semiconductors with the full-visible light response, suppressed electron-hole recombination and optimized redox potential.

PS44
(Late News) Depth-Dependent Photoluminescence Analysis of the Inhomogeneities in Perovskite Solar Cell Eulises Regalado-Perez1,2, Evelyn Diaz-Cruz1,3, Julieta Landá Bautista1, Nini Rose Mathews1 and Xavier Mathew1; 1Universidad Nacional Autónoma de México, Mexico; 2Instituto de Física “Alfonso Pardo Linares” Benemérita Universidad Autónoma de Puebla, Mexico; 3Universidad del Istmo, Mexico

In this work, we report depth-dependent photoluminescence to investigate the vertical inhomogeneity on carrier extraction in perovskite devices. The vertical inhomogeneities which include uneven grains, voids, and grain boundaries are closely linked to the underlying charge transport layer which controls the nucleation and grain growth in the perovskite film. In the present work, we studied devices based on mesoporous TiO₂ and planar SnO₂. By exploring the morphological properties and the PL emission from different depths across the device structures, we show that the lower vertical inhomogeneity leads to more efficient charge carrier extraction in planar SnO₂-based devices. A red shift and line broadening of PL emission was observed when grain size changes in the direction of the incident probe laser. The perovskite deposited over planar SnO₂ electron transport layer (ETL) showed least red shift and broadening compared to that on mesoporous TiO₂, as a consequence of higher vertical homogeneity and structural order. Overall, the devices fabricated with SnO₂ ETL demonstrated least trap-assisted recombination and higher charge extraction leading to better device performance. Our studies reveal that the choice of SnO₂ over TiO₂ is not only because of the higher electron affinity leading to more favorable band alignment but also due to the vertical homogeneity resulting in a more propitious charge extraction-recombination balance in the device structure. This work provides a broader understanding of the impact of vertical inhomogeneity on the charge extraction efficiency, and presents a methodology to study quantitatively the inhomogeneity of perovskite films in device structures.

Acknowledgements: This work was partially supported by the projects PAPIIT-UNAM IT100021 and Texas A&M-CONACyT collaborative grant 19-20-027.

PS45
(Late News) Wurtzite Crystalline Structure Enhances Second-Harmonic Generation in GaAs Nanowires Bin Zhang; Jan Stehn; Ping-Ping Chen; Xingjun Wang; Fumitaro Ishikawa; Weimin Chen; and Irina Buyanova; Linköping University, Sweden; Shanghai Institute of Technical Physics, China; Ehime University, Japan

Nonlinear optical processes, including second harmonic generation (SHG), can be utilized in a wide range of classical and quantum applications, including on-chip integrated nano-photonic systems, non-linear optical microscopy, IR light visualisation and sensing. Using nanowires (NWs) for such applications is advantageous for efficient miniaturization and provides freedom in tailoring their non-linear response. An additional degree of freedom in the engineering of the SHG response is provided by the ability to grow NWs with different lattice structures and, therefore, to explore non-linearity of crystallographic polytypes that cannot be fabricated in bulk under conventional growth conditions. This makes it possible to tailor a polarimetric response of SHG determined by crystal symmetry. The (Al)GaAs material system is especially appealing as non-linear media, as GaAs exhibits large bulk second-order nonlinear optical susceptibility, rendering GaAs NWs highly attractive for diverse nonlinear photonic devices. Though essential for optimization, ascertaining the origin of SHG in thin NWs, including GaAs-based NWs, is not trivial due to sensitivity of non-linear properties to surfaces, interfaces, defects, as well as lattice polymorphism. Until now, however, impacts of these effects on non-linear properties of GaAs NWs are still largely unexplored and are investigated in this work.
The investigated GaAs NWs were grown by molecular beam epitaxy. Both zinc blende (ZB) and wurtzite (WZ) NWs with diameters of around 80 - 100 nm were studied. The crystallographic structure was ascertained by using transmission electron microscopy (TEM). It is found [1] that the SHG intensity is significantly stronger in WZ NWs as compared with ZB NWs (by about 7 times), reaching the value of 2.5×10⁻⁶ W⁻¹. This value is among the highest reported in the literature, including complex waveguide and nanoresonator structures, as well as hybrid plasmonic structures. Such enhancement was directly verified by correlative SHG intensity mapping and TEM characterization performed on the same polymeric NWs. Polarization-resolved measurements show that the increase of the orthogonal SHG component is chiefly controlled by the surface-induced SHG caused by structural and electric field discontinuity at the NW surface. This component, however, remains weaker than the parallel SHG output by about two orders of magnitude, due to weak out-coupling of the generated light from thin NWs. The dominant parallel SHG is proven to be enhanced in WZ via electric-field induced SHG, which is activated by the axial built-in electric field related to spontaneous polarization in WZ NWs, and can be controlled optically and potentially electrically. This SHG enhancement is found to be robust and does not require high structural quality of the NWs as the presence of structural defects in fact facilitates SHG by enhancing the internal electric field. Our results, therefore, demonstrate great potential of thin GaAs NWs for nonlinear nanophotonics and show that their non-linear properties can be manipulated via lattice engineering.


PS46

(Student, Late News, Student) Revealing the Electronic Heterogeneity and Inhomogeneity in Perovskite CsPbBr3 Nanowires Using Contactless Dielectric Force Microscopy
Rahayana Ruth Bautista1, Shuang Liang1, Tuong Trieu1, Zhiquan Lin2 and Yize Stephanie Li1; 1California State University, Bakersfield, United States; 2Georgia Institute of Technology, United States

Dielectric force microscopy (DFM) is a scanning force microscopy (SFM)-based technique that utilizes a double-pass imaging method to probe the electronic properties of low-dimensional materials, such as nanowires, nanorods, and nanotubes. In this work, we employ the DFM technique to identify majority charge carriers in all-inorganic metal halide perovskite CsPbBr3 nanowires (NWs) synthesized using a hot-injection approach. Ambipolar, n-type, and p-type responses have been observed in different CsPbBr3 NWs, revealing the electronic heterogeneities of the as-synthesized CsPbBr3 NWs. Moreover, longitudinal and transverse electronic inhomogeneities have been unveiled in CsPbBr3 NWs with diameters of 10-20 nm and 30-40 nm diameter, respectively. Such findings suggest the potential of further DFM studies on the electronic properties of other perovskite nanostructures.

PS47

(Late News) Thickness Dependence of Electronic Properties of GaN Slabs—A Density Functional Study
Narges Masoumi1, Rasoul Khaledi Alidusti1 and Reza Vatan M edanshahi1; 1Arizona State University, United States; 2Norwegian University of Science and Technology, Norway

GaN with a wurtzite structure is of great interest due to its wide direct bandgap, high breakdown voltage, spontaneous polarization, high electron mobility, and high thermochromical stability. Such distinct properties make GaN a promising material for a broad range of applications in electronic and optoelectronic devices e.g., blue light-emitting diodes (LEDs) and lasers, high power transistors, piezoelectric sensors, etc. As individual devices are continuously scaled-down, the thickness of the GaN layer reaches the nanometer level where the surface-to-volume ratio is significantly higher than its bulk counterpart. In this regime, the thickness and structural details of the surface play critical roles in determining the electronic properties of GaN and affect the GaN-based device fabrication and functionality. Here we use ab initio density functional theory (DFT) to systematically investigate the effect of thickness on the electronic properties of wurtzite-structure Ga-terminated GaN (0001) slabs with 2x2 surface reconstruction which is the most frequently used surface orientation for the epitaxial growth of GaN in the fabrication of GaN-based devices. Therefore, the band structures, band bending, and surface charges of up to 9 bilayer GaN slabs are studied. Moreover, to study the polarity of the slabs, the work function of various slabs has been calculated. We found that after 6 Ga-N bilayers thickness, the electronic bulk properties of GaN are recovered in the middle of the slabs and the surface reconstruction remains unchanged. The bandgap is decreased from 3.4 eV for the slab with 2 Ga-N bilayers to 2.2 eV for the slabs with > 6 Ga-N bilayers. This larger bandgap in thinner slabs could lead to higher breakdown voltage in GaN power electronic devices. Our study reveals that the distortion of atoms from their equilibrium positions at lower thicknesses induces an additional polarization to the spontaneous polarization which consequently creates higher carrier concentration in the inner layer of HEMT devices. We also observed that in GaN slabs, surface charge density and band bending are highly correlated with the thickness such that both quantities increase when the slab thickness decreases. This behavior could potentially affect the fabrication of the low dimension GaN-based devices. Moreover, the obtained work function (electron affinity) for various slabs shows a linear dependence on the thickness with a positive slope.

PS48

(Late News) Effects of Ge Doping on the Properties of Cu2ZnSnS4 Thin Film Solar Cells
T.G Sanchez and Nini Rose Mathews; Instituto de Energías Renovables, México

Effects of Ge doping on the properties of Cu2ZnSnS4 thin film solar cells
T. G. Sanchez1, N. R. M. Mathews1, 1 Instituto de Energías Renovables, Universidad Nacional Autónoma de México, Temixco, Morelos, 62580, México

Cu2ZnSnS4 is a p-type semiconductor with earth abundant and low toxicity constituent elements. It has a band gap of 1.5 eV and an absorption coefficient greater than 10⁴ cm⁻¹ and is considered as a potential candidate to replace other chalcopyrides like CdTe, CIGS. Herein, we report the incorporation of Ge into Cu2ZnSnS4 (CZTS) films and its effect on the structural, morphological, and solar cell properties. CZTS thin films were developed from sputtered Cu2ZnSn/Zn metallic stacks followed by annealing under S atmosphere. Solar cells with the glass/Mo/CZTGS/CdS/i-SiO2 (Student, Late News) Design and Development of Additively Manufactured Hybrid Antennas for Medical Applications in the Human Body
M. A. Mathews2, D. Mathews2, K. Mathews2, T. G. Sanchez2, T. G. Reyes2, and R. G. Martinez2; 1 Arizona State University, United States; 2Alliance University, India

The Ge thickness investigated were 5, 10 and 15 nm. Devices made with the stack Mo/Cu/In/Cu/Zn/Ge with 5 nm thick Ge resulted in best performance and a 27 % efficiency improvement over the reference cell was obtained (from 5.5% up to 7%). The EQE curve showed an improvement in the collection of photo generated carriers. The carrier concentration was determined to be in the range of 1x10¹⁴ - 1x10¹⁵ cm⁻³ for CZTS-G films, which is in the range of the values reported for CZTS.

Acknowledgements: This work was supported by the project PAPIIT: IN10921.
Germanium (Ge) thin film is one of the most promising semiconductor materials for next generation electronic devices. Ge offers several potential features, including higher electron and hole mobilities and a smaller energy bandgap compared with conventional silicon material, which makes it ideal for high-speed thin-film transistors and next-generation MOSFETs. Additionally, Ge has good lattice matching with group III-V semiconductor, which can be applied as a bottom layer for high efficiency GaAs solar cell. Especially, fabricating Ge thin film on plastic substrate could realize the high efficiency flexible solar cell. The metal-induced crystallization (MIC) method using gold (Au) catalyst is one of the most promising crystallization methods for crystalizing Ge thin films on plastic substrates like polymide at low temperature. Nevertheless, the formation of excess Ge islands on the crystalline Ge films are generally found in the MIC method which roughens the surface. Additional processes are required to remove these Ge islands, which is usually done by wet etching processes by H2O2 or peeling off with tape which could damage the sample. In this study, it is found that the four growth conditions including (1) Au/Ge thickness ratio, (2) annealing temperature, (3) heating rate and (4) initial Au layer thickness, are very important factors to obtain a high-quality Ge thin film. The flat and continuous crystalline layer can be obtained by controlling these growth parameters, and no additional process is required. In this work, we successfully obtained a smooth and continuous layer of crystalline Ge thin films with mainly (111) orientation at low temperature crystallization by controlling these growth parameters. This achievement will open up the possibility to fabricate a high-quality Ge thin film on plastic substrate as a buffer layer instead of an expensive single crystalline Ge for the epitaxial growth of GaAs film for the next-generation flexible solar cell application.

The Au/Ge bilayer films were fabricated by RF magnetron sputtering process on Si wafer with 100nm thermally grown oxide (SiOx), layer. The thickness of Au/Ge layer is Au(29nm)/Ge(46nm), which is the optimized value found in the previous study. The bilayer films were crystallized by using the MIC method at 220 and 250°C under N2 ambient for 1hr at different heating rate conditions. Structural properties were examined by X-ray diffraction (XRD), Raman spectroscopy, scanning electron microscope (SEM) and electron backscattered diffraction (EBSD). The results show that Ge thin films are successfully crystallized even at an annealing temperature as low as 220°C, which is low enough to be fabricated on a plastic substrate. Surface coverage of as high as ~99% is achieved for sample annealed at 220°C with a low heating rate of 0.5°C/min. The film surface is very smooth and continuous coverage without excess Ge islands on crystalline Ge. From the Hall effect measurement, hole mobility of as high as 145 cm²/Vs is achieved. Moreover, a smooth and continuous layer of crystalline Ge thin film with mainly (111) orientation is achieved when a thinner Au layer and low heating rate at low annealing temperature are adopted.

**References**


**PS51**

(Student, Late News) Design and Development of Additively Manufactured Passive Heat Sink for Electronics Cooling

Wondwosen F. Demisse and Pawan Tyagi; University of the District of Columbia, United States

The increasing demand for data use in our community results in a massive data processing and computational hours. The state of art electronics uses significant power, and a part of it is converted into heat. This enormous amount of heat may result in overheating and compromise the electronics performance. Overheating can affect the device functions, speed and lead to random shutdowns, unusual sounds, crashes, or blue screen errors. Therefore, it is vital to find an excellent and efficient solution for heat generation due to the kinetic energy of electrons motion. As additive manufacture opened novel avenues for creating innovative components, there is a great interest in the electronics industry for developing additively manufactured heatsinks. Additively manufactured heat sinks could be active, passive, or hybrid in nature. Passive heat sinks rely on natural convection, which utilizes buoyancy of hot air to produce airflow across the heat sink system. A active heat sinks use forced air to increase fluid flow across the hot area. Forced air is commonly generated by a fan, blower, or forward motion of hot object. Hybrid heat sinks blend some aspects of passive and active heat sinks.

We design an additive manufactured passive heat sink, which works on the principle of natural convection. The design is inspired by the natural movement of heat waves (gradient) from the hot surface. In passive heat exchanger the temperature will decrease from bottom to top. That means the heat transfer at the lower part of the heat sink is high. So it is appropriate to add more material to facilitate maximum absorption of heat from the source. We use L9 Taguchi design of experiments (TDOE) to optimize our heat sink design. In TDOE we varied parameters such as the...
channel’s material, shape, size, and pattern. Heat sink fins receive heat from an electronic device and dissipate it into the surrounding coolant fluid. It is common to see vertical fins on most conventional heat sinks. Our heat sink design incorporates a horizontal fin in addition to the vertical fin. The horizontal fins will increase the surface area of additively manufactured heat sink. Hence, horizontal fins are increasing the convective heat transfer between the environment (air) and heat sink. Also, increasing the surface contact between the medium helps to maximize the overall efficiency of heat sink. The performance analysis for the heat sink is performed using COMSOL multiphysics. Results show new heatsink designs, which can be manufactured using additive manufacturing, are highly efficient as compared to conventional heat exchanger in the present day computers.

**PS52**  
*(Late News)* Rhodium Nanoparticles Incorporated Mesoporous Silica as an Active Catalyst for Cyclohexene Hydrogenation Under Ambient Conditions  
Nabil AlZaqri; King Saud University, Saudi Arabia

Rhodium (Rh) nanoparticles were embedded in the mesopores of TUD-1 siliceous material and denoted as Rh-TUD-1. Five samples of Rh-TUD-1 were prepared with various loadings of Rh that ranged from 0.1 to 2 wt% using the sol-gel technique. The prepared samples were characterized by means of several chemical and physical techniques. The obtained characterization results show the formation of highly distributed Rh\(^{0}\) nanoparticles with an average size ranging from 3 to 5 nm throughout the three-dimensional silica matrix of TUD-1. The catalytic activity of the prepared catalysts was evaluated in the solvent-free hydrogenation of cyclohexene to cyclohexane at room temperature using 1 atm of hydrogen gas. The obtained catalytic results prove the high activity of Rh-TUD-1, in which a turnover frequency (TOF) ranging from 4.94 to 0.54 s\(^{-1}\) was obtained. Moreover, the change in reaction temperature during the reaction was monitored, and it showed an obvious increase in the reaction temperature as an indication of the spontaneous and exothermic nature of the reactions. Other optimization parameters, such as the substrate/catalyst ratio, and performing the reaction under non-ambient conditions (temperature = 60 C and hydrogen pressure = 5 atm) were also investigated. Rh-TUD-1 exhibited a high stability in a consecutive reaction of 5 runs under either ambient or non-ambient conditions.
channel’s material, shape, size, and pattern. Heat sink fins receive heat from an electronic device and dissipate it into the surrounding coolant fluid. It is common to see vertical fins on most conventional heat sinks. Our heat sink design incorporates a horizontal fin in addition to the vertical fin. The horizontal fins will increase the surface area of additively manufactured heat sink. Hence, horizontal fins are increasing the convective heat transfer between the environment (air) and heat sink. Also, increasing the surface contact between the medium helps to maximize the overall efficiency of heat sink. The performance analysis for the heat sink is performed using COMSOL multiphysics. Results show new heatsink designs, which can be manufactured using additive manufacturing, are highly efficient as compared to conventional heat exchanger in the present day computers.

PS52

(Late News) Rhodium Nanoparticles Incorporated Mesoporous Silica as an Active Catalyst for Cyclohexene Hydrogenation Under Ambient Conditions

Nabil AlZaqri; King Saud University, Saudi Arabia

Rhodium (Rh) nanoparticles were embedded in the mesopores of TUD-1 siliceous material and denoted as Rh-TUD-1. Five samples of Rh-TUD-1 were prepared with various loadings of Rh that ranged from 0.1 to 2 wt% using the sol-gel technique. The prepared samples were characterized by means of several chemical and physical techniques. The obtained characterization results show the formation of highly distributed Rh0 nanoparticles with an average size ranging from 3 to 5 nm throughout the three-dimensional silica matrix of TUD-1. The catalytic activity of the prepared catalysts was evaluated in the solvent-free hydrogenation of cyclohexene to cyclohexane at room temperature using 1 atm of hydrogen gas. The obtained catalytic results prove the high activity of Rh-TUD-1, in which a turnover frequency (TOF) ranging from 4.94 to 0.54 s⁻¹ was obtained. Moreover, the change in reaction temperature during the reaction was monitored, and it showed an obvious increase in the reaction temperature as an indication of the spontaneous and exothermic nature of the reactions. Other optimization parameters, such as the substrate/catalyst ratio, and performing the reaction under non-ambient conditions (temperature = 60°C and hydrogen pressure = 5 atm) were also investigated. Rh-TUD-1 exhibited a high stability in a consecutive reaction of 5 runs under either ambient or non-ambient conditions.
α-In$_2$Se$_3$ is a two-dimensional (2D), semiconducting material in which ferroelectricity was discovered in 2018. This combination of properties makes α-In$_2$Se$_3$ promising for a material for emerging, low-power computing devices, such as ferroelectric-field effect transistors and ferroelectric Schottky diodes for neuromorphic circuits. Synthesis of large area (>1 cm$^2$) α-In$_2$Se$_3$-thin films with precise control of thickness and defect density is necessary for fabrication of neuromorphic circuits and industrial adoption; however, most reports in the literature of α-In$_2$Se$_3$’s superlative performance in these applications are from studies conducted on a relatively small number of small fabricated from isolated flakes. These flakes are obtained either from mechanical exfoliation of bulk material or from vapor deposition at temperatures far above the thermodynamic stability range of α-In$_2$Se$_3$, resulting in uncoalesced, mixed phase films.

α-In$_2$Se$_3$ is thermodynamically stable below 200 °C and transitions to the 2D, centrosymmetric β-In$_2$Se$_3$ phase upon heating above 200 °C. While the β to α-In$_2$Se$_3$ phase transition is achievable in bulk synthesis via slow cooling, the β to α-In$_2$Se$_3$ phase transition does not occur as readily in thin-films. Two reports from the last two years demonstrate large-area synthesis of β-In$_2$Se$_3$-thin films – metal-organic chemical vapor deposition and molecular beam epitaxy (MBE) – at substrate temperatures greater than 300 °C, but no β to α-In$_2$Se$_3$ phase transition is reported upon cooling.

A recent study reported MBE synthesis of metastable, strained, mixed phase β/γ-In$_2$Se$_3$ films on Si(111) substrates at 180 °C. One study from 2018 claims deposition of large-area α-In$_2$Se$_3$-thin films on graphene at a substrate temperature of 250 °C via chemical beam epitaxy; however, it is difficult to distinguish the α from β phase by the Raman spectra and TEM micrograph along the c-axis. Development of direct synthesis of α-In$_2$Se$_3$−thin films at substrate temperatures below 200 °C would be advantageous to avoid the β to α-In$_2$Se$_3$ phase transition and reduce the thermal budget for CMOS integration.

In this work, In$_2$Se$_3$ films were synthesized on highly oriented pyrolytic graphite (HOPG) in the temperature range 150 - 250 °C and the crystal structures then carefully characterized. HOPG provides a low defect density surface of van der Waals bonds that minimizes heterogeneous nucleation and maximizes adatom surface diffusion to promote layer-by-layer crystal growth. Furthermore, bulk α-In$_2$Se$_3$ powder and exfoliated flakes were annealed and characterized to study the α-β phase transition and correlate with results from thin films. Finally, In$_2$Se$_3$ films were synthesized at high substrate temperature (500 - 700 °C) and the effect of cooling rate on film phase was measured. In summary, a detailed study of the impact of MBE synthesis conditions on the structure and properties of In$_2$Se$_3$ is presented and compared to the structure and phase transitions associated with exfoliated flakes. This material is based upon the work supported by the Georgia Tech Quantum Alliance and Georgia Tech Research Institute and conducted in part at the Georgia Tech Institute for Electronics and Nanotechnology, a member of the NCI, which is supported by the NSF (ECCS-2025462).


SESSION N: 2D Materials Growth and Surfaces
Session Chairs: Soaram Kim and Siddharth Rajan
Thursday Morning, June 30, 2022
Great Hall Meeting Room 1 & 2

8:20 AM N01
(Student) Molecular Beam Epitaxy Synthesis of In$_2$Se$_3$ Thin Films on Graphite in the Temperature Range 150 °C - 250 °C and 500 °C - 700 °C
Cooper A. Voigt1,2, Matthew Reingold1, Lawrence Early1, Alexander Dubé2, Brent Wagner2 and Eric Vogel1; 1Georgia Institute of Technology, United States; 2Georgia Tech Research Institute, United States

8:40 AM N02
(Student) Molecular Beam Epitaxy Growth of Monolayer Hexagonal Boron Nitride on Nickel Substrates Incorporated with Oxygen Atoms
Yuan Li; University of California, Riverside, United States

9:00 AM N03
Kineti cs of Wafer-Scale Epitaxial Growth of MoS$_2$ on Sapphire
Nicholas Trainer1,2, Chen Chen1,2, Yeongok KIm1,2, Dorota Kowalczyk3 and Joan M. Redwing1; 1The Pennsylvania State University, United States; 2The University of Tokyo, Japan; 3University of Lodz, Poland

Two-dimensional transition metal dichalcogenides (TM Ds) such as MoS$_2$ hold great promise in a wide variety of electronic, optoelectronic, spintronic and valleytronic applications. However, fundamental understanding of their growth kinetics is lacking. One useful tool to achieve this is metal organic chemical vapor deposition (MOCVD) as its use of gas phase precursors enables tight control over gas chemistry and growth time. Additionally, sapphire has proven itself as a reliable substrate for MoS$_2$, producing epitaxial films with minimal strain. In this work, we discuss the wafer-scale growth of MoS$_2$ monolayers on sapphire via MOCVD. The growths were conducted in a horizontal cold-wall reactor using H$_2$S and MoO($CO_3$)$_2$ as precursors and H$_2$ as the carrier gas. 2" c-plane...
sapphire wafers were heated using a graphite susceptor to 900-1000 °C, where they were exposed to the precursors at a nominal chalcogen to metal ratio of 20:0. After the growth, the samples were annealed for 10 minutes under H₂S before cooling down. Surface coverage and domain density were measured using atomic force microscopy and scanning electron microscopy. The evolution of the Raman, photoluminescence, and absorption spectra as well as the average domain size from X-ray diffraction will also be presented. Wafer-scale, fully coalesced monolayer MoS₂ films were achieved within only 12 minutes of growth. High nucleation densities between 1-2×10⁹μm⁻² were achieved within 30s of growth, after which the density remained relatively constant. Within the first 3 minutes of the growth, the film grew rapidly with domain size increasing linearly with time at a rate of about 150 nm²/min, indicating that the deposition rate is limited by gas phase transport of the source material to the substrate. After that, the domains began to merge, and the growth rate drops due to reduced adsorption of precursors on the MoS₂ van der Waals surface. Overall, the film coverage was roughly logarithmic with time, with 65% of the coalesced monolayer being deposited within 3 minutes. Past the 12 minutes of growth time, small bilayer regions were observed that eventually developed into spirals and pyramids at longer growth times.

Additionally, the effect of temperature and sapphire surface chemistry (adjusted using pre-anneals) on nucleation density and growth rate will be also discussed. Our results help probe the effects of surface chemistry and growth conditions on the MoOVD growth of MoS₂, thereby enabling a deeper understanding of the fundamental kinetics of the system. This knowledge will be applicable to other TMDs as well as other deposition techniques.

9:20 AM N04
(Student, Late News) Facile Integration of Giant Exchange Bias in 2D Magnet/Oxide Heterostructures Shanchuan Liang, Ti Xie and Cheng Gong; University of Maryland, United States

Exchange bias, a magnetic phenomenon emerging at the interface between a ferromagnet (FM) and an antiferromagnet (AFM), originates from the pinning of spins in the FM layer by the adjacent AFM layer, effectively stabilizing the FM against the environmental strain magnetic fields. This phenomenon has been implemented in a wide range of technological applications including magnetic memories, magnetic read heads, and sensors, and plays the foundational role for advanced spintronics. Here, we report an approach to establishing strong exchange bias in the 2D magnet/oxide heterostructure by a single-step process - atomic layer deposition (ALD). The exchange bias we created is controllable in the range of -300 to 1500 Oe by replacing different oxides in the heterostructure. Hence, this systematic work elucidates the essential role of a LTD-enabled oxidation of layered magnets in the formation of exchange bias and establishes ALD of oxides as a facile, controllable, and generally effective approach to creating giant exchange bias in vdW magnets, representing an integral advance towards practical vdW spintronic devices.

9:40 AM N05
Fast and Easy Optical Imaging and Epitaxial Growth Control of Rotational Domains in SnSe Thin Films Wouter Mertelmanns, Maria Hilsen, Qian Song, Seong Soon, J. Kevin Y. Derr, Rebre Lui, Nitin Samuel, and Rafael Jaramillo; 1MT, United States

Layered chalcogenides are promising materials for future (optoelectronic) applications. The semiconductor tin selenide (SnSe) is a member of the monochalcogenide (M X) family, which feature functionality including domain-switching behavior, ferroelasticity, thermo-, piezo- and ferroelectricity. Orthorhombic α-SnSe has strong in-plane anisotropy with implications for thermal, electronic, and optical properties. It has been studied for next-generation microelectronics, photonics and energy-conversion technologies, and has been the focus of a theoretical proposal for ultra-fast, non-thermal optical domain switching. Control of rotational domains (i.e., twins) during SnSe thin-film synthesis is key to enable high-quality, single-crystalline SnSe for the proposed applications. This work focuses on MBE of SnSe. We demonstrate (1) a fast and easy method to probe rotational domains in SnSe thin films and (2) a solution to overcome the formation of rotational domains by focusing on symmetry and lattice-matched vdW epitaxy of SnSe on a-plane sapphire surfaces.

When orthorhombic SnSe (in-plane lattice parameters; a = 4.15Å and b = 4.44Å) is epitaxially grown on cubic MgO (a = 4.21Å), various rotational domains are formed as a result of the various symmetry structure of both materials. The 2-fold rotational symmetry of SnSe combined with the 4-fold symmetry of MgO results in the formation 90° SnSe twins, and a high density of grain boundaries upon closure of the epitaxial film. Characterizing rotational domains in ultra-thin films of 2D materials is generally challenging (in-plane HR-XRD, “large-area” cs-TFM imaging, etc.). We show that, thanks to the optical anisotropy of α-SnSe in the visible (Δn = 0.88)³, supported by an optical model based on the reflectivity of linearly polarized light, 90° SnSe twins are easily distinguishable using polarized optical microscopy. When studied under cross-polarization at 45° with respect to the SnSe optical axis, slightly increasing or decreasing the angle of the polarizer with respect to the analyzer enables the color splitting of 0°-oriented and 90°-oriented domains into blue and yellow, respectively, when illuminated with white light. We first demonstrate this method on thicker SnSe epitaxial crystallites (~50nm), using polarized Raman spectroscopy for validation, and we then apply it to thinner (~5nm) epitaxial SnSe films. The distribution of blue and yellow pixels in the optical image enables the quantification of rotational domains and confirms the presence of a high density of 90° twins on MgO.

To overcome the formation of 90° twins, we grow epitaxially on a-plane sapphire [011-20] substrates. Similarly as α-SnSe, the surface unit of α-Al₂O₃[011-20] can be constructed using dissimilar in-plane lattice parameters; a = 8.24Å and b = 12.99Å. This favors single-oriented domain epitaxy of (2 x 3) units of SnSe on α-Al₂O₃[011-20], explained by the symmetry match and small lattice mismatch in both in-plane directions, and confirmed experimentally by our polarized reflectivity method.

The developed optical method and epitaxy on a-plane sapphire [011-20] substrates represent a very useful combination of film methodology and growth technology to realize high-quality, single-crystalline epitaxial SnSe thin films free of rotational twin domains. We will also highlight our epitaxial growth techniques, especially a comparison between solid-source and plasma-assisted methods.

1) Singh A et al ACS Photonics 2020, 7 (12)
5) Chang K et al Nano Lett. 2020, 20 (9)
7) Zhao D et al Nature 2014, 508 (7496)

10:00 AM Refreshment Break
Freestanding graphene nano- and microstructures have been shown to exhibit controllable electron emission when carrying a current and immersed in an external accelerating electric field. Through the mechanism of Phonon-Assisted Electron Emission, these structures demonstrate electron emission at electric field intensities and lattice temperatures below what would be expected for carbon to demonstrate field emission or thermionic emission, respectively. Emission currents have been measured primarily out of the plane of the device surface, allowing some directional control before the accelerating field is even considered. Thus far, such demonstrations have tended to involve structural dimensions on the order of only a handful of um, and have commonly been fabricated from CVD transferred graphene, flakes, or carbon nanotubes in various vertical and horizontal arrangements. Applied fields for such devices typically approach hundreds of kV/cm, and emission currents rarely leave the nA range. Herein are presented graphene structures with dimensions up to cm, in fields not exceeding 1 kV/cm, and producing emission currents of nearly 10 μA. Freestanding epitaxial graphene, synthesized from a silicon carbide substrate, offers several advantages compared to transferred graphene or unzipped nanotubes, including greater structural integrity, lower defect density, ease of handling, and ready compatibility with conventional simple photolithographic fabrication techniques. The devices presented here were fabricated with a low-cost, wafer scalable, single-mask process that does not require material transfer to a secondary substrate and is easily tailored to create variations in design parameters, which allowed multiple batches of devices to be rapidly manufactured with precise variations for the purpose of performance testing. The devices exhibit recognizable patterns of emission current performance relative to device and substrate temperature, including an identifiable turn-on point and emission current maintenance. Device behavior relative to substrate heating identifies the electron-phonon interactions that enable function and current emission, both when device temperature is supplied internally and externally. Emission currents are also observed to follow a performance pattern derived from purposeful device morphology, even exhibiting emission currents in accelerating fields as low as 50 V/cm.

Graphene electron emission devices present an opportunity for electron emission in a planar 2D heterostructure environment, beyond even the dimensional capabilities of field emission devices, and below the high operating temperatures of thermionic sources. Through refinements in the design and packaging, such devices, which are arbitrarily scalable between the micron and wafer level, could provide the electron sources for novel applications in X-ray generation or electron microscopy.

High-brightness photoemitters can be employed as electron sources in ultrafast electron diffraction and X-ray free-electron lasers, energy recovery linacs, electron microscopes, electron beam lithography, space propulsion and high-power microwave devices. To yield high quantum efficiencies, high brightness beams require rapid response times and low mean transverse energies (MTE). Recently, negative electron affinity (NEA) photocathodes, consisting of a GaAs wafer and a CsO surface layer, have been reported to exhibit both reasonably low MTE and good external quantum efficiencies (EQE) of $10^{-2} - 10^{-3}$. However, NEA cathodes are rarely used due to their significantly complex fabrication process which includes high temperature processing steps, entirely in-situ activation as well as ultra-high vacuum storage and operating pressures. Their stability is not also up to the mark. In this investigation, we have fabricated a Hot Electron Laser Assisted Cathode (HELAC) using electronically tunable negative electron affinity silicon surface. Briefly, the device consists of a three-layer stack of (i) a semiconductor, which absorbs incident photons, (ii) a monolayer of graphene, which acts as the gate, and (iii) an insulator, which allows a voltage drop between the semiconductor and graphene. In this device, an electric field is generated by applying a bias voltage between the semiconductor and graphene which mimics the surface dipole field in an NEA photocathode. Electrons injected into the graphene do not require transport to the emitting surface due to the monolayer thickness of the graphene. This device is air stable with a simple ex-situ fabrication flow while preserving the advantages of NEA photocathodes. We have demonstrated an initial proof-of-concept HELAC device with a p(-)-silicon substrate, silicon oxide insulator and monolayer graphene stack and evaluated its performance using a 405 nm CW laser at ~40 mW of incident power. Despite having a non-optimized structure, this device has exhibited a current of ~70 μA (~1.1 mA/cm²), resulting in an EQE of ~0.5%. Semiconductor modeling indicated the need of ~10% and response times in the 1-10 ps range are plausible for this device. Additionally, it is expected that low-MTE is achievable by optimizing the quality of the insulator, the barrier height, and the tunneling mechanism. This is analogous to Cs-based NEA devices, where low MTEs are attainable despite a large electric field which is developed due to the surface dipole.

**11:00 AM N08**

**A Multifunctional Manufacturing of Interface Engineered Colloidal 2D-Crystals for Flexible Thermoelectric Energy Harvesting**

Yong He, 1 A. E. Briggs, 2 H. Rajabi, 2 J. M. Enck, 2 H. H. O. Subbarao, 2 D. Estrada, 2 Boise State University, United States; 1 Center for Advanced Energy Studies, United States; 2 Idaho National Laboratory, United States

Bi$_2$Te$_3$, a narrow gap layered semiconductor, and a topological insulator has been reported to have excellent room temperature thermoelectric performances. Alloying and nanostructuring of the material have been widely studied for reducing the lattice thermal conductivity ($\kappa$) of the material to enhance the thermoelectric figure of merit (ZT). In the past, the performance of printed thermoelectric devices is significantly low compared to bulk counterparts due to low density and porosity, here we report interface engineering and nano inclusion in the crystals as an effective way to increase the performance of thermoelectric materials. This work demonstrates the scalable solvothermal synthesis of crystalline nanomaterials with engineered defects and interface engineering to improve the thermoelectric performance of the colloidal nano-inks. The engineered nanomaterials are transferred into devices using multiple additive manufacturing methods including Screen printing, Aerosol Jet Printing, Plasma Jet Printing, and Direct Writing. The low-cost scalable additive manufacturing methods and interface engineering developed in this work demonstrate a significant advance in the field of high-performing low-cost thermoelectric generators, advancing the commercial viability of the technology for energy harvesting, sensing, and cooling applications.
Electronically Tunable Negative Electron Affinity Silicon could provide the electron sources for novel applications in X-ray 50 V/cm.

An identifiable turn-on point and emission current maintenance.

With precise variations for the purpose of performance testing.

Allowed multiple batches of devices to be rapidly manufactured easily tailored to create variations in design parameters, which does not require material transfer to a secondary substrate and is with a low-cost, wafer scalable, single-photomask process that transferred graphene or unzipped nanotubes, including greater carbide substrate, offers several advantages compared to

The electron emission when carrying a current range. Herein are presented graphene structures with dimensions and lattice temperatures below what would be expected for carbon to exhibit controllable electron emission.

Daniels; University of Maryland, United States

Epitaxial Graphene Planar Devices lithography, space propulsion and high-power microwave devices.

lasers, energy recovery linacs, electron microscopes, electron beam assisted cathode (HELAC) using electronically tunable negative electron affinity. In this investigation, we have fabricated a Hot Electron Laser (HELAC) device with a p-silicon substrate, silicon oxide insulator and lattice temperatures below what would be expected for carbon to exhibit controllable electron emission when carrying a current range. Herein are presented graphene structures with dimensions and lattice temperatures below what would be expected for carbon to exhibit controllable electron emission. HELAC device with a p-silicon substrate, silicon oxide insulator and lattice temperatures below what would be expected for carbon to exhibit controllable electron emission when carrying a current range. Herein are presented graphene structures with dimensions and lattice temperatures below what would be expected for carbon to exhibit controllable electron emission. HELAC device with a p-silicon substrate, silicon oxide insulator and lattice temperatures below what would be expected for carbon to exhibit controllable electron emission when carrying a current range. Herein are presented graphene structures with dimensions and lattice temperatures below what would be expected for carbon to exhibit controllable electron emission. HELAC device with a p-silicon substrate, silicon oxide insulator and lattice temperatures below what would be expected for carbon to exhibit controllable electron emission when carrying a current range. Herein are presented graphene structures with dimensions and lattice temperatures below what would be expected for carbon to exhibit controllable electron emission. HELAC device with a p-silicon substrate, silicon oxide insulator and lattice temperatures below what would be expected for carbon to exhibit controllable electron emission when carrying a current range. Herein are presented graphene structures with dimensions and lattice temperatures below what would be expected for carbon to exhibit controllable electron emission. HELAC device with a p-silicon substrate, silicon oxide insulator and lattice temperatures below what would be expected for carbon to exhibit controllable electron emission when carrying a current range. Herein are presented graphene structures with dimensions and lattice temperatures below what would be expected for carbon to exhibit controllable electron emission.

Quasi-freestanding epitaxial graphene, synthesized from a silicon carbide substrate, offers several advantages compared to

We acknowledge funding support from the NSF TAQS QII program (award #1936219) and Army Research Office.

1) Wang, P. et al., (submitted)

SESSION O: Group III-Nitrides—MOCVD Growth

Session Chair: Fatemeh (Shadi) Shahedipour-Sandvik

Thursday Morning, June 30, 2022

Great Hall Meeting Room 3

8:20 AM O.01

(Student) Facet Control by Supersaturation in III-Nitrides

Jack Almeter1, Kewang1, James Loveless1, Will Mcouch2, Pramod Reddy1, Seiji M Ito1, Ronny Kirste1, Ramón Collazo1 and Zlatko Sitar1,2,3,4, North Carolina State University, United States; 2Droid Materials, United States

Heteroepitaxy of AlGaN layers on native GaN and AlN requires strain management schemes to achieve relaxed layers. Facet-controlled epitaxial lateral overgrowth (FACELO) allows for growth on inclined semi-polar facets from a typical c-plane substrate, enabling the generation of misfit dislocations for relaxation. While FACELO processes have been achieved in nitrides, there is no generalized model for the relationship between facet formation and growth conditions. This study presents a framework for controlling facet formation via the control of the vapor supersaturation, which describes the driving force for crystal growth.

GaN/sapphire wafers were patterned via SiO2 stripes along the direction, consisting of alternating 2 μm SiO2 stripes and 2 μm openings. AlN samples were prepared analogously from native AlN substrates following a maskless procedure, consisting of 2 μm wide stripes separated by 2 μm wide trenches etched via RIE to a depth of about 1.5 μm. Subsequent GaN or AlN structures were grown by MOCVD on prepared templates under various metal supersaturation conditions. Face formation was investigated via cross-sectional SEM.

The reference growth conditions for GaN were selected at 900 °C, 80 Torr, 132 μmol/min TEG, 1.5 slm NH3, H2 diluent, and total flow 7.5 slm. Supersaturation increases with decreasing growth temperatures and increasing NH3 flow rate. Observations of the shape at similar supersaturations but at different temperatures and ammonia flows were used to decouple the influence of any particular growth condition and to demonstrate the functionality with supersaturation. At low supersaturations, vertical and c-plane facets are preferred, giving a rectangular profile. As supersaturation increased, inclined facets appear, first in a truncated shape and then a trapezoid at higher supersaturations, eventually forming a triangle. These results were consistent between the temperature and ammonia flow series, demonstrating that the shape is determined specifically by the supersaturation.

For AlN growth, the reference growth condition was selected at 20 Torr, 13.4 μmol/min TMA, 0.3 slm NH3, and 10 slm H2. The growth temperature was varied between 500°C and 750°C, while the NH3 flow rate was varied between 5 sccm and 15 sccm.

Facet formation is controlled by the vapor supersaturation is supported [1]. Furthermore, it is predicted that facet formation is a result of the minimization of the overall surface energy where formation of a specific facet is dependent on its surface energy which is dependent on vapor supersaturation. This proposed facet formation mechanism will be used to engineer templates in native substrates for the controlled relaxation of AlGaN layers and their applications in either optoelectronic or power devices.

predicted shape is identical to the one from SEM. This indicates kinetic Wulff diagram is a powerful tool to determine, for example the shape of interfaces, and the dopant immunity distribution. In addition, comparing Wulff diagrams of two conditions, growth rate anisotropy could be modified and controlled. Lastly, the effects of non-uniform Mg doping, originated from the non-planar growth within the trench, on different device structures are also studied from the perspective of TCD simulations. Demonstrated in Fig. 2, nonuniform Mg doping improves the breakdown voltage of devices with floating field ring termination by alleviating the field crowding at the corner of the trench. On the other hand, non-uniformity has little effect on the performance on JFET structures by comparing the barrier height in the conduction band, as shown in Fig. 3. However, for a more sophisticated structure, such as superjunction devices, a detailed charge balance between electrons and holes is important. Nonuniform doping within the trench will adversely affect the device performance.

Acknowledgements

This work is supported by the Advanced Research Projects Agency-Energy (ARPA-E), U.S. Department of Energy, under Award Number DE-AR0000871 as part of the PNDIODES program managed by Dr. Isik Kizilyali.

9:00 AM 003

Crack Suppression in High Al-Mole-Fraction AlGaN Beyond the Critical Layer Thickness via Non-Planar Growth Approach on Patterned GaN Platforms

Frank M. Ehnhke, Zhiyu Xu, Yuto Ando, Alec Fischer, Fernando Ponce, Shyh-Chiang Shen, Theeradeth Detchprohm, and Russell Dupuis

Gallium nitride's high electron mobility, wide bandgap, and high intrinsic material properties, such as large bandgap, high critical field, and reasonable electron mobility. In order to demonstrate the utility of the CPC scheme in reducing the supersaturation is employed as a representative thermodynamic parameter. Following the CPC framework, increasing the growth rate (LGR) sample and 9.2 µm/h for the high growth rate sample. These growth parameters are, for example, the V/III ratio, diluent gas, temperature, pressure, and input partial pressures.

Chemical Potential Control in p-Type N-Polar GaN

Shashwat Rathkanthiwar, Dennis E. Szymanski, Dolar Khacharya, Pegah Bagheri, Ji Hyun Kim, Ke Wang, A. Hierro, and J. C. Campbell

Due to the high V/III ratio (N-rich growth conditions) improves Mg activation efficiency, but total [Mg] varies only weakly with V/III ratio.

In this work, we study the effects of varying V/III and GaBe precursor flow ratios on Be incorporation and activation efficiency in GaN. Be concentration and incorporation efficiency is determined using secondary ion mass spectroscopy (SIMS), and photoluminescence (PL) is used to determine the relative activation efficiency of the highly resistive GaN:Be.

Because Be is electrically similar to Mg (both are divalent alkaline earth metals), it is expected that activation efficiency will follow similar trends to that of Mg. On the other hand, the structural effects of Be and Mg are not expected to be the same; while Mg has a larger atomic radius than Ga, Be has a smaller atomic radius, which induces opposite-signed strain when each is incorporated into GaN. It is well known that a high V/III ratio (N-rich growth conditions) improves Mg activation efficiency, but total [Mg] varies only weakly with V/III ratio.

In this work, we demonstrate chemical potential control as an effective tool to suppress compensation in M-g-doped nitrogen-polar (N-polar) gallium nitride (GaN) films grown by metalorganic chemical vapor deposition (MOCVD). An increase in nitrogen chemical potential obtained by increasing the process supersaturation is shown to systematically reduce the incorporation of compensating oxygen and nitrogen-vacancy point defects. This is confirmed by photoluminescence and temperature-dependent Hall effect measurements. The suppressed compensation led to an order of magnitude improvement in p-type conductivity with the target 1015 cm-3 for vertical GaN devices and are unlikely to cause voltage drift, minimize leakage current, and allow controlled n- and p-type conductivity, to date, comprehensive growth optimizations for crystal quality and minimizing power and optoelectronic devices.

order of magnitude improvement in p-type conductivity with the room-temperature hole concentration, mobility, and resistivity measuring \(10^9 \text{ cm}^2/\text{V} \cdot \text{s}\) and \(1.1 \text{ k} \Omega \cdot \text{cm}\), respectively. These results are paramount in the pathway towards N-polar GaN power and optoelectronic devices.

GaN with N-polar orientation has attracted growing interest toward the development of high-performance electronic and optoelectronic devices such as high-frequency high electron mobility transistors (HEMTs), solar cells, long-wavelength LEDs, and ultraviolet photocathodes. A reversal of polarization field direction in N-polar GaN from its metal-polar counterpart allows for device designs that lead to improved performance, for example, enhanced carrier extraction efficiency in InGaN solar cells, enhanced hole injection, suppressed electron overflow and decreased droop in LEDs, improved confinement in the two-dimensional electron gas channel in AlGaN/GaN HEMTs, and improved transistor performance in polarization-engineered tunnel field-effect transistors (T-FETs).

These novel device applications based on N-polar GaN can be further improved and optimized with the realization of low-resistivity p-type material. For example, achieving a deep steep turn-on in T-FETs necessitates low resistance p-GaN layers, whereas high hole and electron concentrations are required near the p-n junction for optimal band alignment in these devices.

Achieving high p-type doping in GaN is understood to be challenging due to an interplay between large \(M\) acceptor ionization energy (150-220 meV), incorporation of compensating point defects and point defect complexes during epitaxial growth, and low mobility values of holes as compared to electrons. Moreover, N-polar GaN offers additional material challenges that need to be addressed to achieve high p-type conductivity. For instance, if not controlled, p-type doping in GaN can degrade the growth uniformity characterized by hexagonal hillocks, and high unintentional defect incorporation, notably oxygen, which incorporates at concentrations \(>10^{19} \text{ cm}^{-3}\). Oxygen on the nitrogen site \((O_n)\) acts as a shallow donor in N-polar GaN with an activation energy of \(-29 \text{ meV}\), which leads to significant difficulties in achieving p-type conductivity. In addition, the incorporation of nitrogen-vacancy \((V_N)\)-related compensating defects is favored in p-type GaN due to low formation energy. While much work has focused on p-doping of Ga-polar GaN, to date, comprehensive electrical characterization and compensation control in p-type N-polar GaN is lacking in the literature.

The chemical potential control (CPC) is a predictive approach wherein the dependence of the defect formation energy is theoretically estimated as a function of MOCVD growth parameters. These growth parameters are, for example, the V/III ratio, diluent gas, temperature, pressure, and input partial pressures of gas species. Instead of these individual MOCVD “knobs”, supersaturation is employed as a representative thermodynamic parameter. Following the CPC framework, increasing the supersaturation can be shown to increase the formation energy of both compensating defects, \(O_n\) and \(V_N\). In this work, we demonstrate the utility of the CPC scheme in reducing the compensation in p-type N-polar GaN to realize state-of-the-art hole concentration and resistivity.

10:00 AM Refreshment Break

10:20 AM 006

(Student) Characterization of Traps in High-Growth-Rate MOCVD GaN

Wenbo Li, Yuxuan Zhang, Vijay G. Thirupakuzhi, Vangipuram, Hongping Zhao, Steven A. Ringel and Aaron A. Rath; The Ohio State University, United States

Gallium nitride's high electron mobility, wide bandgap, and high breakdown field would be ideal for thick vertical devices if higher growth rates could be obtained to meet the demand for faster, more power-efficient devices. A key challenge in maintaining low defect concentrations to minimize threshold voltage drift, minimize leakage current, and allow controllable n-type doping in the low- to mid-\(10^{15} \text{ cm}^{-3}\) range. In metal-organic chemical vapor deposition (MOCVD) growth, ammonia cracking efficiency is one of the limiting factors of achieving higher growth rate. To facilitate this, a laser is introduced in the MOCVD reactor to improve the ammonia cracking efficiency enabling higher MOCVD growth rates. Higher growth rates and the laser require many new growth optimizations for crystal quality and minimizing traps. In this study, deep level transient/optical spectroscopy (DLTS/DLOS) are used to characterize traps in MOCVD GaN films grown with growth rates up to \(9.4 \text{ µm/h}\) and with and without laser-assistance to understand the trap incorporation. The MOCVD films were grown on 2 in. Nitride Specialty Supply GaN-on-sapphire templates. First, an n+-doped layer for lateral conduction and where the Ti/Al/Ni/Au Ohmic contact was formed. Second, a lightly-doped n-type layer was grown with a semitransparent Schottky Ni contact deposited on top. The DLTS and DLOS measurements proved the traps in the lightly-doped layer. The Si doping was targeted at \(5 \times 10^{15} \text{ cm}^{-3}\) in the lightly doped layer. For samples grown without laser-assistance, the growth rates were \(2.0 \text{ µm/h}\) for the traditional/optimized low growth rate (LGR) sample and \(9.2 \text{ µm/h}\) for the high growth rate (HGR) sample. For the laser-assisted MOCVD growth, the growth rate was \(9.4 \text{ µm/h}\) using a \(CO_2\) laser at 250 W parallel to the growth surface to more efficiently crack ammonia. More details on the growth conditions can be found in Ref. 1 and measurement details in Ref. 2.

The HGR and LA samples have traps from DLTS at \(E_c - 0.25, E_c - 0.45, E_c - 0.65, E_c - 0.72\), and \(E_c - 0.9 \text{ eV}\) with concentrations ranging from high-\(10^{11} \text{ cm}^{-3}\) to mid-\(10^{14} \text{ cm}^{-3}\) but are overall up to \(2X\) lower in the LA sample than the HGR sample. One exception is the Fe-related \(E_c - 0.57 \text{ eV}\) level in the LA sample with a concentration of \(\sim10^{13} \text{ cm}^{-3}\) that was not detected in the HGR sample. Although the \(E_c - 0.45\) and \(E_c - 0.65 \text{ eV}\) levels were not detected in the LGR sample, both high growth rate samples’ total DLTS trap concentrations are overall \(2X\) lower than the LGR sample. These concentrations are well below the target \(10^{13} \text{ cm}^{-3}\) for vertical GaN devices and are unlikely to cause significant compensation. Conversely, traps were detected via DLOS at \(E_c - 1.35, E_c - 2.6\), and \(E_c - 3.28 \text{ eV}\) in all samples. Here, the trap concentrations are in the mid- to high-\(10^{13} \text{ cm}^{-3}\) range in the LGR and LA samples. Like the DLTS results, the LA sample trap concentrations were \(2X\) lower than the HGR sample, but the traps, related to \(C\) and \(V_{GaN}\), remain well above the LGR concentrations. Further mitigation of these traps is required to enable controllable low doping and mitigate other trap-related issues that cause reduced performance and reliability while simultaneously achieving with high growth rates for economical vertical GaN devices.

Reference


10:40 AM 007

High-Speed MOCVD Growth of GaN Assisted by TBC

Bingjun Li and Jung Hahn; Yale University, United States

GaN is a perfect candidate for high-power applications due to its intrinsic material properties, such as large bandgap, high critical electrical field, and reasonable electron mobility. In order to achieve extremely high breakdown voltage, vertical power devices need a thick drift layer (30–100 \(\mu\)m), which cannot be feasibly produced by MOCVD processes due to low growth rate. On the other hand, hydride vapor phase epitaxy (HVPE) is capable of growing GaN at a very fast rate (\(\sim 100 \mu\)m/h), but it is not practical (growing \(>50\) wafers/run) for mass production. Therefore, turning MOCVD into HVPE-like reactor is of great significance.
During MOCVD growth of GaN, gas-phase parasitic reaction of TM Ga to form GaMe₃ and followed by (GaMe₃), nano-clusters or particles greatly limits the growth rate under high TM Ga partial pressure. As a result, under a constant pressure and temperature, the measured growth rate increases linearly with TM Ga flow rate at the beginning and then saturates if not decreasing. There have been reports of co-flowing HCl during the GaN growth, demonstrating a growth rate above 25 μm/h. However, HCl is highly corrosive to the stainless-steel apparatus and a hot wall reactor is needed to prevent the depletion of HCl by NH₃. In this study, we introduced tertiarybutyl-chloride (TBCl) into our MOCVD reactor. It doesn’t decompose to form either HCl or Cl₂ under room temperature (RT). Therefore, it is less corrosive and it doesn’t get consumed by NH₃, forming white powders (NH₃Cl) at the upstream of the reactor. In order to identify whether TBCl is capable of suppressing parasitic reaction or not, two different experiments were conducted. As shown in Fig. 1 (a), under a constant TM Ga flow rate without co-flowing TBCl, growth rate decreased by a factor of 5 when the reactor pressure was increased from 200 mbar to 500 mbar. However, a relatively pressure-independent growth rate was observed when co-flowing 2.5 sccm of TBCl. On the other hand, a saturation of growth rate was observed at around 7.5 μm/h when we continuously increased the TM Ga flow rate to 300 sccm without TBCl as shown in Fig. 1(b). Instead, after co-flowing TBCl, growth rate increases linearly with TM Ga flow rate, without showing any sign of saturation even above 22 μm/h. Both experiments indicate that TMGa has been replaced by GaCl, a same precursor of Ga in HVPE system having little parasitic reaction. An atomically smooth surface with step-flow patterns has been confirmed by AFM (Fig. 2) for a sample grown at 15 μm/h. Besides, TBCl is also capable of modifying the growth rate anisotropy. The kinetic Wulff diagram with or without TBCl has been plotted in Fig. 3. TBCl tends to decrease the relative growth rate of c-plane and (10-11), while it increases (11-22) and r-plane (10-12) dramatically. This modification of growth anisotropy is potentially related to a different surface kinetics of GaCl precursor.

Acknowledgements

This work is supported by the Advanced Research Projects Agency-Energy (ARPA-E), U.S. Department of Energy, under Award Number DE-AR0000871 as part of the PDINDIES program managed by Dr. Isik Kizilyalli.

11:00AM 008

(Student) High to Ultralow Si-Doped GaN Grown by Metalorganic Chemical Vapor Deposition at 550 °C for Heterogeneous Integration

Vineeta R. Muthuraj, Caroline E. Reilly, Shiju Nakamura, Steven DenBaars and Stacia Keller; University of California, Santa Barbara, United States

The heterogeneous integration of III-nitride materials with other semiconductor systems for electronic devices is attractive because it combines the excellent electrical properties of the III-nitrides with other device platforms. Pursuing integration through metalorganic chemical vapor deposition (MOCVD) is desirable because of the scalability of the technique, but the high temperatures required for the MOCVD growth of III-nitrides (>1000 °C) are incompatible with heterogeneous epitaxy on some semiconductor systems and fabricated wafers. Thus it is critical to develop III-nitride films with good electrical properties at growth temperatures compatible with temperature sensitive substrates. High crystal quality GaN films with reduced impurity levels have been achieved at temperatures as low as 500 °C using pulsed growth methods such as atomic layer epitaxy and flow modulation epitaxy (FME). However, the electrical behavior of doped LT III-nitride films is relatively unexplored.

In this work, thin Si-doped LT GaN films were grown at 550 °C by atmospheric pressure MOCVD using an FME scheme. Triethylgallium and ammonia were used as the GaN precursors and disilane as the Si dopant. Because of the very low growth rate (0.006 Å/s), 1200 FME cycles resulted in approximately 16 nm-thick films. Two different FME Si-doping schemes were investigated. The first series varied the fraction of cycles in which disilane was injected into the growing film. Samples were grown with disilane injected every 20, 10, 5, 3, 2, and 1 cycle. The second series varied the disilane flow while using the standard frequency of disilane injection (1 in 5 cycles). Samples were characterized by Hall measurements and secondary ion mass spectrometry (SIMS).

For the disilane injection series films, electron concentrations up to 6.97 x 10¹⁸ cm⁻³ were achieved, with electron mobilities from 34 to 119 cm² V⁻¹ s⁻¹. The peak electron concentration was achieved for samples with disilane injected in 1/3 of FME cycles during growth. The charge dropped off for samples with higher frequencies of disilane injection, likely because of degraded morphology. The Si concentrations measured by SIMS were somewhat lower than the electron concentrations measured by Hall. The background atmospheric impurity concentrations averaged 2.1 x 10¹⁷ cm⁻³ for oxygen and 3.9 x 10¹⁷ cm⁻³ for carbon, with no apparent dependence on Si concentration.

The disilane flow series resulted in films with electron concentrations from 5.98 x 10¹⁷ cm⁻³ to 5.9 x 10¹⁸ cm⁻³ and electron mobilities from 52 to 115 cm² V⁻¹ s⁻¹, with the highest charge achieved with the highest disilane flow. The sheet resistance of this sample was 1068 Ω, which is comparable to low resistance GaN films grown at high temperature, which range from 100-500 Ω. These results demonstrate the potential for LT III-nitrides in electronics applications. This work supported in part by Intel Corporation and the Solid State Lighting and Energy Electronics Center.

11:20AM 009

(Student) Demonstration of Single Crystal InN & GaN/InN Heterostructures by MOCVD

Tianhao Wu, Po Chun Chen and Shadi Dayeh; University of California, San Diego, United States

III nitride semiconductors have recently disrupted several industries and have remarkable potential to address unmet needs in electronics and optoelectronics. While gallium nitride (GaN) is the champion nitride material in solid state lighting and high power and high frequency electronics, there is abundant untapped potential in other nitrides that are otherwise harder to grow and to gain control over their electronic properties. Among these, Indium nitride (InN) that promises the highest saturation velocity in the nitride group poses two difficult challenges to realize its potential: (1) The epitaxial growth of high-quality InN films or structures is very challenging due to the competitive decomposition of InN at the temperatures for which efficient cracking of nitrogen sources occur, and (2) the difficulty in growing a larger bandgap barrier layer at the surface which requires even higher temperatures than the InN decomposition temperature, and with the presence of such layer, surface Fermi energy pinning challenges the modulation of the electron charge density to make functional transistor devices from any grown InN layers. Yet, there is has been outstanding progress in the growth of InN layers by molecular beam epitaxy or plasma assisted metal-organic chemical vapor deposition (MOCVD), but the growth of smooth InN surfaces and the growth of larger barrier layers on InN has not been accomplished before. This work demonstrates by standard pulsed MOCVD growth the ability to grow defect free InN structures with smooth surfaces and the ability to grow with control GaN barrier layers and to demonstrate excellent transport characteristics in these structures. We hypothesized that coalescence of InN islands in constrained growth methods such as lateral Fins can accelerate the formation of void-free and defect free InN growth within the first few nanometers of growth. We further hypothesized that we can raise the effective V/III ratio by pulsing the tri-methyl-indium source to avoid droplet formation, ripening and segregation which otherwise leads to the growth of defective and porous InN layers.
We validated these hypotheses by studying growth parameters and Fin widths in the range of 65 nm to 2000 nm (and control planar samples) and demonstrated FinGaN with defect-free surfaces and single crystal structures. Unannealed Ti/Au metal contacts on packed Fin arrays resulted in effective (un-corrected) specific contact resistance of approximately 612 \pm \mu\text{m}, which is much smaller than that obtained for current GaN ohmic contacts, with an extracted contact transfer length less than 1 \mu m. To leverage these structures for high electron mobility applications and un-pin their surface Fermi energy, we successfully grew in-situ GaN/InN heterostructure without compromising the smooth InN surface. Transmission electron microscopy showed clear interface between GaN and InN and single crystal structure. We then demonstrated that GaN can be selectively etched in the source/drain regions of the heterostructure and that unannealed Ti/Au metal contacts retain their low specific contact resistance on these structures. We are now investigating the fabrication of GaN/lnN and AlN/InN HEMTs and their DCRF performance.

11:40 AM O10

(Student) Effects of Pre-Metallization on the MOCVD Growth and Properties of Ge-Doped AlGaN on AIN Templates

Tianhai Wu, Po Chun Chen and Joan M. Redwing; The Pennsylvania State University, United States

AlGaN is an important ultra-wide bandgap material of interest for UV optoelectronics and vacuum nanoelectronics. However, the growth and n-type doping of Al-rich AlGaN is challenging due to the limited availability of AlN single crystal substrates and the increased ionization energy and compensation of donors, making it challenging to achieve highly doped n-type layers. AlN templates on sapphire are commonly used as substrates for AlGaN epitaxy; however, the crystalline quality and surface morphology of AlGaN is highly dependent on both the growth conditions and the presence of interlayers used to mediate the AlGaN/AlN epitaxial mismatch stress. Prior studies have demonstrated that pre-metallization of the AlN surface prior to AlGaN growth can be used to promote growth under metal-rich conditions which are beneficial to reduce surface roughness and point defects in the layers. However, the impact of pre-metallization on film stress, dislocations, and surface pitting in the AlGaN layers has not been examined in detail, particularly for highly n-type doped layers.

In this study, we investigate the effects of pre-metallization on the structural and electrical properties of Ge-doped Al_{x}Ga_{1-x}N (x \approx 0.5-0.6) epilayers grown by MOCVD on 500 nm thick HVPE AlN templates on sapphire (Nitride Solutions). Germanium was used as the n-type dopant to achieve high n-type doping while avoiding problems associated with tensile stress and film cracking observed in highly Si-doped AlGaN.

The epilayer growth was carried out in a vertical cold wall MOCVD reactor with a k-Space multibeam optical stress (MOS) sensor. Trimethylaluminum (TMAI), trimethylgallium (TMGa), ultrahigh purity ammonia gas (N\text{H}_{3}), and germane (GeH\text{e}_{4}, 2\% in H\text{e}) were used as Al, Ga, N and Ge sources, with hydrogen (H\text{e}) as the carrier gas. The pre-metallization step was performed by switching N\text{H}_{3} out of the reactor following the AlN layer and initiating the TMAI and TMGa flow prior to reintroducing the NH\text{e} and growing the AlGaN layer. For the unintentionally doped AlGaN, the effect of a 10 second pre-metallization step was investigated against a normal non-metallization AlGaN with the same flow rates and V/III ratios. The effect of a 5 second pre-metallization step was investigated for Ge doped AlGaN, where the flow rate was altered while maintaining the same TMAI/TMGa fraction to study the effects of strain and growth rate at a constant Al composition. Characterization of these samples through AFM, XRD, wafer curvature measurements, and dark-field TEM aid in the quantitative imaging of the threading dislocations. STEM/EDS was used to investigate the composition changes as a function of thickness. AlGaN typically grows under compressive stress, due to larger lattice parameters relative to AIN. Comparatively, our results show that a pre-metallization step will alter the AlGaN stress from a compressive to a tensile state under the same flow conditions. This tensile grown AlGaN is also shown to reduce surface roughness in the undoped case, and v-pitting in the Ge doped case. From XRD measurements, the tensile AlGaN shows an increase in screw type dislocations while maintaining similar edge type dislocations as the nominal growth condition. Cross sectional TEM imaging is used to analyze the evolution of increased screw-type dislocations when using pre-metallization steps. Additionally, we show that the transition from compressive to tensile growth is not only dependent on the pre-metallization step but the growth rate of the AlGaN layer at the AlGaN/AlN interface. By utilizing a pre-metallization step and a lower growth rate, it is possible to maintain low surface v-pitting and threading dislocation densities in Ge doped AlGaN. Our results explore the stress, strain, and defect evolution at the AlGaN/AlN pre-metallization interface. Ultimately, these experiments help us establish a better understanding of AlGaN heteroepitaxy, and an effective pathway towards material improvement.

**SESSION P: Quantum, Strongly Correlated and Topological Materials**

**Session Chair:** Stephanie Law and Quang To

**Thursday Morning, June 30, 2022**

US Bank Conference Theater

8:40 AM P01

(Student) Nonlocal Measurement as a Probe of the Spin Hall Effect in Topological Insulators

Jennifer E. Delmâ; Gregory Stephen; Owen Van; Aubrey Hambicki; Patrick Taylor and Adam Friedman; Laboratory for Physical Sciences, United States; U.S. Army Research Laboratory, United States

Topological insulators (TIs) are promising candidates for alternative computing device designs. In particular, they have great potential for spintronic devices, where utilization of electron spin rather than charge would allow for lower-power and higher-performance computing in next-generation architectures. Efficient conversion between spin and charge signals is crucial to spintronic technology. TI is provide highly efficient spin-to-charge conversion as a result of their unique topological properties. One way to electrically quantify conversion efficiency is with the spin Hall effect (SHE). Here, we present SHE measurements of the topological insulator Bi\text{2}Te\text{2}.5Se\text{0.5}. Because of the topological nature of this material, we can measure the SHE without the use of ferromagnetic injectors or detectors. Using the nonlocal resistance, we measure spin Hall angles up to 2.4 with spin lifetimes up to 9 ps. Furthermore, ferromagnet-free measurement allows for quick diagnostics of the spin properties without the need to fabricate multilevel devices.

9:00 AM P02

Magnon-Mediated Entanglement of Solid-State Spin Qubit

Dennis R. Candal and Michael E. Flatté; University of Iowa, United States

In this work we propose a hybrid quantum system that allows the creation of entanglement between solid-state qubits through magnon modes of a magnetic material [1,2]. Our first hybrid quantum system is composed of a diamond nitrogen-vacancy (NV) center spin coupled to a magnon mode of the low-damping, low-moment organic ferrimagnet vanadium tetracyanoethylene [1,3]. According to a new model, we derive an analytical expression for the spinmagnon cooperativity as a function of NV position under a
perpendicular magnetization losses. We predict that the spin-magnon-magnitude coupling strength is \( g \) = 2×10 kHz, yielding cooperativity \( C_t \) = 15 for a narrow range of NV spin locations within the diamond, well within the spatial precision of NV center implantation [1]. Thus our proposal describes a practical pathway for single-spin-state-to-single-magnon-occupancy transduction and for entangling NV centers over micron-length scales [1]. Secondly, we generalize the same finding for rectangular bars made of Yttrium Iron Garnet (YIG) [2]. Additionally, we compare on-resonant transduction and off-resonant virtual-magnon exchange protocols and discuss the generation of entanglement for different temperatures, and under realistic experimental conditions [2].


9:20 AM P03 Entanglement of Circularly Polarized Light with the Quantum Zeno Effect Ian C. Nodzuft1, Brian T. Kirby1,4, Ryan T. Glasser1, Harry C. Shaw1 and Thomas Sears1; 1University of Illinois at Chicago, United States; 2Peraton, United States; 3US Army Research Laboratory, United States; 4U. Illinois University, United States; 5NASA Goddard Space Flight Center, United States

The quantum Zeno effect reveals that a continuously observed quantum system exhibits a natural suppression of its time-evolution. And, as a consequence, the system experiences a measurement-dependent restriction of accessible quantum states. Therefore, one should be able to force a group of particles into an entangled state with the quantum Zeno effect. Here, we present a scheme, supported by numerical simulations, where an unentangled photon pair enters each side of a coupled waveguide and evolves into a polarization-entangled state. Additionally, we find that a very similar setup with three photons can generate W-states. Our findings present a robust avenue for photonic-based quantum applications without the need for distribution protocols.

9:40 AM P04 (Student) Visible Light Emission During Electrical Threshold Switching of NbO2 Mott Switches Mahnaz Islam1, Stephanie M. Bohaichuk1, John A. Roberts1, Chengyang Zhang1, Tae Joon Park1, Victoria Chen1, A. A. Talin1, Shriram Ramanathan1, Jonathan A. Fan1, Suhas K. Kumar2 and Eric Pop1; 1Stanford University, United States; 2Purdue University, United States; 3Sandia National Laboratories, United States

Post-CMOS computing aims to integrate both electrical and optical components that offer high on-chip functional density. Here we demonstrate simultaneous electrical and optical functions in a single device based on NbO2, a Mott insulator-metal-transition (MIT) material. On one hand, the device displays volatile electrical threshold switching, a key ingredient in building artificial neurons [1] and selector devices for non-volatile memory [2]. On the other hand, we discover that during threshold switching the device also emits visible and infrared light, which represents a physically new phenomenon (for NbO2 switches) with potential applications for metrology, electro-optical transduction, and on-chip light sources [3].

We constructed lateral two-terminal NbO2 devices using 100-200 nm of NbO2 grown on c-plane sapphire, with L = 2-8 μm of separation between metallic electrodes. A bode a threshold voltage, the devices display abrupt tunable switching in current, a known behavior due to a Joule-heating-driven MIT at a transition temperature of ~1100 K. Devices with L in the range 2-5 μm switched at quasi-statical voltages of ~50-90 V, in vacuum at room temperature ambient.

Operando visible optical microscopy of these devices with a visible-range camera revealed light emission during electrical switching. The intensity of the emission was highest during the transient current overshoots upon MIT threshold switching. The light emission was also present when the device is held in the low-resistance metallic state, albeit at a lower intensity. In this state, the intensity of the emission increased with increasing current, while the color of the emission for a given device remained the same irrespective of intensity. No light emission was observed in the high-resistance insulating state of the NbO2 devices.

To identify the physical origins of the light emission, we obtained its spectroscopic information in visible wavelengths, which revealed the tail of a peak that is likely in the infrared. While this observation indicates elevated local temperatures, fitting with a blackbody emission model (with variable emissivity) did not yield a reasonable agreement with the experimental data, suggesting an electronic origin of the light emission. Further, comparison of optical and atomic force micrographs (AFMs) of devices before and after electrical switching showed permanent changes, revealing apparent current path formation between the electrodes, indicating local temperatures that exceeded the known MIT temperature of NbO2 (~1100 K).

We also performed operando visible optical microscopy on devices with different sizes and at different ambient temperatures. In general, when the switching voltage was significantly lower, which was the case with a channel length of ~50 μm, light emission at elevated ambient temperatures, light emission was not observed. In contrast, the observed emission was brighter for longer channel lengths with higher MIT voltages at any given ambient temperature. These observations indicate that a higher input power, and thereby increased local temperatures due to Joule heating, was required for light emission. At the same time, the inconsistency with a pure blackbody model and the color of the light remaining invariant, indicate possible electronic origins of the light.

Interestingly, devices which were switched only at a higher ambient temperature did not show a permanent current path formation, and light emission was also absent.

In conclusion, we present the discovery of a light emission process which occurs during the electrical threshold instability in NbO2 devices. The process is likely both thermal and electronic in origin, paving the way for new metrology approaches and electro-optical components based on the MIT material NbO2.


10:00 AM Refreshment Break

10:20 AM P05 MBE Growth of Bi2Se3 with Reduced Twin Defect Density Patrick Taylor, George de Coster, Wendy Sarney, Blair Connelly and Harry Hier; U.S. Army Research Laboratory, United States

Topological Insulator (TI) materials promise a wide variety of disruptive new spintronic and electronic device technologies by leveraging the attractive spin-momentum-locked surface currents. The family of (Bi1-xSb1-x)2(Te1-ySey) Tl materials are an interesting platform because they are three-dimensional TIs with robust Dirac surface state dispersion. Generally, the epitaxial growth of these materials contain a high volumetric density of anti-phase and other unwanted rotational domain disorder such as twinning. That disorder causes issues such as a small-angle carrier scattering, reduced response to circularly polarized light, and persistently high background carrier density4 which degrades the efficiency and operability of devices.

In this work, we present results from a novel approach to reduce the twinning and anti-phase disorder in epitaxially grown TIs. The strategy involves the choice of a vicinal substrate orientation that yields a 60 degree zig-zag-like morphology of atomic ledges on the surface. The 60 degree bends in the ledges accommodate and seed the trigonal growth symmetry of (Bi1-xSb1-x)(Te1-ySey) Tl materials. The
success of this approach is demonstrated by a 4X reduction in twins for Bi$_2$Se$_3$ grown on (111)B InP substrates with a 2 degree miscut toward (010). We will present measurement results including terahertz emission, RHEED, as well as x-ray diffraction pole scans that all are consistent with a reduction in twin density. To help explain the significantly (about 10X) larger terahertz response using circularly polarized light, we calculated the Bi$_2$Se$_3$ band structure including spin-sensitivity near the Γ-point along the M direction.

Reference:

10:40 AM P06
(Student) Epitaxial Growth of Kagome Ferromagnet Fe3Sn2 and Sn-M-O Modulated Heterostructures Shouy Cheng, Binbin Wang, Igor Lyalin, Nuria Bagues Salguero, Alexander J. Bishop, David M C comb and Roland Kawai kim; The Ohio State University, United States

Kagome magnets are interesting due to the coexistence of Weyl points and spin frustration in these materials. The thin-film form of these materials is particularly desired for both fundamental research and practical application. Here we report the molecular beam epitaxy (M BE) growth of kagome magnet Fe3Sn2 on epitaxial Pt(111) buffer layer on Al2O3 (0001) substrate. Using our unique atomic-layer M BE (AL-M BE) technique, we are able to grow these materials at a lower temperature, which reduces interdiffusion and generates a sharp interface. The structure of Fe3Sn2 is confirmed by a combination of reflection high-energy electron diffraction (RHEED), X-ray diffraction (XRD), and transmission electron microscopy (TEM), while the magnetic properties of Fe3Sn2 are demonstrated by magneto-optical Kerr effect (M OKE), SQUID magnetometry, and anomalous N ernst effect (ANE) imaging. Furthermore, AL-M BE technique allows us to grow Sn layer modulated [Fe3Sn2/Fe3Sn2] superlattices, whose structure is also confirmed by TEM and Energy-dispersive X-ray spectroscopy (EDX). These results demonstrate our ability to control the sample structure at the atomic level using AL-M BE.

11:00 AM P07
(Student) Fermi Level Tuning and Band Alignment in Mn Doped InAs/GaSb Logan Kinyon1, Joaquin B. Ortiz2, Gauthier Krimmari3, Seul-I Bae3, Jiashu Wang3, Magyuk Zhukovskyi3, Tatyana Orlova3, Louis Anne DeVaulchiers4, Yves Guilmoto5, Roland Winklerj, Jack K. Furdy6, Xin Yu Li7 and Badih Assaf8; 1University of Notre Dame, United States; 2Purdue University, United States; 3Sandia National Laboratories, United States; 4Notre Dame Integrated Imaging Facility, United States; 5Northern Illinois University, United States

InAs/GaSb hosts a broken gap band alignment that has been shown to generate helical topological edge states. Upon the introduction of Mn into the structure, it has been predicted to host a quantized anomalous Hall effect. Here, we show that dilute Mn doping on InAs in InAs/GaSb, allows a tuning of the Fermi level, the introduction of paramagnetism, but also has a non-trivial impact on the band alignment of the system. The measurement of Shubnikov-de Haas oscillations, cyclotron resonance, and a non-linear Hall effect in Mn-doped samples indicate the coexistence of a high mobility two-dimensional electron gas and a hole gas. Conversely, in undoped InAs/GaSb, pure-n-type transport is observed. We hypothesize that Mn acceptor levels can pin the Fermi energy near the valence band edge of InAs, far from the interface, which introduces a strong band bending to preserve the band offset at the InAs/GaSb interface. The realization of the QAHE in this structure will thus require a careful control of the band alignment to preserve topological insulating character.

11:20 AM P08
(Student) Confinement-Induced Topological Phase Transition in Thin-Film Rare-Earth Pnictides Quoc Dai Ho1, Ruiqi Hu2, Quang To1, Garnett Bryant3 and Anderson J anotti1; 1University of Delaware, United States; 2National Institute of Standards and Technology, United States

Metal-insulator phase transition is a classic phenomenon induced by various reasons. The transition caused by quantization effect when going from bulk materials to a very thin film limit is rather well-known. In this work, by using first principles calculations, we investigate the phase transition when 3D bulk semimetallic rare-earth pnictides having simple rock salt structure become as thin as quasi 2D materials with growth direction chosen to be along [001]. The electronic structure of 3D rare-earth pnictides typically consists of three equivalent electron pockets at X points and two hole pockets at Y point in the Brillouin zone. These charge carriers are very sensitive to external stimuli such as strain or dimensional confinement. We find that due to its unique electronic structure, the electron pockets of these rare-earth pnictides show unique behavior upon quantum confinement in thin films. More specifically, the two in-plane electron pockets in reciprocal space moves up in energy, opening a gap at the X, and Y points while the out-of-plane electron pocket at X point, projected onto the Γ point, does not change, maintaining the system in a metallic state. This characteristic prevents a semi-metal to semiconductor transition. However, in the ultra-thin limit of few monolayer thick, we observe a topological phase transition from a trivial 3D semi-metal to a 2D spin Hall insulator with a sizeable band gap due to the spin-orbit coupling. This finding introduces a new member to the 2D spin Hall insulator family and offers a new platform to realize the 2D spin Hall insulator experimentally.

SESSION Q: Oxide Semiconductor Devices, Defects and Transport

Session Chairs: Leonard Brillon and Sarah Swisher
Thursday Morning, June 30, 2022
Ohio States Inc. Traditions Room

8:20 AM Q01
Large-Area Photonic Lift-off Process for Flexible Thin-Film Transistors A dam _Weidling1, Vikram S. Turkan1, Vahid Akhavan2, Kurt A. Schroder3 and Sarah L. Swisher3; 1University of M innesota, United States; 2Novel, Entrix, United States

As the complexity of flexible electronic devices such as displays and sensors has increased, new plastic-compatible manufacturing
methods are becoming necessary to produce high-yield, low-defect flexible circuits. While solution-processed methods such as printing can be used to fabricate circuits on low-temperature substrates, printing is not always a feasible option to realize complex, high-density circuits with small devices. In particular, high-resolution display applications typically require single-micron feature sizes and excellent uniformity over large-area substrates. For these applications, more precise fabrication techniques such as photolithography are required. However, due to the poor dimensional stability of polymers, even low-temperature processes such as soft bakes during lithography can alter the substrate dimensions. The problem of dimensional stability can be overcome by attaching the polymer film to a rigid carrier during device fabrication, then releasing the polymer substrate with the fully fabricated device layer on top. For this reason, the separation of polymer films from rigid carriers remains a crucial step in creating next-generation flexible electronics.

In this talk, we will discuss a large-area, high-throughput photonic lift-off (PLO) process to rapidly separate polymer films from rigid carriers. PLO uses broadband light (200 nm - 1100 nm) from a flashlamp to lift off a polymer film from a rigid carrier coated with a LAL, where the polymer film may contain functional devices. When compared to a laser lift-off process such as an excimer laser lift-off, the PLO process is advantageous as it can enable large area lift-off (150 mm x 75 mm) in one flash of light lasting between 100-200 µs, thus enabling higher throughput. Furthermore, the LAL prevents direct illumination of the polymer substrate during lift-off and facilitates cleaner lift-off without polymer ashing. The LAL also makes PLO a polymer-agnostic process, enabling lift-off of a wide range of polymers.

We will discuss our recent work fabricating flexible thin-film transistors (TFTs) using PLO [2]. Polyimide with a low coefficient of thermal expansion (CTE) was used to minimize residual film stress. Indium zinc oxide (IZO) TFTs were fabricated on the polyimide films and subsequently released from the carrier using PLO. The released devices demonstrated no significant changes after the PLO process, yielding a mobility of ~3 cm²/Vs before and after lift-off. The flexible TFTs were robust to bending stress, showing no noticeable decrease in mobility while bent with a 10 mm radius of curvature. When combined with the ability to successfully separate the PI from the carrier, the low-CTE PI creates a robust fabrication platform for flexible electronics that allows conventional patterning and deposition techniques to be used on a plastic substrate while maintaining dimensional stability with processing temperatures up to 380 °C. A 3D finite element model indicates that the polymer/LAL interface reaches above 800 °C during PLO, but the top surface of the PI remains below 120 °C. The model shows that the maximum temperature at the device layer during PLO is strongly impacted by the thickness and material properties of the polymer film, highlighting the value of the model to guide PLO device design. This work demonstrates the feasibility of PLO to successfully release polyimide substrates containing flexible electronic devices from glass carriers after withstanding conventional lithographic processing methods.

We have contributed to oxide electronics, particularly on transition metal oxide semiconductors of which the cations include In, Zn, Sn and Ga. We have integrated these oxide semiconductors into thin film transistors (TFTs) as active channel layer in light of the unique combination of electronic and optical properties that high carrier mobility (5-10 cm²/Vs), optical transparency in the visible regime (˃90%) and mild thermal budget processing (200-400°C).

In this study, we achieved four different results. The first result is that unlike several previous reports on oxide p-n junctions fabricated exploiting a thin film epitaxial growth technique (known as molecular beam epitaxy, MBE) or a high-powered laser beam process (known as pulsed laser deposition, PLD) that requires ultra-high vacuum conditions, a large amount of power, and is limited for large-area processing, we demonstrate oxide-based heterojunction p-n diodes that consist of sputter-synthesized p-SnOx and n-IGZO of which the manufacturing routes are in-line with current manufacturing requirements. The second result is that the synthesized p-SnOx films are devoid of metallic Sn phases (i.e., Sn³⁺ state) with carrier density tunability and high carrier mobility (> 2 cm²/Vs). The third result is that the charge blocking performance of the metallurgical junction is significantly enhanced by the engineering of trap/defect density of n-IGZO, which is identified using photoluminescence microscopy and valence band measurements. The last result is that the resulting oxide-based p-n heterojunction exhibits a high rectification ratio greater than 10⁴ at ±3 V (highest among the sputter-processed oxide junctions), a low saturation current of ~2x10⁻⁶ A, and a small turn-on voltage of ~0.5 V.

The outcomes of the current study are expected to contribute to the development of p-type oxides and their industrial device applications such as p-n diodes of which the manufacturing routes are in-line with the current processing requirements.

References:
The released devices demonstrated no significant changes of thermal expansion (CTE) was used to minimize residual film transistors (TFTs) using PLO [2]. Polyimide with a low coefficient of thermal expansion is advantageous for its dimensional stability. We will discuss our recent work fabricating flexible thin-film transistors (TFTs) using PLO [2]. Polyimide with a low coefficient of thermal expansion is advantageous for its dimensional stability. Furthermore, the LAL prevents direct illumination of the polymer during exposure, lasting between 100-200 µs, thus enabling higher throughput.

enable large area lift-off (150 mm x 75 mm) in one flash of light from a flashlamp to lift off a polymer film from a rigid carrier coated with a thin layer of polyimide. For this reason, the separation of channel and metalization is achieved with high precision and large area coverage.

The role of band-tail states (BTS) on the operation of IGZO TFTs is well established, however there is wide variation in the interpretation of the interaction and/or independence of channel mobility and charge trapping. In many reports the influence of BTS on the level of free charge is accounted for by an effective mobility which is dependent on the applied gate bias. While this may accurately match current-voltage characteristics, this treatment is lumping together the effects of charge trapping and carrier scattering. It should remain distinct. When these effects are combined, a model which can accurately represent device behavior over a wide temperature range is not possible due to fundamental differences in temperature dependence.

Bottom-gate TFTs were fabricated with a 50 nm IGZO film sandwiched between a 50 nm gate oxide and a 50 nm passivation oxide layer. The working metal was molybdenum for the gate electrode and source/drain contacts. A passivation anneal was done and a capping layer was added to promote electrical stability; full process details are provided in a previous report. Devices were tested using a Lakeshore cryogenic probe station, with transfer characteristic measurements taken from room temperature to below 100 K.

Electrical measurements made on long-channel devices (L = 12 µm) have revealed temperature-dependent behavior that is not explained by existing TCAD models employed for defect states and carrier mobility. An IGZO TFT device model has been recently developed using Silvaco ATLAS, which accounts for the role of donor-like oxygen vacancy defects, acceptor-like BTS, acceptor-like interface traps, and a temperature-dependent intrinsic channel mobility. The model demonstrates a remarkable match to transfer characteristics measured at T = 150 K to room temperature. The temperature-dependent behavior follows a power-law relationship, resembling behavior consistent with ionized donor defects. The model is independent of carrier concentration, without dependence on the applied gate bias. Details of the material and device model, and associated defect distribution parameters will be presented.

9:20 AM Q04
(Investigator) Study of p-Type SnO Sub-Bandgap Defects by Comparing Experimental Transistor Data to Numerical Device Simulations
Jishwar A. Singh, J. Jun Song, R. L. Peterson, University of Michigan Ann Arbor, United States

Metal oxide semiconductors have gained a lot of attention for applications in thin film transistor (TFT) technology, large-area displays and flexible electronics. Although n-type metal oxide semiconductors have already been commercialized, extensive research is being conducted to find a suitable p-type counterpart. Among the p-type oxide semiconductors available, SnO has gained a lot of attention as its hybridization of O 2p and Sn 5s orbitals at the valence band maximum enables it to avoid charge localization, which limits hole mobility in other p-type oxides. Although there are many reports of SnO TFTs, most show a relatively low field effect mobility ($\mu_F$) of $1-2 \text{cm}^2\text{V}^{-1}\text{s}^{-1}$ and a poor on-off current ratio ($I_{ON}/I_{OFF}$) of $10^2$ to $10^3$. To understand and improve SnO TFT performance, it is necessary to have a quantitative study of sub-bandgap defect states in SnO and its dielectric interface. In this work, we extracted the SnO sub-bandgap defect parameters by comparing experimental TFT data with 2D numerical device simulations using Silvaco TCAD ATLAS. We found that the accuracy of the defect state models can be improved significantly by concurrent fitting of $I_{ON}/I_{OFF}$ and $\mu_F$ to $I_{OFF}$ curves. To obtain experimental data, we RF sputtered polycrystalline SnO on SiO$_2$/n-$\text{Si}$, which acts as the gate stack. To form a TFT, we deposited 20 nm Ni/80 nm Au source/drain contacts by e-beam evaporation. For numerical simulation, the material properties of SnO were taken from literature [1,2]. To model the sub-bandgap defect states in p-type SnO, the model for density of states in a SnO model in ATLAS was used. We established a SnO defect state model by first fitting the experimentally-obtained $I_{ON}/I_{OFF}$ to $I_{OFF}$ curves to simulation. Although the preliminary model showed a good fit between experimental and simulated transfer curves, a discrepancy was observed between modeled and measured $\mu_F$ values. So, to improve the SnO defect state model accuracy, we performed concurrent fitting of $I_{ON}/I_{OFF}$ and $\mu_F$ to $I_{OFF}$ curves. Using our optimized SnO sub-bandgap defect state model, we identified the dominant traps limiting SnO TFT performance. In the high density of interface donor-like tail states and high contact resistance limit $\mu_F$, while the high density of shallow, bulk Gaussian acceptor-like defects leads to poor $I_{ON}/I_{OFF}$ by addressing these specific defect states, SnO TFT performance can be improved significantly.

The authors thank Intel Components Research for helpful discussions and funding.

composition, and substrate choice on grain size, topology and crystallinity as studied by atomic force microscopy and x-ray diffraction. The working of MBE of reactive sputtering and voltage-discharge hysteresis experiments are utilized to optimize for the reactive gas partial pressure in the vacuum chamber. Temperature-dependant resistivity for epitaxial versus polycrystalline films is evaluated by four-point probe method and correlated to the high temperature bandgap-collapse observed by near-IR optical absorption.

Two terminal switching devices are fabricated on SiC, sapphire, and Lanthanum Luminate substrates. Voltage-triggered switching results could support the theory of a critical power density criteria for LCO devices, rather than the Mott criterion established in vanadium dioxide devices. Finally, we will briefly discuss evaluation of various e-beam evaporated metals and annealing procedures via the transmission line measurement method. These methods are used to determine the most thermally stable, lowest contact resistance materials to aid in integration of LCO into power devices.

10:00 AM Refreshment Break

10:20 AM Q06 Controlling the p Type Conductivity of SnO (001) Films by Group-III Doping During Molecular Beam Epitaxy Kingsley Egbo1, Georg Hoffmann1, Jonas Lähnemann1, Andreas Falkenstein1, Joël Varley2 and Oliver Bierwagen1; 1Paul Drude Institute for Solid State Electronics, Germany; 2Institute of Physical Chemistry, RWTH Aachen University, Germany; 3Lawrence Livermore National Laboratory, United States

Reliable bipolar carrier transport remains a challenge in most transparent semiconducting oxides and this limits the widespread device adoption of oxides for optoelectronic devices [1]. Most widely applied transparent semiconducting oxides can only be doped n-type, their p-type doping remains challenging. However, few oxides show p-type character, Ti (III) oxide (SnO) is among the few p-type oxide semiconductors. Its optical bandgap of ~2.7 eV and high hole mobility ~3-5 cm^2/V.s relative to other binary p-type semiconducting oxides makes it a candidate material for transparent oxide heterojunctions with n-type materials [2][3].

Unintentional (UID) p-type conductivity is believed to be controlled primarily by Sn-vacancies [4] or their complex with hydrogen [5]. Few theoretical studies have also suggested the possibility of bipolar doping in SnO [6]. However, experimental studies exploring the effect of intentional impurities in SnO are lacking. Solely, the doping of SnO with >8 cation % of Sb has been experimentally shown to produce 10^6 cm^2-V.s electrons to other binary p-type semiconducting oxides makes it a candidate material for transparent oxide heterojunctions with n-type materials [2][3].

Here we show an experimental and theoretical study on the effects of group III dopants on SnO. SnO (001) films doped with the group III In, Ga, and La species were grown on YSZ (100) substrates by molecular beam epitaxy (MBE). We explore two growth techniques for SnO; plasma-assisted MBE with a metallic Sn source [8] and suboxide MBE using a SnO2+Sn mixture as pure SnO source without the use of additional oxygen[9]. In both growth techniques, the dopant elements were incorporated using the metal effusion cells and the dopant concentration, measured by energy-dispersive x-ray spectroscopy and secondary ion mass spectrometry, was varied by changing the dopant cell temperatures for different growths. The grown films were then analyzed by reflection high-energy electron diffraction (RHEED), and ex situ structurally investigated by x-ray diffraction (XRD), atomic force microscopy (AFM), and Raman spectroscopy. The structural characterization showed that the solubility limit of Ga, In and La in SnO are ~6.0 cation%, 2.0 cation %, and 3.3 cation % respectively. Detailed electrical properties of the doped films are obtained from Hall Effect measurements and Seebeck coefficient analysis. Hole concentration, p ~ 1.2 x 10^19 cm^3 and resistivity, ρ of 0.2 Ω-cm respectively is obtained for UID SnO (001) films grown using plasma-assisted MBE and we find that p increases to ~ 5.0 x 10^19 cm^3 and ρ decreases to 0.063 Ω-cm for ~2.3at% Ga doped films. While SnO (001) films grown using a SnO2+Sn mixed source show lower unintentional p ~ 1.2 x 10^19 cm^3 and p ~ 0.4 Ω-cm and ρ decreases to ~ 0.07 Ω-cm with Ga doping. In contrast, thin films doped with increasing concentrations of La show reduction in p and remarkable increase of ρ up to ~80 Ω-cm without transition to an n-type conductivity. We found that Ga acts as an acceptor defect in SnO while La acts as compensating donor. Our results reveal that p-type conductivity in SnO can be controlled by intentional Ga- and La-doping over four orders of magnitude, whereas the successful n-type doping remains challenging.

References:
9. G. Hoffmann et al., APL Materials 8, 031110 (2020)

10:40 AM Q07 (Student) Defects, Doping and Electronic Structure of Indium Tin Oxide (ITO) Thin Films Ade Cowsky1, Oliver Bierwagen1, Leonard J. Brillson1, D.C. Look2 and K.D. Leedy1; 1The Ohio State University, United States; 2Paul Drude Institut für Festkörperlektronik, Germany; 3Wright State University, United States; 4Air Force Research Laboratory, United States

Indium Tin Oxide (ITO) is a widely used transparent conducting oxide (TCO) with a 3.5 eV and higher band gap with high conductivity. Degenerately doped In2O3 with Sn enables ITO to serve as very thin conducting yet transparent films for touchscreens, solar cells, and light-emitting diodes. A challenge for ITO is to achieve the high conductivity of thicker crystalline films while maintaining the optical smoothness of ultrathin films. Central to the conductivity of such films are the density, spatial distribution, and physical nature of native point defects, which can scatter and trap free carriers in multiple ways to degrade mobility. We use depth-resolved cathodoluminescence spectroscopy (DRCLS) to measure the electronic band structure of ITO, the electronic states of dominant ITO native point defects, their dependence on In2O3 band structure and defects on Sn doping levels. Furthermore, these results can now be compared between films grown by molecular beam epitaxy (MBE) and pulsed laser deposition (PLD).

Optical spectroscopy of ITO band structure and defects can be challenging because of contributions from both direct and indirect band structures and as well as its degenerate doping, which produce Burstein-Moss Fermi level movements out of the band gap well into the conduction band. The presence of defect states within the band gap enables additional transitions into and out of these states. In addition, the non-momentum-conserving nature of cathodoluminescence transitions allows observation of indirect transitions which might not be observed via photoluminescence spectroscopy. These multiple transitions are evident in Figs. 1 and 2, which exhibit peaks corresponding to all the aforementioned transition types and which correspond to the arrows between ITO conduction, valence, and defect gap levels in Fig. 3. Energies of the peaks assigned to direct and indirect transitions are in good agreement with those reported previously [1]. Furthermore, shifts in these energies due to doping, BM-induced Fermi level lift, and thereby effective band gap changes are consistent with changes in free carrier densities measured via Hall effect. Relative to the direct and indirect transition intensities, defect transition intensities increase.
toward the free surface by >5x over tens of nm. (Fig. 4.) These defects and their spatial distributions (Fig. 5) appear to be similar for both MBE- and PLD-grown films, suggesting similar types of defects and depth-dependence even with different growth processes.

The DRCLS peak features lend themselves to interpretations of their physical nature. DFT theory of thermodynamic stability and charge state transition energies (2) in Fig. 6 provides support for identifying the 2.7-2.9 eV defect transition with oxygen vacancies V_o. Since it is the most thermodynamically stable point defect under O-poor conditions, and it has a charge state transition near the 2.7 eV indirect band gap edge. Other defects with transitions deeper within the band gap may be related to oxygen interstitials O_i or cation vacancies complexed with hydrogen, e.g. V_in-H.[3] Studies to further identify and control these defects are presently underway.


11:00 AM Q08
(Student) Study of Hole Scattering Mechanisms in P-Type Cu2O
Jaeung Jo, Zhihao Deng, Nocona Sanders, Emanouel Kourakis and Rebecca L. Peterson; University of Michigan, United States

P-type oxide semiconductor development is a bottleneck that limits complementary metal oxide semiconductor thin film circuitry. One of the most famous p-type oxides is cuprous oxide, Cu2O. This well-known p-type semiconductor has been widely explored for photovoltaic applications due to its high mobility and wide bandgap. The high hole mobility is also attractive for high-performance p-type oxide semiconductor electronics. In our previous work investigating RF sputtered Cu2O thin film transistors (TFTs), we identified two main issues that limit device performance [1]. One is that the field effect mobility of the TFT is much lower than the material’s Hall mobility due to device level problems such as contact resistance and interface traps. The other is that the Hall mobility is lower than the theoretically-estimated value or previously-reported mobility obtained under different thin film deposition conditions. To understand the scattering factors that fundamentally limit the Hall mobility of Cu2O, we investigated thin film transport via experimental, analytical models, and density function theory (DFT). We compared an RF-sputtered polycrystalline Cu2O thin film and a single-crystalline bulk substrate, which is a natural crystal. Temperature-dependent Hall measurements were performed from 200 K to 400 K. Temperature-dependent hole carrier concentration data was analyzed using a two-acceptor state model. The experimental results showed that both the Cu2O thin film and the Cu2O bulk substrate have relatively deep acceptors. The measured mobility data was analyzed using analytical models that incorporate scattering due to ionized impurities, neutral impurities, optical phonons, acoustic phonons, and grain boundaries. We found that neutral impurity and grain boundary scattering are the dominant scattering mechanisms for the Cu2O thin film. On the other hand, phonon scattering is the dominant factor for the Cu2O bulk substrate. Our DFT calculations, focusing on phonon scattering, indicate that the hole mobility of Cu2O at 300 K should be >100 cm2/V·s. The two most dominant phonon modes were identified. This high mobility indicates that Cu2O is a promising material compared to other p-type oxide semiconductors. Our results showed that, to achieve the high hole mobility in Cu2O thin films, it is important to reduce the impurity concentrations and increase the grain size. This work provides insights toward high performance Cu2O-based p-type devices. The authors thank Intel Components Research for helpful discussions and funding. [1] J. B. Varley et al., J. Phys.: Condens. Mater. 23, 334212 (2011)

11:20 AM Q09
(Student) Electron Transport Mechanism and Mobility Prediction in Amorphous InxOy for BEOI Transistors Yaqiao Hu and K yeongjai Cho; The University of Texas at Dallas, United States

Amorphous semiconducting metal oxides like InxOy, IGZO are now being investigated for back-end-of-line (BEOI) transistors due to their wide band gap, high electron mobility, and ease of synthesis at low temperature. In this work, we use density functional theory (DFT) based first principles calculations to investigate the electron conduction mechanism in a-InxOy, and compare the theory with experimental data. Useful insights and practical guidance are provided for device engineers to further optimize the performance of a-InxOy based transistors.

Aromatic structure of a-InxOy was first generated by melt quench method with ab-initio molecular dynamics simulations. Local bonding distortion was observed in a-InxOy, which effectively elongates the In-O bonding distance and negatively impacts electron transport. The electronic density of states was calculated, showing that amorphous disorder and n-type W dopants can induce defect states in the band gap. These defect states could become electrically active and trap electrons, causing threshold voltage instability. Band structure calculation on crystalline phase InxOy (c-InxOy) reveals the In-In direct orbital overlap forms the electron conduction pathway (ECP) in c-InxOy. The local amorphous disorder in a-InxOy effectively decreases the In-In medium range connectivity and therefore reduces the electron transport pathway. The electron mobility in a-InxOy was further calculated based on the degree of electronic spacial localization, which determines the amorphous mobility at 30–50 cm2/V·s. This value is well consistent with the experimental measured mobilities in W doped a-InxOy devices. The effect of oxygen vacancy (V_o) is also investigated, which unveils that higher V_o reduces the In-In connection and impedes electron transport in a-InxOy films. Lastly, we studied the influence of film density on electron mobility, which shows that higher film density leads to compact atomic connectivity and enhanced electron mobility. These findings will contribute to the current general understanding of electron transport in amorphous solids. Our results provide useful guidance and predictive capability for device engineers on enhancing the electron transport in a-InxOy to achieving better device performance.

SESSION R: Detectors and Narrow Bandgap Materials

Session Chairs: Ganesh Balakrishnan and Daniel Wasserman

Thursday Morning, June 30, 2022

Senate Chamber

8:20 AM R01
Undoping Band Anticrossing in Highly Mismatched Alloys Qian M eng1, Tu hiin D ey2, Moham mad S. Reza2, Augustus Arbogast3, Seth R. Bank4 and Mar k W isney2,4; The University of Texas at Austin, United States; The Texas State University, United States

Highly mismatched alloys (HM As) are mixtures of atoms of very different size and electronegativity, as in Ge_xC_y or GaAs_xN_y. In conventional alloys, bandgap (E_g) and lattice constant follow an inverse trend. But small-atom HM As often decrease E_g, giving device designers additional design freedom. The reduction in E_g is usually attributed to band anti-crossing (BAC): repulsion between the conduction band (CB) and a new state within the band introduced by the isoelectronic impurity, splitting the CB into E+ and E- bands. Anions (e.g. B), cations (e.g. N), and carbon (C) can all cause the effect.
However, past results from another HM A, GaInNAS, showed that nearest neighbor arrangements can also have a significant effect on bandgap, leading to a blueshift or increase in bandgap upon anneal. In this work, ab-initio modeling of different nearest neighbor arrangements of 54 and 128 atom supercells of Bi$_{1}$In$_{3}$Ga$_{1-x}$As and Ge$_{1-y}$Sn$_{y}$C$_{y}$, respectively, was performed. HSE06 hybrid functionals were used to improve accuracy of bandgaps, and all supercells were fully relaxed in both configuration and volume, i.e. their native (computational) lattice constant.

The results show that band anticrossing effects in different HM A, particularly bandgap, can be reduced and even eliminated by atomic arrangement in ternaries and quaternaries. A highly mismatched atom may not be sufficient in itself to cause band splitting if compensating atoms are within 2 bond lengths from it. Instead, distortion of the host lattice appears to be necessary. We also note that, as one might expect based on local strains, the lowest energy state is always the one in which Sn atoms are bonded directly to C rather than farther away.

The consistent results across three different HM A's suggests this is a general property applicable to many materials. Furthermore, this may explain the wide variation in properties reported by different groups, since nearest-neighbor arrangement in the growth can be highly sensitive to growth temperature, surface reconstruction, flux ratios, and the presence of surfactants such as Sn or Sb.

8:40 AM R02
(Student) Growth and Characterization of AlIn1-xAsySb1-y Digital Alloys Grown on InP
Ellie Y. Wang, Joshua A. M. Arthur, Ann K. Rockwell and Seth R. Bank; The University of Texas at Austin, United States

Al$_{1-x}$In$_{x}$As$_{y}$Sb$_{1-y}$ (referred to as AlInAsSb) grown as a digital alloy lattice-matched to GaSb substrates has been shown to have characteristics useful for avalanche photodetectors (APDs). In addition to a broadly tunable bandgap over a wide compositional range, the material system has favorable band offsets, with most of the bandgap change occurring in the conduction band, and it exhibits low excess noise due to impact ionization coefficient ratios as low as k = 0.01 [1]. The digital alloy method of growing thin binary layers to form extremely short-period superlattices enables the growth of high quality AlInAsSb within the miscibility gap. It also allows for more consistent parameters and finer control over compositional gradings in the growth of complex heterostructures when compared to alloy growth [2]. In some cases, the technique improves the noise characteristics of the material. For example, digitally grown Al$_{1-x}$Ga$_{x}$Sb$_{y}$As$_{1-y}$ on InP exhibits a lower impact ionization ratio than the Al$_{1-x}$Ga$_{x}$As$_{y}$ random alloy, with k = 0.05 and k ∼ 0.2, respectively [3]. Similarly, when grown as a digital alloy on InP, Al$_{1-x}$Ga$_{x}$Sb$_{y}$As$_{1-y}$ also exhibits reduced k as low as ∼0.005 [4], compared to the random alloy with k ∼0.1 [5].

Noteworthy, Al$_{1-x}$In$_{x}$As$_{y}$Sb$_{1-y}$ and Al$_{1-x}$Ga$_{x}$Sb$_{y}$As$_{1-y}$ represent the lattice-matched extremes of the AlInAsSb quaternary on InP, with Al compositions of x = 0.48 and x = 1.00, respectively, suggesting the low-noise potential of the digital alloy system on InP across the full compositional range. Although Al$_{1-x}$In$_{x}$Ga$_{1-x}$As$_{y}$Sb$_{1-y}$ random alloys on InP have shown low noise, growth over other Al compositions is challenged by phase separation that could potentially be overcome by digital alloying [6, 7]. The benefits of using InP substrates instead of GaSb for AlInAsSb growth are twofold: first, the maximum accessible bandgap would extend to ∼1.8 eV, compared to ∼1.25 eV on GaSb. Second, the more mature InP manufacturing infrastructure could be leveraged to produce high-quality APDs. The advances of AlInAsSb grown on GaSb substrates and the potential to enhance device performance using a mature InP platform motivated this study.

Here we present AlInAsSb grown as a lattice-matched digital alloy on InP substrates. AlInAsSb digital alloys of different aluminum compositions were grown using the molecular beam epitaxy (MBE) growth approach described in [8], where the aluminum composition is calculated as the sum of the number of Al and As monolayers divided by the total number of monolayers. Lattice-matching to InP at each composition was achieved by adjusting the AlAs/AlSb thickness ratio while maintaining a constant InAs thickness. X-ray diffraction (XRD), photoluminescence (PL) and atomic force microscopy (AFM) measurements were performed on preliminary samples of AlInAs (x = 0.48) and AlInAsSb (x = 1.00) to verify the structural, optical, and surface qualities at the compositional limits. XRD scans suggest high-quality crystal structures, as indicated by the sharp superlattice peaks and strain-balancing to the InP substrates. Room temperature PL was observed for both samples, showing optical emission at wavelengths of ∼1.2 µm (x = 0.48) and ∼0.9 µm (x = 1.00). AFM showed smooth surface morphology with RMS roughnesses of 0.3 nm (x = 0.48) and 1.1 nm (x = 1.00). In order to fully explore the compositional space of the material, the growth and characterization of additional AlInAsSb digital alloys with intermediate aluminum compositions are underway and will be reported at the conference.

References

9:00 AM R03
(Student) Exploring the Impact of Sn Alloying on Structure and Luminescence in PbSnSe Epitaxial Films on GaAs

The narrow gap IV-VI semiconductor PbSe is an intriguing option for heterogeneously integrated mid-infrared light emitters in the 3 - 5 µm wavelength range. Thanks to its rare combination of ionic, covalent, and metallic bonding, PbSe has an anomalously low bulk Auger recombination coefficient, high tolerance of its minority carriers to crystal defects, and favorably low temperatures for epitaxy. The growth of PbSe and related IV-VI materials on substrates like GaAs is of great interest as these exciting optoelectronic properties of PbSe may be paired with the superior mechanical, chemical, and thermal properties of III-V materials and potentially even in functional heterostructures with III-V optoelectronic devices. Recently, we demonstrated epitaxial thin films of PbSe on 8%-lattice mismatched GaAs that nevertheless emit brightly, indicating high internal quantum efficiency for photoluminescence at room-temperature.

Moving beyond the binary compound, we may tune the bandgap across the mid-IR and into the far-IR by substituting Pb with the isovalent element Sn as Pb$_{1-x}$Sn$_{x}$Se.$^1$ This alloy was also recently discovered to be a topological crystalline insulator past ~22% Sn following a complete band gap closure.$^3$ This motivates us to explore how alloying Sn alters the microstructure and otherwise excellent luminescence properties of PbSe films. Strain-induced structural distortions, stemming from lattice-constant and thermal expansion mismatch with GaAs, are an important parameter in understanding the electronic properties of these thin films. The lattice constant for Pb$_{1-x}$Sn$_{x}$Se spans a range from 6.126 for PbSe to roughly 6.00 Å for cubic SnSe (a roughly 2% lattice mismatch between the two binaries).

We grew Pb$_{1-x}$Sn$_{x}$Se epitaxial films on (001)-oriented GaAs substrates by molecular beam epitaxy at 280–300 °C using PbSe and SnSe compound source effusion cells, following a 400 °C surface pretreatment with PbSe flux that we find is essential for good photoluminescence, and a 330°C PbSe buffer layer. Across a Sn composition range of x = 0–0.4, full-width-at-half-maximum of

---

$^1$Supported by the NSF (No. ECCS-1542159). This work was also supported by the NASA EPSCoR Grant NNX13AM76A.

$^2$Amberly Ricks, Rachel C. White, Morgan Bergthold, Aaron J. Muhowski, Leland J. Nordin, Ellie Y. Wang, Joshua A. M. Arthur, Ann K. Rockwell and Seth R. Bank; The University of Texas at Austin, United States.

$^3$Amberly Ricks, Rachel C. White, Morgan Bergthold, Aaron J. Muhowski, Leland J. Nordin, Ellie Y. Wang, Joshua A. M. Arthur, Ann K. Rockwell and Seth R. Bank; The University of Texas at Austin, United States.
(004) rocking curves increase from 350 to 515 arcseconds, suggesting a slight decrease in structural quality despite a decreased lattice mismatch to the GaAs substrate. We also find an increase in the in-plane residual tensile strain from 0.37-0.55% at room-temperature as the Sn content is increased, determined via high resolution x-ray diffraction reciprocal space maps. At growth temperatures, the nearly 8% lattice mismatch between PbSe and GaAs is fully relaxed. However, a tensile strain develops upon cooldown from growth temperature due to the large thermal-expansion mismatch between PbSe and GaAs. The increased tensile strain in the higher Sn alloys is attributed to tensile strain with respect to the higher lattice constant PbSe buffer. While higher Sn-content PbSnSeSnSe ternaries suffer from a loss in structural quality, only less than 20% Sn is required to tune the emission wavelength from 4 to 10 µm. Preliminary room-temperature photoluminescence show redshifted peak wavelengths out to 4.6 µm for a film of PbSnSeSnSe, but with decrease in emission intensity compared to PbSe. We will present results investigating and comparing loss mechanisms in PbSe and PbSnSeSnSe to understand whether these are fundamental in nature or if they may be overcome by engineering.

While III-V-bismide alloys have received substantial attention due to the significant bandgap reduction induced by the incorporation of dilute concentrations of bismuth, the need for a highly optimized growth regime so disparate from the host alloy’s ideal growth conditions has hindered their development relative to traditional III-V semiconductors. In particular, lower substrate temperatures are necessary to minimize bismuth desorption and promote substitutional incorporation, however, this parameter must be carefully balanced to minimize defects. InSnSb, Bi, while relatively unexplored, is a particularly promising candidate material system for accessing the longwave-infrared due to the similar growth temperatures that are ideal for InSb and III-Bi materials. We recently demonstrated the growth of high-quality InSb, Bi, and, consequently, reported the first photoluminescence (PL) measurements from InSbBi alloys. Alloying very small concentrations of arsenic to form the quaternary InAsSbSbBi results in a flexibility to decrease the bandgap energy, which enables infrared emission, and increases spin orbit (SO) split band properties, which can suppress Auger recombination when larger than the bandgap energy. Current approaches for photodetector operation in the mid-wave and long-wave infrared, such as HgCdTe and InSb-based devices, suffer from large dark currents. While nBi structures can suppress many sources of dark current, the use of AlInSb barriers in InSb-based nBi detectors result in a difficult tradeoff between undesirable valence band offset and high barrier layer strain. A flexible method to mitigate these challenges in InSb-based nBi detectors is to introduce small amounts of Bi and Al to InSb to tune the bandgap of InSbBi absorber regions and AlInSbBi barriers, while simultaneously minimizing strain. However, AlInSbBi remains largely unexplored, in part due to the difficulties of growing Bi-containing III-V alloys. Noteworthy are the tradeoffs in temperature and growth rate, which pose challenges in the ability to grow quality III-V-Bi materials. In this work, material properties such as bandgap energy, lattice constant, surface morphology, and photoluminescence of AlInSbBi alloys were investigated to optimize material quality for barrier layer applications.

A InSbBi grown by solid-source molecular beam epitaxy on n-type InSb substrates was used to promote bismuth incorporation. Photoluminescence (PL) and atomic force microscopy (AFM) measurements were performed to quantify the optical quality and surface morphology of the films. X-ray diffraction (XRD) 20 scans are in progress to confirm the bismuth and arsenic concentrations in the films and will be reported at the conference. PL measurements of InSbBi and InAsSbSbBiBi films both targeting ~1% Bi incorporation demonstrated an expected redshift in emission wavelength from the film with additional As incorporation. By targeting further increased As and Bi concentrations, wavelength extension out to approximately 6.6 µm was achieved from InAsSbSbBiBi alloys on InSb. While AFM measurements of the InSbBi film showed a relatively smooth surface, the InAsSbSbBiBi films exhibited some droplet formation. We expect this can be mitigated through careful optimization of the growth parameters. Current work includes optimizing the growth of InAsSbSbBiBi for enhanced structural and optical quality as well as investigating the limits of Bi incorporation in this material system. Progress towards these goals will be reported at the conference.

This work was supported by Lockheed Martin and NSF (ECCS-1933836). This work was performed in part at the University of Texas Microelectronics Research Center, a member of the National Nanotechnology Coordinated Infrastructure (NNCI), which is supported by the NSF (No. ECCS-1542159). This work was also supported by an NSF Graduate Fellowship (RCW).

Bi-containing III-V alloys have attracted attention over the past few decades due to their suitability for optoelectronic devices operating across a wide spectrum of the infrared region. Integrating small amounts of Bi into III-V materials offers the flexibility to decrease the bandgap energy, which enables infrared emission, and increases spin orbit (SO) split band properties, which can suppress Auger recombination when larger than the bandgap energy. Current approaches for photodetector operation in the mid-wave and long-wave infrared, such as HgCdTe and InSb-based devices, suffer from large dark currents. While nBi structures can suppress many sources of dark current, the use of AlInSb barriers in InSb-based nBi detectors result in a difficult tradeoff between undesirable valence band offset and high barrier layer strain. A flexible method to mitigate these challenges in InSb-based nBi detectors is to introduce small amounts of Bi and Al to InSb to tune the bandgap of InSbBi absorber regions and AlInSbBi barriers, while simultaneously minimizing strain. However, AlInSbBi remains largely unexplored, in part due to the difficulties of growing Bi-containing III-V alloys. Noteworthy are the tradeoffs in temperature and growth rate, which pose challenges in the ability to grow quality III-V-Bi materials. In this work, material properties such as bandgap energy, lattice constant, surface morphology, and photoluminescence of AlInSbBi alloys were investigated to optimize material quality for barrier layer applications.

A InSbBi grown by solid-source molecular beam epitaxy on n-type InSb substrates was used to promote bismuth incorporation. Photoluminescence (PL) and atomic force microscopy (AFM) measurements were performed to quantify the optical quality and surface morphology of the films. X-ray diffraction (XRD) 20 scans are in progress to confirm the bismuth and arsenic concentrations in the films and will be reported at the conference. PL measurements of InSbBi and InAsSbSbBiBi films both targeting ~1% Bi incorporation demonstrated an expected redshift in emission wavelength from the film with additional As incorporation. By targeting further increased As and Bi concentrations, wavelength extension out to approximately 6.6 µm was achieved from InAsSbSbBiBi alloys on InSb. While AFM measurements of the InSbBi film showed a relatively smooth surface, the InAsSbSbBiBi films exhibited some droplet formation. We expect this can be mitigated through careful optimization of the growth parameters. Current work includes optimizing the growth of InAsSbSbBiBi for enhanced structural and optical quality as well as investigating the limits of Bi incorporation in this material system. Progress towards these goals will be reported at the conference.

This work was supported by Lockheed Martin and NSF (ECCS-1933836). This work was performed in part at the University of Texas Microelectronics Research Center, a member of the National Nanotechnology Coordinated Infrastructure (NNCI), which is supported by the NSF (No. ECCS-1542159). This work was also supported by an NSF Graduate Fellowship (RCW).
~1 μm/hr. Atomic force microscopy (AFM) and photoluminescence (PL) measurements were performed on an AlInSbBi thin film targeting ~1% Bi and ~5% Al incorporation. AFM measurements showed droplets on the film surface, however further optimization of the growth parameters may be able to mitigate droplet formation. PL measurements at 83K demonstrated that the AlInSbBi film emitted at roughly 5.1 μm, whereas the AlInSb and InSbBi control films emitted at 4.9 and 5.6 μm, respectively, suggesting ~0.5% Bi incorporation into AlInSb. To investigate the bandgap change with Bi incorporation, preliminary density functional theory (DFT) simulations with hybrid functionals (HSE) were performed using a 54-atom supercell with 1 A1 and 1 Bi atom (corresponding to 3.7% Al and Bi). DFT predicts that the direct bandgap of Al0.93In0.07Sb0.96Bi0.03 is reduced by ~20 meV from that of InSb, in qualitative agreement with the observed reduction in PL emission energy. Further growths are underway for additional alloy compositions to fill out the AlInSbBi growth space and optimize the bandgap energy, lattice constant, surface morphology, and photoluminescence to act as a barrier layer.

2. L. Wang et al., Crystals 7, (2017).

10:00 AM Refreshment Break

10:20 AM R06
Low Growth Temperature Epitaxial PbSe for Heterogeneous Mid-Infrared EmitterS Leland J. Nordin, Jaron M. eyer, Pooya J. Reddy and Kunal M. ukherjee; Stanford University, United States

The mid-infrared (MIR) wavelength range is vital for an abundance of sensing, health/biological monitoring, security and defense, and fundamental science applications. For compact solid-state sources of MIR light, III-V semiconductor heterostructures, such as quantum cascade lasers (QCL), interband cascade lasers (ICL), or type-II superlattice light emitting diodes (SLED), are often used. However, QCL, ICL, and SLED structures all suffer from substantial growth complexity and, in addition, SLEDs struggle to achieve high performance at room temperature. Moreover, typical III-V growth temperatures (>550 °C) prevent III-V based MIR emitters to be heterogeneously integrated during the back-end-of-line (BEOL) portion of Si fabrication. Recently, thin films of PbSe grown epitaxially on III-V GaAs(001) substrates have shown remarkably high internal quantum efficiency (IQE) of nearly 30% at room temperature and comparatively low growth temperatures of 300 °C, compatible with BEOL [1]. However, the total film thickness is restricted (<200 nm) for growth on GaAs(001) due to thermal mismatch induced crack formation and thus the prospect of heterogeneous devices is narrow.

In this work, we show that the growth window for high optical-quality PbSe-III-V extends to substantially lower temperatures than previously demonstrated and investigate the recombination dynamics of the low growth temperature films. A high temperature (300 °C) PbSe film [Figure 1(a)] and a lower temperature (170 °C) PbSe film [Fig. 1(b)] were grown on oxide-desorbed and arsenic-capped GaAs(001) substrates in a Riber Compact 21 molecular beam epitaxy (MBE) system using a compound PbSe source. Both growths started with a PbSe dose procedure and nucleation layer [2]. Following the nucleation layer, the growth temperature was lowered to the either 300 °C or 170 °C, and 80 nm of PbSe was grown. Following growth, room temperature MIR photoluminescence (PL) was measured on both films and is shown in Fig. 1(c).

Notably, the magnitude of PL is nearly identical for both the high growth temperature and low growth temperature films, suggesting that SRH recombination rates, often associated with poor growth quality, are comparable in both films. We attribute the slight redshift of the PL-peak to a lower strain energy contribution. This strain energy is accumulated when cooling down from growth temperature to room temperature. To better understand the impact of growth temperature on luminescence efficiency we performed power dependent PL (PDPL) measurements and shown in Figure 2. is PL efficiency (PL magnitude divided by laser power, the optical analog of wall plug efficiency) versus laser power. Remarkably, we do not see a substantial deviation in PL magnitude for lower pump powers, further corroborating the similar SRH recombination rates. However, we do not observe a pump power independent PL magnitude, suggesting that we have not reached low injection in these measurements, so we cannot claim identical SRH recombination rates.

We have grown PbSe films on GaAs substrates at 300 °C and 170 °C and investigated their luminescence properties, both spectral and power dependent PL. PL magnitude is not dramatically impacted by the lower growth temperature, corroborated by both the magnitude of spectral dependent PL, which was performed at high injection, and power dependent PL. Most importantly, the low growth temperature PL magnitudes are compatible with BEOL processes, likely extend the accessible crack-free film thicknesses, and possess bright PL. The confuence of these properties suggests that low growth temperature PbSe films are an ideal candidate for MIR heterogeneous emitters. Additionally, these low growth temperatures enable the investigation of more esoteric ternaries, such as PbSe, which require extremely low growth temperatures.

undertaken CV measurements at 295, 150 and 77 K (see Fig.1). We found that the capacitance varies with the top mesa diameter for both material systems, and not the bottom mesa diameter, indicating that the unintentionally doped intrinsic region is n-type in nature.

11:00 AM R08

(Student) Majority Carrier Concentration and Minority Carrier Lifetime in Mid-wave Infrared InGaAs/InAsSb and InAs/InAsSb Superlattice nBn Detectors

Alexander T. Nwewi1,2, Preston T. Webster1,2, Chris P. Hains2,3, Julie V. Logan4, Rigo A. Carrasco2, Perry C. Grant2, Zinah M. Alsaa’d2,3, Diana M aetas2,3, Christian P. M oral2 and Ganesh B alakrishnan1; 1University of New Mexico, United States; 2Air Force Research Laboratory, United States; 3A-tech, LLC, a BlueHalo company (ATA BlueHalo), United States

Infrared unipolar barrier detectors based on III-V materials have progressed tremendously due to success in improving material quality and bandgap engineering. In the standard nBn detector, the single unipolar barrier extends into the conduction band, blocking the majority carrier dark current and significantly inhibiting the generation-recombination and surface contributions to the dark current. The barriers serve to create a minority carrier, diffusion-limited device, however doping still has a dominant impact on device performance due to its relationship with the minority carrier lifetime and minority carrier concentration. Increasing doping degrades the minority carrier lifetime, and thus the quantum efficiency of the photodetector. Diffusion dark current in the nBn detector, which is proportional to the minority carrier concentration, is initially reduced by increased doping until it begins to have an adverse effect on the minority carrier lifetime. Ultimately, absorber doping density significantly affects nBn photocollection and noise characteristics and must be precisely controlled to optimize photodetector performance.

Recent advances leading to high minority carrier lifetime in strained InAs/InAsSb superlattices have led to it being considered as a higher mobility drop-in replacement to the InAs/InAsSb superlattice nBn. Two InAs/InAsSb and three InGaAs/InAsSb nBn structures designed for maximum electron-hole recombination wavelength over 5.1-5.3 μm wavelength cutoffs have been grown with different absorber doping profiles by molecular beam epitaxy. The material is examined by time-resolved and steady-state photoluminescence, X-ray diffraction, and Nomarski surface imaging. The samples are then processed into variable-area mesa arrays using standard lithography and contact metal deposition. The devices are packaged in and wire-bonded to 68-pin leadless-chip carriers, which are then mounted in a vacuum-sealed dewar for temperature-controlled measurements of the photocurrent, dark current, and capacitance-voltage to evaluate the doping concentration profile in each device. The undoped Ga-free nBn’s exhibited the lowest background n-type majority carrier concentration of 6x10^13 cm^-3 with a minority carrier lifetime of 3 μs. The undoped InGaAs/InAsSb superlattice exhibited a -4x higher majority carrier concentration of 2x10^16 cm^-3 with a minority carrier lifetime of 2 μs. Si-doped samples with constant and graded doping profiles are also examined, and the minority carrier lifetime is observed to degrade with increased doping. An analysis of the minority carrier lifetime’s dependence on doping, impact on detector performance and other characterization results will be presented. 

Approved for public release: Distribution is unlimited. AFMC PA number xxxxxxx

11:20 AM R09

(Student) Graded-Mode Resonance Enhanced Room-Temperature Infrared Detectors

Abhilasha Kamboj1, Leland J. Nordin2, David Woolf3 and Daniel Wasserman3; 1University of Texas at Austin, United States; 2Physical Sciences Inc., United States

The mid-infrared wavelength range (3−30 μm, mid-IR) is a spectral range of significant importance. The mid-wave infrared (MWIR, 3−5 μm) transmission window, specifically, is vital for applications such as gas sensing and free-space communication, as well as thermal imaging of mechanical objects (engines, turbines, etc) that have temperatures ~580−970 K. For an infrared detector, efficient operation at high temperatures is typically the primary goal. While M encry-Cadmium-Telluride (HgCdTe) detectors are the current state-of-art infrared detectors, the type-II superlattices (T2SL) have shown to be a promising alternative material system. However, the comparatively lower absorption efficiency of the T2SL detectors presents a challenge, due to the trade-off (as a function of the absorber thickness) between large external quantum efficiency and higher collection efficiency/reduced dark current. This limitation can be addressed by incorporating thin detector absorber regions in resonant photonic architectures. One such architecture is the guided-mode resonance structure, comprising a high-refractive-index grating layer sandwiched between two low-index layers.[1] Incident light diffracts into guided modes in the grating layer, which can then couple out to free space. When the outcoupled light interferes constructively/destructively with reflected/transmitted light, strong and narrow resonant peaks/dips can occur in the reflection/transmission spectra. We design a GMR structure where index-mismatch required is achieved with highly doped (n−) semiconductor layers, which can be modeled with the Drude formalism, allowing for a lattice matched material system with extremely low refractive index in the MWIR, which can serve as a waveguide cladding layer.

In this work, we build on our previous efforts[2], to demonstrate GMR-enhanced all-epitaxial uncooled (room-temperature) M WIR nBn InAs/InAsSb T2SL detectors. We have designed, grown, fabricated and characterized GMR detectors showing such enhancement in a T2SL absorber only 250 nm thick. GaSb serves as a high-index grating layer which, together with the nBn detector (serving as a waveguide core), is sandwiched between a low-index n− virtual substrate and air. For grating periods Λ = 1.6 μm and 1.8 μm, resonances with enhancement of ≈ 8x & 14x are shown at wavelengths λ = 4.4 μm & 4.7 μm respectively which is very close to the band-edge of the absorber (≈5 μm). Typically, due to the steep drop in absorption coefficient close to the band-edge, it is extremely difficult to obtain sufficient external quantum efficiency near the absorber band edge. Thus, detectors must be grown with lower energy cut-off, which will significantly increase dark current and degrade device detectivity. The ability to enhance EQE at the band edge of the absorber T2SL, allows us to use higher energy cut-off absorbers without degrading absorption efficiency. Moreover, the ultra-thin absorber, when compared to a typical M WIR detector, offers a significant reduction in dark current, when compared to traditional M WIR III-V detectors operating in same wavelength range, at similar temperatures. Significant improvement in both the optical and electrical performance of the GMR detectors results in superior specific detectivities. TE-polarized estimated specific detectivity D′ = 1.2 x 10^10 cm Hz^½/W and 1 x 10^10 cm Hz^½/W are reported for the Λ = 1.6 μm and 1.8 μm devices, respectively. Future work will investigate polarization-independent detectors with substrate-side illumination for potential incorporation into focal-plane array architectures.

The authors gratefully acknowledge United States Army under Prime Contract W909M Y-20-P-0010 and National Science Foundation (ECCS-1926187 and ECCS-2025227).

References:
The primary focus of mid-wave (M WIR) and long-wave infrared (LWIR) detector research has been to optimize detector detectivity and operating temperature. However, emerging applications such as free-space optical communication, lidar sensing, and dual-comb spectroscopy require, in addition to high detectivity and operating temperature, detectors with fast time response (high bandwidth). Traditional high-speed device structures, such as p-i-n photodiodes, have been proven highly suitable for the shorter near-infrared telecommunication wavelengths, but are difficult to design and implement in the M WIR and especially LWIR due to the increasingly narrow material bandgap, which causes a number of undesired effects that undermine device performance. In the LWIR spectral region (8-12 μm), high-speed detection is usually achieved with the intersubband quantum well infrared photodetectors (QWIP) or quantum cascade detectors (QCD), which generally have much lower responsivity than detectors leveraging bulk, narrow bandgap absorber materials.

Here, we demonstrate a LWIR detector using a plasmonically enhanced type-II superlattice (T2SL) material as the absorber. The detector has an nBn device architecture, where the barrier (B layer) blocks the flow of majority carriers (electrons) and thus reduces the dark current. Previous work has shown that by using a highly doped layer as a plasmonic backplane, optical absorption in the ~300 nm thick (~λ/33) absorber can be strongly enhanced, achieving an external quantum efficiency and detectivity similar to detectors that have much thicker absorber layers [1]. In addition to improvements in the magnitude of the response, the ultrathin absorber layer should also lead to a fast time response, enabling high-speed operations. To investigate the temporal response of these ultra-thin plasmonic detectors, we fabricate the material into mesa structures of varying areas, with coplanar waveguide metal contacts, and measure the time response of the detectors using an optical parametric amplifier (OPA) configured to output λ=5 μm ~200 fs pulsed light. The devices are biased using an external voltage source connected to a bias tee, and the DC-filtered time response signal is captured with a digital sampling oscilloscope and subsequently Fourier transformed to determine the 3dB cutoff bandwidth.

The time response measurements show that for a 50 μm diameter circular mesa device, at an operating voltage of -0.6 V and temperature of 180 K, the device exhibits a bandwidth of 530 MHz, equivalent to a 300 ps time constant. The detector bandwidth increases with increased bias voltage but not significantly, indicating that drift is unlikely the dominating transport mechanism in this detector. Although the carrier transport is expected to be diffusion-dominated, the bandwidth achieved in this ultrathin detector is comparable to other thick detectors that need to operate in a high bias, drift-dominated regime. These results show the promising potential of the ultrathin plasmonic LWIR detectors as a material platform for high-speed LWIR detector applications.


Session Chair: Joshua Zide
Thursday Morning, June 30, 2022
Cartoon Room #1

8:20 AM S01
Wafer-Scale Ferromagnetic Fe3GeTe3 Thin Films by Molecular Beam Epitaxy
K. Zhou, The University of British Columbia, Canada

Until now, two-dimensional ferromagnets still remain mostly limited to exfoliated micron-sized samples. Large-scale thin films are desirable for the fabrication of integrated devices for spintronics and memory storage applications. Among this group of materials, Fe3GeTe3 (FGT) can host ferromagnetic states at room temperature upon optimized gating. We achieve, by molecular beam epitaxy, the synthesis of high-quality monolayers and ultrathin FGT films. Surface x-ray diffraction confirms its quintuple layer substructures with hexagonal symmetry. Thickness-dependent transport measurements are used to characterize and probe for magnetic order. Ferromagnetic states exist in 1–10 layer thick FGT, with Curie temperatures ranging from ~75 K in one layer samples to above 175 K in ten layer samples. A ferromagnetic phase with significant magnetic anisotropy is revealed for all layer numbers.

8:40 AM S02
(Student) MBE Growth of CrbixSb1-xTe for Enhancing Spin-Orbital-Torque Switching and Stabilizing Quantum Anomalous Hall Effect
Y. Tan, University of California, Los Angeles, United States

CrBixSb1-xTe is a magnetic topological insulator which could achieve quantum anomalous Hall (QAH) effect and spin-orbit torque (SOT) switching in the same structure. This is promising for its future applications in memory or switching applications with its robust surface properties by topological protection. In this work we have grown CrBixSb1-xTe on GaAs (111) substrate through modulation doping (of Cr) by MBE (Molecular Beam Epitaxy). The doping level and the thickness of each layer is examined to tune the bandgap and the Fermi level of the whole sample. In this way, we can tune the Fermi level into the bandgap and optimize the total resistivity of the sample to achieve quantization. The influence of electrical field is also examined. This will help us optimize materials properties and design the device structure to enhance the performance of future SOT switching applications.

9:00 AM S03
(Student) Epitaxial Thin Films of Chalcogenide Perovskites and Related Phases
S. Surendran, H. Chen, B. Zhao, A. Thind, S. Singh, T. Orvis, H. Zhao, H. Boton, M. Kawasaki, R. Mishra, J. Ravichandran, University of Southern California, United States

Chalcogenide perovskites have recently emerged as a new class of semiconductors composed of earth abundant, non-toxic elements with large chemical and structural bandgap tunability in the visible-infrared region and desirable opto-electronic properties. Past investigations on single crystals of perovskites such as BaZrS3 (BZS) and the corresponding Ruddlesden-Popper phases such as Ba3Zr2S7, both with corner shared ZrS5 octahedral connectivity, show that these materials are suitable for solar energy conversion due to their optimum band gaps and strong light absorption. On the other hand, Quasi-1D hexagonal chalcogenide perovskites with face shared octahedral connectivity such as
BaTiS$_3$ (BTS)\textsuperscript{[2]} and Sr$_{1-x}$TiS$_x$\textsuperscript{[3]} exhibit optical anisotropy resulting in large birefringence and linear dichroism in the mid-wave and long-wave infrared (MWIR) regime. The demonstration of high-quality epitaxial thin film growth of these chalcogenide perovskites is a critical next step to improve our understanding of their physical properties and to realize heterostructures of these materials that host emergent physical phenomena. Recently, multiple groups have developed innovative but multi-step approaches\textsuperscript{[4]-[6]} to achieve thin films of the prototypical chalcogenide perovskite BZS. Nevertheless, the direct epitaxial growth of chalcogenide perovskites is challenging due to a large mismatch in the vapor pressure for the cations and chalcogens, and the corrosive and reactive nature of most chalcogen precursors.

Here we report single-step epitaxial growth of BZS thin films on perovskite oxide substrates by pulsed laser deposition\textsuperscript{[9]} from stoichiometric polycrystalline targets. X-ray diffraction (XRD) shows that the films are strongly textured out of plane and have a clear in-plane epitaxial relationship with the substrate. Electron microscopy studies confirm the presence of epitaxy despite the polycrystalline nature, with a large number of extended defects away from both the substrate and the film. The films show strong light absorption and fast photo response.

Further, we used the same approach of growth to realize thin films of BTS. XRD shows the films are polycrystalline with a strong out of plane texture and multiple in-plane domains. Extensive structural characterization was performed to understand the orientation of these domains. XRD and AFM show film surfaces and interfaces with relatively large roughnesses ($\sim 1-2$ nm), which hinder the growth of large grains with low defect density. The role of processing parameters such as substrate temperature, background gas composition and pressure, laser fluence and the choice of single crystal substrates on controlling the structure and improving the quality of these films will also be discussed.

References:

\textsuperscript{[2]} S. Niu, et al., Nano Letters 2018, 12, 392.
\textsuperscript{[3]} S. Niu, et al., Chemistry of Materials 2018, 30, 4897.
\textsuperscript{[5]} X. Wei, et al., Nano Energy 2020, 68.
\textsuperscript{[6]} M. Surendran, et al., Chemistry of Materials 2021, 33, 7457.
This work sets the stage for developing chalcogenide perovskites as a family of semiconductor alloys with properties that can be tuned with strain and composition in high-quality epitaxial thin films, as long-established for other semiconductor materials, while also displaying rich solid-state chemistry and physics familiar in complex oxides. Our methods also represent a revival of gas-source chalcogenide MBE, with potential for impact on research on chalcogenide perovskites and other sulfur- and selenium-containing compounds.


10:00 AM Refreshment Break

SESSION T: Epitaxial Growth of Highly Mismatched Alloys
Session Chair: J. Joshua Zide
Thursday Morning, June 30, 2022
Cartoon Room #1

10:20 AM T01
Critical Evaluation of Thermal and Compositional Dependences in a Finite Strain Model of Ge-Si-Sn Alloys on Ge(100) and GeSn Buffer Layers from DFT
Narges M asoumi and Andrew Chizmeshya, Arizona State University, United States

Ge rich Si-Ge-Sn alloys typically adopt the a-phase (diamond) structure of Ge, while the b-phase is expected to prevail in the limit of large Sn concentration. Strain has an important influence on the stability of the a-phase (diamond) structure of Si-Ge-Sn alloys, but its role in the a-b non-isomorphism has to our knowledge not been studied or reported to date. Here we report the outcome of ab initio thermochemistry calculations based on DFT and special quasi-random supercell representations, which show that the a-phase exhibits a stability field spanning −90% Sn in the Si0.5Sn0.5 and Ge0.5Sn0.5 systems for T between 300-500K. Another key aspect of epitaxial stability is the strain response of thermodynamically stable alloys grown on either pure Ge clad Si, or various GeSn buffers. In the small strain limit linear elasticity theory can be used to relate the perpendicular and parallel strains. In this paper we develop a thermodynamics model for fully relaxed hetero-epitaxial alloys over the entire 0-100% Sn composition range corresponding to 0-13% compressive biaxial strains on Ge (001), beyond linear elasticity estimates commonly used (Hooke’s law). The numerical results are fitted to an analytic model which includes compositional and thermal bowing corrections to Vegard’s law, and the elastic ratio, and reproduces known strained lattice parameters over the wide composition range. For Ge0.5Sn0.5 alloys we predict the existence of a “sweet spot” in the viscosity of strain values of 6%. Below this value the linear elasticity theory appears to overestimate the perpendicular strain, while above this value the converse behavior ensues.

Ge has a nearly direct bandgap because the direct Γ valley (k = 0 in momentum space) is only 140 meV above the indirect L valley. Tensile strain (>2%) and alloying (Ge1-xSnx or Ge1-yCy) are the two most common approaches to make Ge-based direct bandgap materials. Although Ge0.5Sn0.5 becomes a direct bandgap material with >10%, strained growth on Ge or GaAs adds undesirable compressive strain. Worse, the very small electron effective mass (m* = 0.02m0) loses the direct bandgap when confined in a quantum well (QW) or dot.

Our group has previously demonstrated that Ge0.3Cy, with y ≈ 1%, has a direct bandgap, and reported GeC using a special precursor (4GeMe) as a C source in molecular beam epitaxy (MBE), with no defects detected in transmission electron microscopy (TEM)3. In this work, we instead grew Ge0.5Sn0.5C0.05 using a simpler precursor. GeSnC adds additional control in epitaxial growth: Sn and C partially compensate local strain and distortion of the host Ge bonds. Ab-initio calculations predict that C-Sn-C bonding would be energetically favorable over C-C bonds in the Ge lattice. This is likely to increase both C and Sn substitutional incorporation and provides a more stable material, similar to InGaAsN4. We saw no evidence of Sn segregation as surface droplets, nor C incorporation as undesirable C-C or C=C bonded nano-clusters. Therefore, adding Sn might reduce the carbon clustering at the surface which would be a great achievement compared with past growths by other groups. As an added benefit, GeC offers a larger electron effective mass (m*), which would preserve the direct bandgap in GeSnC even when confined in a QW. Tensile strained Ge0.5Sn0.5C0.05 was grown on GaAs (001) substrate in hybrid MBE using thermal Ge, Sn sources and commercial carbon tetraamide (CB4) as the carbon source. We believe sp2-C-C pairs are likely defects in the carbon containing alloys, so we also used hydrogen to preferentially remove sp2 carbon, as is done in growth of epitaxial diamond. High resolution x-ray diffraction (HRXRD) reveals good crystallinity in the epilayer with maximum 3% of substitutional carbon and 4% tin. Raman observation of the C local mode at 530 cm−1 confirms substitutional incorporation into the crystal. Atomic Force Microscopy (AFM) shows mostly flat surfaces. Unlike most other carbon sources, no sp2 (graphitic) or amorphous carbon bonds were detected in Raman spectroscopy from 1200-1600 cm−1 (not shown). The successful incorporation of C into Ge substitutionally, without cluster carbon, is a major step toward efficient Group IV lasers for silicon photonics. We have also observed emissions in 0.50-0.60 eV range both from bulk and multiple quantum well (MQW) GeSnC samples. These peaks could be from different atomic arrangements, from defects, or from non-uniform QW compositions. The detailed origins of the emission spectrum are currently under investigation and will be reported at the conference.

Reference
1. Jifeng Liu, Photonics 3 (3), 162 (2014)
GeSn offers a route to on-chip lasers, amplifiers, and compact modulators for dense silicon photonics. The addition of either C or Sn to Ge can modify the band structure to create a direct bandgap and adding both can improve growth quality of both C and Sn. More important for devices is the electron effective mass, $m_e^*$. In GeSn, $m_e^*$ in the direct conduction band (CB) valley ($\Gamma$) can be as small as 0.015$m_0$. When confined in a quantum well (QW), this light effective mass gets pushed up by quantum confinement to higher energies much faster than the indirect (L) CB valley, converting the quantum well back to an indirect bandgap. Therefore, quantum wells offer a stringent but necessary test of whether GeSn alloys can be made suitable for lasers and other direct bandgap photonic devices.

In this work, we grew stacks of 25 Ge$_{0.5}$Sn$_{0.5}$ quantum wells separated by Ge barriers using hybrid solid+gas source molecular beam epitaxy to yield high quality GeSn crystal growth over various temperature regimes based on previous bulk growths. The M QW structures were grown on GaAs substrates with a 300 nm Ge buffer layer. The quantum wells were 5 nm GeSn with 18.6 nm Ge barriers, ending with a 20 nm Ge cap layer. Based on samples of bulk GeSn grown under similar conditions, we estimate the QW composition to be at 4% Sn and 3% substitutional C. As reported in a separate talk (T. Dey), Raman observation of the C local mode at 530 cm$^{-1}$ from these previous growths also confirmed substitutional carbon incorporation into the QW layers. Compared with its parent GeSn bulk materials, we observed several new peaks in photoluminescence from the MOW samples, around 0.35 eV and 0.5 eV. Recent ab-initio results suggest that the mixture of C and Sn could lead to both increased and decreased bandgaps depending on nearest neighbor ordering, which may explain the multiple peaks. Further studies are underway to determine if some of the emission might also be due to defects or non-uniform QW compositions, and these will be reported at the conference.

In summary, this work presents the first growth and PL of GeSn QW's. These samples showed emission at significantly smaller photon energies, as low as 0.35 eV, compared with bulk GeSn and previous reports of Ge alloys. This emission range may be useful for LIDAR and other mid-IR light sources, as well as IR photodetectors.

11:20 AM T 04
(1) Mechanical and Electronic Effect of B on the Band Structure of BGaAs Alloys
Qian Meng1, Rasha El-Jaroudi2, Rachel C. White1, Tuinh Dey1, Mohamad S. Reza1, Seth R. Bank1 and Mark Wistey2; 1The University of Texas at Austin, United States; 2Texas State University, United States

The addition of boron into conventional III-V alloys provides a method for strain engineering of near-infrared, direct-bandgap materials and to lattice-match with silicon$^1$ and other substrates.$^2$ However, the addition of boron into conventional III-V material forms a highly-mismatched alloy whose material properties are underexplored. In other highly-mismatched alloys, such as dilute-nitrides and dilute-bismides, small amount of nitrogen or bismuth can perturb the host band structure, resulting in a reduction in the bandgap while undesirably degrading material properties. In contrast, boron is predicted to have a higher solid solubility, and B-III-V is predicted to degrade material properties less severely than other highly mismatched alloys.$^3$ This suggests that higher B concentration with superior material quality is achievable. A significant reduction in carrier mobility has been found in the dilute-nitrides and -bismides, which was attributed to alloy scattering in the band edges due to band anticrossing (BAC) and materials degradation due to growth.$^4$ In contrast, we observed a weaker reduction in carrier mobility in BGaAs compared with dilute nitrides, and the hole mobility of p-type doped B$_{85}$Ga$_{15}$As$_{0.5}$Sb$_{0.44}$ can be at around 180 cm$^2$/V·s.$^5$ Here we investigate the effects of boron incorporation on the electronic band structure of III-V alloys to determine their fundamental properties and ultimate device potential.

Theoretical calculations of the electronic properties were performed using the density function theory (DFT) package Vienna Ab initio Simulation Package (VASP) using HSE06 hybrid functionals. The influences of mechanical structure change in lattice because of the small size of the B and the influences of electronic differences between B and Ga/As were separated creating different configurations: substitutionally incorporated BGaAs; BGaAs$_{0.5}$Ga$_{0.5}$As$_{0.5}$ replace single B atom with Ga and keep the lattice constant and local distortion of substitutional BGaAs; pristine GaAs; Ga$_{0.5}$B$_{0.5}$ replace single Ga atom with B and keep the perfect zincblende structure of GaAs. We found a split conduction band minimum (CBM) created by the existence of B and the conduction band 1 (CB1) and conduction band 2 (CB2) states were changing between extended states and localized states according to the wavefunction and energy change with pressure. The band splitting and pressure-dependence are consistent with the hallmarks of band-anticrossing. The decreased lattice constant and local distortion had more influences on the band splitting and changing the lattice constant proportionally changed the bandgap, clarifying that the presence of the highly-mismatched boron atom drives the anticrossing. Further analysis of the origin of CB1/CB2 states in BGa(In)As alloys is underway and will be reported at the conference. Experimental characterization of the band splitting in BiGa(Al)As alloys, grown by solid-source molecular beam epitaxy, will also be reported.

This work was performed in part at the University of Texas Microelectronics Research Center, a member of the National Nanotechnology Coordinated Infrastructure (Nanoc), which is supported by the NSF (No. ECCS-1542159). This work was also supported by the National Science Foundation (A Ward Nos. ECCS-1933836, DMR-1508846, and CBET-1438608). The authors also acknowledge the Learning, Exploration, Analysis, and Processing (LEAP) cluster at Texas State University for computing resources.

1 M. Nicholas et al. 60th Electronic Materiais Conference (2018)

11:40 AM T05
(1) Impact Ionization Coefficients and Excess Noise in AlGaAs$_{0.2}$Ga$_{0.8}$As$_{0.15}$Sb$_{0.85}$
Avalanche Photodiodes
Harry Lewis1, Xiao Jin2, Bingtian Guo2, Seung Heun Lee2, Hyemin Jung2, Sri Harsha Kodati2, Baolai Liang4, Sanjay Krishna1, Joe Campbell2 and John David2; 1The University of Sheffield, United Kingdom; 2University of Virginia, United States; 3The Ohio State University, United States; 4California State University, Los Angeles, United States

Avalanche Photodiodes (APD) provide a very high sensitivity of -33dBm at 100Gb/s, with a
100

600nm thick multiplication region. AlGaAsSb provides advantages of reduced dark currents and increased device reliability over AlAsSb and recent research has indicated that it also exhibits very low excess noise. Unfortunately, there is currently a lack of data of the material’s impact ionization behavior across a wide electric-field range, making it difficult to design APDs for different applications. This work presents the first comprehensive analysis of the electron and hole impact ionization coefficients for AlGaAsSb, calculated from avalanche multiplication data and the excess noise characteristics, on a wide range of structures with thicknesses from ~400-1020nm. M measurements have been performed under pure electron injection conditions, pure hole injection conditions (using 455nm light), and a range of mixed injection conditions on AlGaAsSb p-i-n structures grown on InP substrates using MBE. M esa diodes were fabricated using standard wet etching and very low dark currents were obtained on unoptimized devices. M multiplication measurements were carried out using phase-sensitive detection to differentiate the photocurrent from the dark current. Excess noise measurements were performed using a transimpedance amplifier-based phase-sensitive detection system enabling measurements of multiplication >37. The ionization coefficients were extracted by fitting the multiplication data using a numerical model which takes any electric-field variations into account. These ionization coefficients are capable of replicating the multiplication data even in significantly thinner AlGaAsSb structures where the effect of the ‘dead-space’ can be observed at low multiplication values. The $\alpha/\beta$ ratio in AlGaAsSb is only slightly smaller than in AlAsSb and still much larger than other comparable semiconductors. There is a significant difference obtained in the excess noise from electron and hole-initiated multiplication, further confirming the presence of a large $\alpha/\beta$ ratio in this material system. The excess noise from pure electron injection ($F_E$) in p-i-n structures with 1020nm, 600nm and 400nm widths increases as the device width decreases. $F_E$ is obtained at multiplication values of 25, 12 and 10 in these structures as the avalanche width decreases. Note that the shape of the $F_E$ vs $M$ characteristic does not follow the classical McIntyre behaviour, suggesting that the ionization probability in these structures is not a simple exponential function. Based on the $\alpha/\beta$ ratio which changes with electric field, these multiplication regions would give a 3dB bandwidth (excluding the absorber) of 8.4GHz, 23GHz and 31.3GHz respectively for the multiplication values stated earlier. Despite the increasing $F_E$ with decreasing structure thickness, these results are still significantly better than those for InAlAs or InP. The lowest excess noise, seen in the 890nm p-i-n structure under pure electron injection conditions, gives an $F_E$ of 2.34 at a multiplication of 37. Our findings indicate that, in this alloy system, the benefit of the larger $\alpha/\beta$ ratio in thicker structures at lower electric fields will outweigh the improvement in noise performance which occurs in thin APD structures due to the effects of the carrier dead space. This offers the possibility of extremely high sensitivity 1550nm APDs for LiDAR and sensing applications as we shall show.

SESSION U: Nano-Magnetic, Magnetic Memory and Spintronic Materials

Session Chairs: Denis Candido and Pawan Tyagi
Thursday Afternoon, June 30, 2022
Great Hall Meeting Room 1 & 2

1:30 PM U01
Spin-Polarized Scanning Tunneling Microscopy of Epitaxial Fe3GeTe2
Alexander J. Bishop, Robert Walko, Wenyi Zhou, Jay Gupta and Roland Kawakami; The Ohio State University, United States

In recent years Fe3GeTe2 (FGT) has become an exciting material due to its perpendicular magnetic anisotropy and high Curie temperature while maintaining a 2D van der Waals structure. These properties have led to the manifestation of skyrmions and room temperature ferromagnetism in exfoliated FGT heterostructures and thin films. A new mechanism for the manifestation of skyrmions and room temperature ferromagnetism in exfoliated FGT heterostructures and thin films. A new mechanism for the manifestation of skyrmions and room temperature ferromagnetism in exfoliated FGT heterostructures and thin films.

1:50 PM U02
(Graduate) Kinetically-Controlled Epitaxial Growth of vdW Fe3GeTe2 Ferromagnets and Their Heterostructures with Topological Insulators
Wenyi Zhou, Alexander J. Bishop, M englin Zhu, Igor Lyalin, Shuyu Cheng, Jinwoo Hwang and Roland Kawakami; The Ohio State University, United States

As a 2D van der Waals material, Fe3GeTe2 (FGT) stands out because of its strong perpendicular magnetic anisotropy and high Curie temperature ($T_C$). A lot of interesting phenomena have been studied in FGT thin films and heterostructures, such as skyrmions and room temperature ferromagnetism. However, most studies are based on exfoliated FGT. Here, we utilize molecular beam epitaxy (MBE) for high-quality epitaxial monolayer and multilayer FGT. Cross-sectional transmission electron microscopy (TEM) shows an atomically-sharp interface between the FGT film and Ge(111) substrate. Our study also demonstrates that the magnetic interaction between magnetic molecules and FM electrodes' type, thermal energy, and several other factors play an important role in the epitaxial growth of FGT films by MBE. By varying the deposition rate, we observe control the formation or suppression of an initial tellurium-deficient non-van der Waals phase (Fe3Ge) prior to realizing epitaxial growth of the vdW FGT phase. This demonstrates how the interplay of energetics and kinetics can help tune the re-evaporation rate of chalcogen atoms and interdiffusion from the underlayer, which paves the way for future studies of van der Waals epitaxy.

In addition, we developed heterostructures with topological insulators such as FGT/Bi2Te3 and FGT/SnTe which are very interesting for spin-orbit torque and magnetic topological phases. M agneto-optic Kerr Effect (M OKE), magnetic circular dichroism (MCD) and Anomalous Hall Effect (AHE) were used to confirm square hysteresis loops and M OKE microscopy made it possible for us to catch a glimpse of its domain structure during magnetization switching.

This work is supported by A FOSR MURI 2D MAGIC (FA9550-19-1-0390), DOE (DE-SC0016379), NSF-M RSEC (DMR-2011876), DARPA (D18A P00008).
Magnetic skyrmions are ideal bits for next generation information storage due to their small size, low depinning current, and topological stability. Co/Si/Pt heterostructures are a promising platform to host small skyrmions because of the system’s tunability. In our work, we use spin polarized Scanning Tunneling Microscopy (STM) on Co/Cu/Co heterostructures to detect and characterize individual skyrmions at cryogenic and room temperatures. We grow our heterostructures with molecular beam epitaxy and keep them under ultra-high vacuum to preserve the surface’s quality. Topographic STM images of the surface show small granular domains with a typical diameter of 30 nm; the surface is atomically flat even over 10-100’s of μm with a variation of grain heights of less than 1 nm. Spinned polarized STM, with a magnetic Ni tip, can detect skyrmions through differential conductance measurements. Our differential conductance scans reveal skyrmions as small as 30 nm in diameter. We have preliminary evidence of tip-induced motion of skyrmions. Future high resolution (–k) images will allow us to identify pinning sites and study the energetics of skyrmion motion, creation, and annihilation.

We acknowledge funding support from the DARPA TEE program (award #D18AP00008).

2:00 PM U03
(Student) Spin Polarized STM Imaging of Magnetic Skyrmions in Metallic Thin-Film Heterostructures Brad Goff, Jake Repicky, Shuyu Cheng, Roland K awakami and Jay Gupta; The Ohio State University, United States

Magnetic skyrmions are ideal bits for next generation information storage due to their small size, low depinning current, and topological stability. Co/Si/Pt heterostructures are a promising platform to host small skyrmions because of the system’s tunability. In our work, we use spin polarized Scanning Tunneling Microscopy (STM) on Co/Cu/Co heterostructures to detect and characterize individual skyrmions at cryogenic and room temperatures. We grow our heterostructures with molecular beam epitaxy and keep them under ultra-high vacuum to preserve the surface’s quality. Topographic STM images of the surface show small granular domains with a typical diameter of 30 nm; the surface is atomically flat even over 10-100’s of μm with a variation of grain heights of less than 1 nm. Spinned polarized STM, with a magnetic Ni tip, can detect skyrmions through differential conductance measurements. Our differential conductance scans reveal skyrmions as small as 30 nm in diameter. We have preliminary evidence of tip-induced motion of skyrmions. Future high resolution (–k) images will allow us to identify pinning sites and study the energetics of skyrmion motion, creation, and annihilation.

We acknowledge funding support from the DARPA TEE program (award #D18AP00008).

2:30 PM U04
(Student) Tuning Magnetic Properties of [Pt/Co/Cu] Multilayers Shuyu Cheng1, Nuria Bagues Salguero2, Camelia Selcu1, Binbin Wang2, Ziling Li3, Shekhar Das4, David M Combr2, Chris Hammel5 and Roland K awakami2; The Ohio State University, United States; 2Ohio State University, United States

Skyrmions, which are nanometer-sized vortex-like magnetic textures, stand out as a strong candidate for next-generation information storage and processing. The main advantages of skyrmion-based devices are topological robustness, high energy efficiency, and small sizes. Using molecular beam epitaxy (MBE), we have successfully synthesized [Pt/Co/Cu] magnetic multilayers, a skyrmion-hosting material. The broken inversion symmetry in this type of material gives rise to non-zero Dzyaloshinskii-Moriya interaction (DMI), which plays a key role in skyrmion formation. We have established the connection between the sample structure (thickness of each layer and number of periods) and magnetic properties revealed by magneto-optical Kerr effect (MOKE) measurement. Based on these results, we are able to engineer the sample structure to tune various magnetic interactions (exchange interaction, interfacial magnetic anisotropy, magnetic shape anisotropy, DM, etc.) and controllably generate skyrmions in our designed multilayer samples. The room-temperature skyrmions have been observed in these samples by magnetic force microscopy (MFM) and Lorentz transmission electron microscopy (LTEM). Furthermore, we have also successfully realized skyrmions nucleation/motion by applying current pulses.

2:50 PM U05
(Student, Late News) Electromagnetic Interference (EMI) Shielding Techniques for Simulated PVDF-TrFE/FEOx M ultiferroic Monopolar Antenna Richard L. Harry, Shaik Zainuddin and Shaik J eelan; Tuskegee University, United States

Magneto-electric materials have widely been used as a conducting medium for monopolar, dipolar, and conical antennas based off of their interaction with electromagnetic fields and transverse wave absorption properties. Upon application, these antennas tend to perform extraordinary due to their tailorability properties at a nanoscale, and have opened doors for many applications in large scale sensor, detection, and radar systems. In this study, we investigated the potential of nanocomposite films made from PVDF-TrFE/FEOx loaded with SWNMs and 3wt% Fe3O4 nanoparticles as receiving microstrip patch antennas. Simulation of device was conducted using 2021 ANSYS HFSS software. Electronic properties such as electro-conductivity, magnetic permeability, dielectric constant, elastic modulus, and loss values of nanocomposites were incorporated to model storage/reflectance behavior under increasing electromagnetic frequencies up to 5GHz.

3:00 PM Refreshment Break

3:30 PM U06
(Student) The Effect of Spin Fluctuations on Temporal and Spatial Evolution of Magnetic Moment in A Magnetic Tunnel Junction-Based Molecular Spintronic Device (MTJ MSD) M arzieh Savadkoohi, Bishnu R. Dahal, Christopher D’Angelo, Andrew C. Grizzle and Pawan Tyagi; University of the District of Columbia, United States

Spintronics in conjunction with molecular electronics can lead to the development of quantum computers and highly efficient logic and memory devices [1]. Spin is an intrinsic property of atoms that exist in infinite states compared to electric charges which are available only in a binary state. Superposition of spin-up and spin-down states enables computational devices to function much faster than today’s computers. They can also increase hard drives’ storage capacity significantly. Spintronic properties can be tailored with organic molecules. Controlling and manipulating electrons’ spin of ferromagnetic (FM) materials via magnetic molecules can lead to novel magnetic phenomena and numerous computational applications.

Here, we report the preliminary result of our computational and experimental study on a magnetic tunnel junction-based molecular spintronic device (MTJ MSD). Using Monte Carlo Simulations (MCS) we have simulated an MTJ MSD composed of two ferromagnetic layers separated by a nano-scale insulator and magnetic molecules attached to the exposed edges of the device [2-4]. The interaction between magnetic molecules and FM electrodes, strengths and nature of couplings, molecules and electrodes’ type, thermal energy, and several other factors play important role in defining MTJ MSD ultimate properties. In our previous research, we have shown that the strength and nature of Heisenberg exchange coupling between magnetic molecules and FM layers dictate MTJ MSD’s magnetic properties [5]. Here, we are investigating the effect of spin fluctuations on MTJ MSD’s magnetic moment and other physical properties such as heat capacity.

Our MCS preliminary results showed that spin fluctuations impact temporal and spatial evolution of magnetic moment of MTJ MSD at room temperature. The magnetic instability caused by spin fluctuation also increased MTJ MSD’s heat capacity when molecules made FM coupling with both electrodes, antiFM coupling with both electrodes and FM coupling with one electrode, and antiFM coupling with another electrode. Our computational work agrees with the experimental research in which MTJ MSD was exposed to the external magnetic field. A cooling to our observations, MTJ MSD produces a symmetric hysteresis loop with saturated magnetic moment on both negative and positive range of applied field. The low magnetic coercivity represents a soft magnetic behavior in the presence of spin fluctuation. To gain a better insight we will use MCS to investigate MTJ MSD magnetic behavior in the presence and absence of spin fluctuations for both parallel and antiparallel molecule-FM electrodes couplings.
Molecular spintronics is gaining attraction because molecules possess a weak spin-orbit coupling and longer relaxation time[1]. Therefore, molecular spintronics devices (M SD) are considered highly promising for the future of quantum computing technology. However, the fabrication of robust and mass-producible M SD at the nanoscale is a major concern[2]. To overcome this issue, we have designed a magnetic tunnel junction-based molecular spintronics device (MTJ M SD). An MTJ M SD utilizes a tunnel barrier to ensure a robust and mass-producible physical gap between two ferromagnetic electrodes. Molecular device channels are covalently bonded between two ferromagnets across the insulating barrier. MTJ M SD approach may benefit from MTJ's industrial practices; however, the MTJ M SD approach still needs to overcome additional challenges arising from defects of nearly 4 nm thin insulating layers[3]. An insulating barrier may possess a variety of potential defects arising during the fabrication or operational phase. This study describes the Taguchi Design of Experiment (DOE) approach to make robust AIO insulator between two ferromagnetic layers. The DOE parameters for AIO, insulator deposition were sample position, deposition rate, deposition power, the flow rate of Ar/O2 inside the sputtering chamber, pressure of the chamber, and argon-etching rate and wait time after etching. Based on the DOE approach, we tailored the most appropriate parameters to fabricate the robust insulator. We successfully achieved a >95% yield of robust 4 nm tunnel barrier with 20-40 nA tunneling current at 100 mV to serve as testbed for MTJ M SD realization. In this paper, we will present the experimental data based on the electrical and magneto-transport properties of MTJ and its effect on the transport properties after creating the conducting molecular channel between two ferromagnetic electrodes.

This research is supported by National Science Foundation-CREST Award (Contract # HRD-1914751), Department of Energy/ National Nuclear Security Agency (DE-FOA-0003945).


is accomplished by a conceptually new approach of defect-engineered remote spin filtering and amplification of InAs quantum-dot (QD) electrons via an adjacent tunneling-coupled GaNAs quantum well acting as a spin filter. The extraordinary spin filtering effect in GaNAs is enabled by spin-dependent recombination via spin-polarized defects, i.e. grown-in Ga self-interstitials, which selectively deplete conduction electrons with an opposite spin orientation to that of the defect electron. In sharp contrast to the general trend of deteriorating spin polarization with increasing temperature seen in all other approaches of spin generation, our approach is gifted with an opposite temperature dependence up to RT thanks to a thermally accelerated remote spin-filtering effect as a result of thermally activated recombination via the defects. We further show that the QD electron spin can be remotely manipulated by spin control in the adjacent spin filter, paving the way for remote spin encoding and writing of quantum memory as well as for remote spin control of spin-photon interfaces. The fact that the demonstrated spin functionality is implemented in a commonly used semiconductor optoelectronic nanostructure system (i.e. InAs/GaNAs QDs) based on the mature GaN technology can greatly facilitate the integration of spin functionalities with the existing electronic and photonic devices. It could also pave the way for a range of potential applications based on opto-spintronics exploiting the state-of-the-art GaN technology platform, such as spin-LEDs, spin lasers, spin-polarized single-photon sources, spin-photon interfaces, spin qubits, etc. This work demonstrates the feasibility to implement opto-spintronic functionality under practical device operation conditions in a semiconductor nanostructure system based on the mature III-V semiconductor technology commonly used for today’s optoelectronics and photonics.


SESSION V: Group III-Nitrides—Light Emitting Diodes

Session Chair: Theeradetch Detchphrom
Thursday Afternoon, June 30, 2022
Great Hall Meeting Room 3

1:30 PM V01
(Student) Enhancing the External Quantum Efficiency of Micro-LEDs via Optimized Dry Etecching Condition [maohwun Park1, Heajung Cheong2, Y. asuhisa Ushida3, Yuta Furusawa3, Tae-Yeon Seong2, and Hiroshi Amano2; 1Nagoya University, Japan; 2Nagoya University, Nagoya, Japan; 3Department of Materials and Systems for Sustainability (IMaS), Nagoya University, Nagoya, Japan]

Micro- and nano-scale light-emitting diodes (µLEDs) based on III-V compounds can realize next-generation displays with attractive properties, such as high resolution, long lifetime, and low power consumption. Even though µLEDs have better physical properties than organic LEDs, performance issues such as external quantum efficiency (EQE) remain as the LED chip size decreases due to plasma damage at the sidewall. To overcome this issue, chemical treatment or passivation layer deposition have been reported by many researchers; however, these methods require additional processes after dry etching. In this study, we evaluated the influence of dry etching conditions on the performance of µLEDs. We found that the chemical reaction between Cl2 (i.e., etching gas) and GaN dominated the etching process, rather than physical plasma etching, as the dry etching power (PBA) decreased during the mesa fabrication process. The dominant effect of the chemical reaction led to low plasma damage on the etched GaN surface and created a rough sidewall morphology. This effect is shown in Figure 1a. It was observed that the maximum external quantum efficiency (EQE) differed depending on etching bias and were 3.23%, 2.65%, 2.43%, and 2.25% for 2.5 W, 5 W, 15 W, and 30 W, respectively as shown in Figure 1b, which behavior enhancing maximum EQE could be attributed to the suppressed plasma induced sidewall damage on micro-LED; thus, the EQE improved without requiring an additional process. The effect of low PBA was further investigated by cathodoluminescence using various substrates, demonstrating that low PBA is related to the chemical reaction; that will be explained in the presentation in detail.

1:50 PM V02
(Student) Impact of Photon Recycling on Absorption Losses in Tunnel Junction-Based III-Nitride LED Structure [Ahmed A. Awwad, Betty L. Anderson and Siddharth Rajan; The Ohio State University, United States]

III-Nitride light emitting diodes have been successfully adopted in visible display and illumination applications, and are very promising for ultra-violet wavelength applications. Tunnel junctions can provide the significant advantages of an operation of both visible (for multiple active region LEDs) and UV LEDs (to act as transparent spreading layers). Recent work on tunnel junctions have demonstrated excellent characteristics for both GaN, as well as ultra-wide bandgap AlGaN. A though tunnel junctions (TJs) have been demonstrated with excellent electrical efficiency, and low voltage drop, especially for GaN-based LEDs, the absorption introduced by them has not been well-understood. Design of tunnel junctions for low voltage drop often requires the use of ultra-thin layers of lower bandgap material (such as InGaN) which could have substantial absorption at emission wavelengths. Previously used methods to calculate tunnel junction absorption losses, such as ray tracing and finite-difference time-domain (FDTD) [1] do not take into account photon recycling in the TJ. In this work we propose a theoretical model that can provide an intuitive understanding of the impact of photon recycling on the optical absorption losses in tunnel junction-based LEDs. The proposed model is derived using a 1-dimensional N-cascaded GaN LED structure. The top metal contact is considered as a perfect reflector, and the output optical power is collected at the bottom side. GaN layers are assumed to be transparent, while any power absorbed by the TJ is recycled by generating an electron-hole pair (EHP) that is injected back to the active region to recombine there. The efficiency, η, by which the generated EHPs produce new photons in the active region is assumed to be the mathematical product of the IQE and the injection efficiency. The proposed closed form model takes into account the infinitely repeated photon recycling process. The model enables an estimate of the normalized light extraction efficiency, and can be compared with estimates from simple ray tracing model single and cascaded multiple active region TJ LEDs. It is shown that as the number of TJs increases and/or its absorption increases, the recycled power increases. Consequently, while ray tracing models would predict significant absorption losses, taking into account photon recycling shows that the effective loss is significantly lower. The model can also describe the impact of the internal quantum efficiency on the effective light extraction efficiency. For InGaN polarization engineered TJs, a comparison between the two models at various Indium compositions and thicknesses shows that for In0.23Ga0.77N TJ LED, ray tracing model predicts absorption losses that are significantly higher. For example, for 3 nm 24% In-content tunnel junction, the ray tracing model predicts total absorption loss of 7.95%, whereas the loss including the photon recycling is only 2.94%.

In summary, our work shows that absorption effects in tunnel junctions can be significantly overestimated if photon recycling is not taken into account. The work presented enables rational design
of tunnel-junction based LEDs with accurate estimation of absorption losses. 


2:10 PM V03 (Student) High In-Content InGaN Platelets as Underlayer for Light-Emitting Diodes Toward Long Wavelength Application Wintao Ca,1, Yuta Furusawa,1, Jeong-Hwan Park,2, Heajeong Cheong,1, Shugo Nitta,2, Yoshiro Honda1 and Hiroshi Amano1,2,3,4,1 Nagoya University, Japan; 2 Institute of Materiales and Systems for Sustainability (IMASS), Nagoya University, Japan; 3 V enture Business Laboratory, Nagoya University, Japan; 4 Akaiki Research Center, Nagoya University, Japan.

It was both theoretically and experimentally proved that the growth of InGaN quantum wells (QWs) on InGaN underlayer (x > y) would significantly improve the light emitting diodes (LEDs) performance, attributing to the reduction of non-radiative recombination centers, the decline of the internal electrostatic field, and the improvement of indium composition uniformity in QWs. Moreover, the reduced lattice mismatch between QWs and underlayer greatly suppresses composition pulling effect, which improves indium incorporation rate grown at the same temperature, resulting in In-rich InGaN with highly crystalline. However, to serve as templates of red emission QW, a thicker InGaN pseudo-substrate with closer indium mole fraction to QWs grown beyond the critical layer thickness is desired.

In this work, we present an approach to achieve a sub-micron size InGaN underlayer with high to 30 % indium composition, while the thickness is around 90 nm, far exceeding the critical layer thickness of such In-rich InGaN layer on planar c-plane GaN (reported less than 5 nm). The InGaN platelet is demonstrated by selective area growth (SAG) on arrays of GaN seed from circle openings with a diameter of 400 nm in a SiN mask. To our best knowledge, SAG of InGaN results in random nucleation and uneven shape due to the low diffusion length of gallium precursor at relatively low growth temperature. It was reported that the selectivity of InGaN can be enhanced by introducing pyramidal shaped GaN seed first, resulting in InGaN pyramid. However, the local indium composition fluctuation on the semipolar facet of the InGaN pyramid hinders pure red emission of QWs with small full width at half maximum (FWHM). In this work, planar polygonal shape of GaN seed was introduced first before SAG of InGaN, leading to the formation of uniform InGaN platelets with c-plane domain morphology. The optical properties of the InGaN platelets were characterized by photoluminescence (PL) excited by a He–Cd laser of 325 nm, 15 mw, room temperature), showing PL peaks around 530 nm with FWHM of 141 meV, suggesting around 30 % indium incorporated. A FM scan of the top c-plane surface of the InGaN platelet indicates an atomically flat surface without v-pits or trench defects while the thickness is over 90 nm. Cross-sectional TEM characterization of InGaN platelet suggests homogenous crystalline and sharp interface between InGaN and GaN seed.

According to localized EDX line measurements recorded with the same area, the InGaN platelet shows indium composition almost linearly increased from InGaN/GaN interface to c-plane surface. Detailed line profiles show indium composition of 25 % to 30 % at the top surface and 15 % to 20 % at InGaN/GaN interface. Such high indium-content InGaN platelets are competitive candidates for the development of high-quality yellow-to-red emission InGaN micro-LED, by increasing the indium incorporation rate and reducing the lattice mismatch for later In-rich quantum wells.

2:30 PM V04 (Student) Significant Improvement in Quantum Efficiencies and Wall-Plug Efficiency of Flexible AlGaN-Based Deep-Ultraviolet Light-Emitting Diodes M Iad Yarali1,2,1, Sara Pouladi1,1, Shahab Shervin1,1, Hanyoul Ryu1,1, Ja Yeon Kim3,4, Min-Ki Kwon1 and Je-Hyun Ryu1,1;1 University of Houston, United States; 2Inha University, Korea (the Republic of); 3 Korea Photonics Technology Institute (KOPTI), Korea (the Republic of); 4 Chosun University, Korea (the Republic of).

AlGaN-based deep ultraviolet light-emitting diodes (DUV LEDs) are considered as the foremost promising candidate for environment-friendly DUV light sources. III-N-based LEDs with the emission wavelength range of 400 - 200 nm (UV A, UV B, and UVC) can be produced only by adding aluminum nitride (AlN) to the GaN alloy system. As a result, emitted photon wavelength becomes as short as 210 nm. DUV LEDs are potentially powerful, harmless to the ecosystem, and can display extremely long lifetimes. Its remarkable properties assign DUV-LEDs as a key enabling segment for various new applications that cannot be accessed by regular UV sources such as food and medical equipment sterilization, water and air purification, plant lighting, and non-line-of-sight communication. Nevertheless, the current status of DUV LEDs is not mature enough and they suffer from low efficiency and optical power therefore significant improvement is highly needed in the performance of these devices. The highest external quantum efficiency (EQE) of DUV LEDs reported so far is less than 10%. Spontaneous polarization and strain-induced or piezoelectric polarization charges exist in the active region leading to Quantum Confined Stark Effect (QCE) in which the conduction and valence bands are tilted thus electron and hole wave functions are separated leads to less radiative recombination and poor internal quantum efficiency. On the other hand, a small barrier height exists as a consequence of QCE and electrons leaking from the active region. Meanwhile, the tendency of photon emission mode changes from transverse-electric (TE) mode to transverse-magnetic (TM) mode when mole fraction of AlN is getting higher in ternary AlGaN heterostructure resulting in low light extraction efficiency (LEE). All these technical challenges hinder the progress to fully replace widely used toxic mercury UV lamps.

In this study, we report a new approach to fabricate and characterize flip-chip AlGaN based DUV LED by introducing flexibility to the device to mitigate QCE, improve barrier height for electron leakage, and enhance TE polarized mode of emission by external strain applied in the flexible structure. The device consists of n and p types AlGaN active region, and p-GaN as a p-contact layer, all grown on a sapphire substrate. This rigid substrate is lifted off via laser lift-off process then the device is flipped and a thick layer of copper is electroplated as a flexible substrate. We investigate the effect of bending degree on the device performance and according to the simulation results, the device gets the highest IQE, LEE, and wall-plug efficiency when it is bent upward with a radius of 2.5 mm. Additionally, we report the ohmic contact configuration on N-face Al-rich n-AlGaN for the first time. This high efficiency flexible AlGaN-based DUV LED has great potential to replace conventional UV light sources since the performance is significantly improved.
SESSION W: Group III Nitrides—MBE, CVD and Sputtering
Session Chair: W. Alan Doolittle
Thursday Afternoon, June 30, 2022
Great Hall Meeting Room 3

3:30 PM W01
(Student) Observation of Compositional Modulation in AlGaN Self-Assembled Superlattices by Transmission Electron Microscopy K esuke Motoki, Zachary Engel, Christopher M. Matthews and W. Alan Doolittle; Georgia Institute of Technology, United States

AlxGa1-xN, AlxGa1-xN, and AlxGa1-xN superlattices (SLs) have been studied with interest for strain relief layers, defect reduction buffers, high-performance ultra-violet (UV) light emitting diodes (LEDs) and distributed Bragg reflectors (DBRs). SLs typically require compromises in growth conditions such as changes in metal fluxes and substrate temperatures for each SL layer and these growth interrupts involve undesired accumulation of contaminants at the interfaces leading to a loss of optical emission and/or creating structural defects in the film. Furthermore, strain from lattice mismatch in the SLs can cause plastic deformation and is thought to be exaggerated by growth interrupts. Therefore, eliminating the interrupts is key for improving the film quality. Material modulated Epitaxy (MME) has demonstrated its ability to grow self-assembled SLs (SASLs) at a growth rate of 1 μm/hour, providing uninterrupted rapid growth of abrupt and coherent SLs by using a shuttered scheme on the metal effusion cells (Al and Ga) in a metal-rich condition using surface segregation to achieve composition steps1. This method facilitates the design of the period, thickness, and compositions of the well and barriers in the SLs. However, structural information, detailed compositional distributions, and its mechanisms for the creation of SASLs are not well known up to now. Transmission electron microscopy (TEM) is used to provide detailed examination of the composition changes, coherency and unintentional compositional modulation within the SASLs. Unintentionally doped (UID) MME SASL AlGaN films were grown on MBE AlN on hydride vapour phase epitaxy (HVPE) AlN templates on c-plane sapphire substrates as described elsewhere2. Using plasma-assisted molecular beam epitaxy (PA-MBE), the thickness and coherency of the AlGaN SASLs have been investigated by TEM. The cross-sectioned sample is prepared by standard mechanical polishing methods, followed by argon ion milling. High-resolution (HR) TEM images close to [1 -1 0] zone axis shows highly coherent SASLs of 910 nm total thickness consisting of 13 nm periods of Al0.12Ga0.88N barriers and Al0.25Ga0.75N wells for a film grown at 2.8 μm/hour. This period thickness corresponds with the amount of material grown per shutter cycle, TEM images with a two-beam condition g = {0 0 0 2} show large contrast between Al-rich (bright) and Ga-rich (dark) layers. The thickness of the Al-rich layer is 10 ±1.5 nm and the Ga-rich layer is 3.5 ±1.5 nm. A finer contrast modulation, on the order of ~2 nm within the Al-rich layer is also observed in the image and in the line intensity scan corresponding to unintentional compositional modulation along the growth direction during the MME cycle where both Ga and Al metal shutters are open. Such a compositional modulation has not been previously observed in MME grown films. A strain map calculated from 4D-STEM shows strain relaxation in both and direction in the SASLs especially near dislocations suggesting the SASLs are effective in modifying defect structures. Further investigation quantifying the compositions and strain in the AlGaN SASLs are ongoing.


3:50 PM W02
(Student) Molecular Beam Epitaxial Growth of AlGaN Epilayers on Si Using a Nanowire Template Qibin Zhang, Xue Yin, Eli M. Ardel, Heemal Parimoo and Songrui Zhao; McGill University, Canada

A aluminum gallium nitride (AlGaN) on silicon (Si) represents a technologically important platform, not only for the ultraviolet, direct, and tunable bandgap energies of AlGaN alloys, but also for the advantages of Si substrate such as low cost, easy removal by chemical wet etching, and so on. However, owing to the large lattice mismatch between AlGaN alloys and Si, obtaining high quality AlGaN epilayers on Si remains to be a challenge in the field. This is in particular the case for the growth of AlN epilayers on Si. In this context, we present a new method of growing AlGaN epilayers on Si by molecular beam epitaxy. Such a method involves the usage of a thin nanowire template. The growth of AlN epilayers is described first. Such AlN epilayers are grown in nitrogen- (N-) rich conditions; and compared to the typical growth conditions of AlN nanowires on Si, the AlN growth temperature promotes the coalescence of AlN [1]. This coalescence is reflected by the appearance of streaky pattern from the reflection high-energy electron diffraction (RHEED). Characterizations using electron microscopes and atomic force microscopy (AFM) further indicate a relatively smooth surface can be obtained within a small thickness (~200 nm), with a root-mean-square (rms) roughness of ~2 nm, within the range of typical AlN nitride epilayers grown in N-rich conditions. RHEED 3x3 reconstruction and potassium hydroxide (KOH) etching experiments further indicate that the AlN epilayers are N-polar. Using such AlN epilayers as a buffer layer, the growth of AlGaN epilayers is further demonstrated. The AlGaN epilayers in this case are also grown in N-rich conditions and are found be of AlN as well, following the polarity of the AlN epilayers underneath [2]. The rms roughness of such AlGaN epilayers is similar to that of AlN epilayers. Current progress on a more detailed growth investigation of AlGaN epilayers and recent deep ultraviolet (UV) light emitting devices development will be presented as well.


4:10 PM W03
(Student) Transition-Metal-Alloyed Group-III-Nitride Piezoelectric Thin Films Grown by Hybrid Chemical Vapor Deposition and Sputtering Deposition Techniques Mina Moradi, Sara Pouladi, Nam-In Kim, Rebecca Forrest and Jae-Hyun Ryu; University of Houston, United States

Transition-metal alloyed III-V nitride thin films have been considered because of their significant impact on the enhancement of the piezoelectric properties in Group III-N (III-N) films, such as wurtzite AlN, by group IIIb transition metals. For example, Sc incorporation as an alloying element to substitute aluminum (Al) in wurtzite-structure AlN, forming ScAlN, is a promising approach to improve the piezoelectric coefficients of AlN-based materials on the piezoelectric devices to enhance their performance, hence extending their applications in wireless communication, sensors, mechanical energy harvesting, and semiconductor-based ferroelectrics. Several deposition techniques have been employed to grow the transition-metal-alloyed III-N films. We are focusing on the DC reactive magnetron sputtering system and a new hybrid chemical vapor deposition (HybCVD) thin film growth method. The ScAlN deposited thin film by the physical vapor deposition of the sputtering technique relies on a
dual target sputtering method using an aluminum target and a scandium target, which are sputtered at the same time. The HybCVD is a CVD with a combination of different types of precursors. Hydride vapor phase epitaxy (HVPE) has been employed for the alloying of group-IIIa elements, such as AlGaN. However, this technique cannot be extended to III-N with transition metal alloys, due to the problems related to the chloride form of Sc. Therefore, the new HybCVD employs chloride, elemental source, and hydride for the precursors of the group-III element, transition-metal element, and nitrogen, respectively, for ScAIN thin films to address the issue regarding the HVPE growth method. The phase equilibria between transition-metal nitride (ScN) and III-N (AIN) to form ternary alloy system, such as ScAIN, show a phase separation with the formation of cubic rock-salt structure ScN in wurtzite III-N film with increasing alloy composition of transition-metal nitride, resulting in degradation and eventually the disappearance of its piezoelectric properties. HybCVD growth method provides accurate control of alloy composition along with the high crystalline quality required in designing highly functional piezoelectric materials. In this regard, we numerically investigate the thermodynamics of precursors and vapor-solid reactions on the alloy composition of ScAl1-xN by HybVPE. The equilibrium partial pressures of the gaseous species and the driving force for AlN and ScN solid composition at various temperatures, reaction gases, and partial pressure of hydrogen in the carrier gas have been thermodynamically calculated in source and growth zones. Equilibrium partial pressures of gaseous species over Al metal in the Al source zone can be controlled at different values of temperature which suggests the temperature range of the source zone up to 620 °C to avoid any damage to the CVD furnace. The reaction in the Al source zone happens below 620 °C to produce enough partial pressure of AlCl3 as the desired group III input from the Al source zone for AlN deposition in the growth zone. Elemental Sc source precursor is capable to provide high precursor input and enough driving force for the ScN formation. According to the thermodynamic calculations, the Sc composition in the alloy can be accurately controlled by the mixture ratio of the cation precursors. Here, the combination of M OCCVD and HVPE growth methods simultaneously provides well control on the uniformity and quality of piezoelectric films based on transition-metal-alloyed III-N materials.

4:30 PM W04  
(Stud)ent Use of a TIN Seed Layer to Enhance (0002) Epitaxy and Piezoelectric Coupling of AIN Thin Films  
Zhehua Li, Morton Greenslitt, Mauricio P. da Cunha and Robert J. Lad; University of Maine, United States

A aluminum nitride remains piezoelectric up to at least 1000°C and has higher phase velocity than other high temperature piezoelectrics such as langasite and potential for reduced acoustic loss. The ability to grow epitaxial (0002) oriented AIN thin films using PV D techniques makes these attractive materials for use in bulk acoustic wave (BAW) or surface acoustic wave (SAW) sensors that can operate in high temperature harsh environments. High quality epitaxy of AIN (0002) grain growth has been reported on single crystal sapphire and GaN substrates by several groups. In this work, we report on the use of an ultrathin TIN seed layer that targets the formation of AIN (0002) oriented grains independent of the underlying substrate.

TIN seed layers were grown on different substrates including sapphire, silicon, M o, steel and Inconel by using nitrogen plasma-assisted e-beam evaporation of Ti at a growth temperature of 930°C. A highly textured TIN (111) seed layer was formed as confirmed by high-resolution x-ray diffraction and in situ RHEED. AIN (0002) oriented films were grown on the TIN seed layers using nitrogen plasma-assisted e-beam evaporation of A I also at a growth temperature of 930°C. The TIN seed layer on sapphire induced a larger population of (0002) grains and a reduction in the mosaic grain spread compared to growth of AIN on thermally nitride sapphire without the TIN layer. The enhancements in AIN (0002) epitaxy can be attributed to the highly textured growth of TIN (111) grains and the 1.8% lattice mismatch between (0002) AIN and (111) TIN. In situ RHEED and X-ray diffraction pole figures verify the highly oriented AIN (0002) grains as well as in-plane texture of the nucleated AIN grains.

The degree of piezoelectric coupling of AIN films grown on the TIN seed layers was evaluated by measuring the acoustic responses from surface acoustic wave resonator (SAWR) devices fabricated using the epitaxial AIN films. By measuring the reflection coefficient (S11) frequency response from one-port SAWR devices, the admittance, conductance, susceptance, and electromagnetic coupling coefficient (K2) were determined. The addition of the TIN seed layer led to a doubling in K2 value compared to AIN growth on c-sapphire alone. The TIN seed layer can be used to induce AIN (0002) epitaxy and piezoelectric coupling on other substrates as well.

4:50 PM W05  
(Stud)ent Sputter Deposition of III-N Thin Films  
Josue Noriega1, Ramón Collazo2, Zlatko Sitar3 and Jon-Paul Maria3; 1The Pennsylvania State University, United States; 2North Carolina State University, United States

In this presentation, we demonstrate that reactive High-Power Impulse Magnetron Sputtering (HiPIMS) is an effective alternative for depositing high quality, epitaxial III-N thin films. In contrast to conventional direct current (DC) or radio frequency (RF) sputtering, HiPIMS provides the needed kinetic energy and ionization fraction to establish a sufficiently reactive environment to promote full nitridation. Specifically, the low duty cycle regime of HiPIMS provides access to kW/cm² peak power densities without target degradation and thus dramatically increased metal reactivity. In addition, adding an opposite polarity voltage pulse between the target bombarding events, known as a kick pulse, further allows one to tailor both the adatom landing energy on the substrate surface, and mitigate target poisoning.

This unique capability set enables us to prepare high crystal quality epitaxial InN thin films with low out-of-plane mosaicity and electron mobilities in excess of 400 cm²/Vs with a step-and-terrace microstructure when deposited on AIN-nucleated sapphire substrates. InN grows epitaxially strained and the electron concentration decreases with increasing film thickness in films up to about 200 nm until significant cracking is observed.

In addition, homoepitaxial GaN thin films can be deposited at temperatures below 600°C with smooth surface morphologies characterized by c<2 steps and terraces. The presentation will focus on the relationships between sputtering parameters and III-N thin film crystal quality, surface morphology, and growth rate.
designing highly functional piezoelectric materials. In this regard, composition along with the high crystalline quality required in and eventually the disappearance of its piezoelectric properties.

The phase equilibria between transition-metal nitride ScAlN thin films to address the issue regarding the HVPE growth element, transition-metal element, and nitrogen, respectively, for growth temperature of 930°C.

ScAlN thin films to address the issue regarding the HVPE growth element, transition-metal element, and nitrogen, respectively, for growth temperature of 930°C. Therefore, the new HybCVD employs chloride, transition metal alloys, due to the problems related to the chloride loss. The ability to grow epitaxial (0002) oriented AlN thin films has higher phase velocity then other high temperature

The TiN seed layer on sapphire induced a larger population of TiN (111) grains and the 1.8% c/2 steps and terraces. The presentatio

Epitaxially-grown III-V semiconductor nanostructures — quantum dots (QDs) in particular — are considered nearly ideal single- and entangled-photon emitters for applications in quantum information technologies. They offer high efficiencies, ease of integration with existing photonic/electronic components and hold records for photon purity and indistinguishability. State-of-the-art approaches for realizing III-V QDs include: (I) the Stranski-Krastanov (SK) growth mode, where the strain between a substrate (e.g., GaAs) and QD material (InAs) leads to 3-dimensional island formation; and (ii) the droplet epitaxy (DE) method which uses the controlled crystallization of metal nanodroplets into nanostructures. While both techniques have their individual merits, epitaxial QDs are currently at a disadvantage in three areas: lack of control over size/shape, location; SiQDs need specific material combinations leading to a limited emission wavelength range; DE QDs suffer from low efficiencies. To that end, research into alternative methods of realizing epitaxial nanostructures is relevant and ongoing. In this work, we present an in-situ etching technique using arsenic (As2) to form nanostructures on III-V surfaces.

As2 is known to aggressively react with GaSb through both an anion exchange reaction and an isoelectronic AsSb compound formation. In a previous study, prolonged exposure of GaSb surfaces to an As2 flux was shown to form highly faceted nanoscale pits. The original aim of our work was to use these nanoscale pits as seedling locations and to infill the voids to form QDs. However, on close examination of the pit-etching process, we found that the interaction of As2 with the GaSb surface initially forms 3-dimensional nanostructures which evolve into nanoscale pits with higher exposure flux and/or longer exposure times. Since the As2-induced etch itself yielded QD-like features, it eliminated the need to develop an etch + infill process. These nanostructures were found to be mainly GaAs and have dimensions similar to SK or DE QDs and their size/shape and areal density could be controlled using As2 flux density, exposure temperature and duration.

Methods: The samples described in this study were grown on GaSb substrates in a molecular beam epitaxy (MBE) reactor equipped with valved cracker sources for both As and Sb. Following thermal oxide removal at 540°C, a 200nm GaSb smoothing layer was grown. The substrate temperature was then adjusted for the As2 etch process (if needed) and the GaSb surface was exposed to a controlled As2 flux. The beam flux monitor equivalent pressures (BFM) for As2 were in the range of 7E-7 to 1E-5 Torr and the exposure time was varied from 60s to 600s. The As2 etch was followed by a 300s Sb soak to aid the formation of nanostructures. In samples for structural measurements, the growth was terminated at this point. For optical measurements, a 4 nm GaSb layer sandwiched in between Al0.5Ga0.5Sb barrier layers was etched using As2. Cross-sectional transmission electron microscopy (TEM) and energy dispersive x-ray analysis (EDX) were performed to analyze the dimensions and compositions of the nanostructures. Areal density and structural properties were measured using atomic force microscopy (AFM). Cryogenic photoluminescence (PL) measurement efforts are ongoing and will also be presented.

The samples described in this study were grown on GaSb substrates in a molecular beam epitaxy (MBE) reactor equipped with valved cracker sources for both As and Sb. Following thermal oxide removal at 540°C, a 200nm GaSb smoothing layer was grown. The substrate temperature was then adjusted for the As2 etch process (if needed) and the GaSb surface was exposed to a controlled As2 flux. The beam flux monitor equivalent pressures (BFM) for As2 were in the range of 7E-7 to 1E-5 Torr and the exposure time was varied from 60s to 600s. The As2 etch was followed by a 300s Sb soak to aid the formation of nanostructures.

The samples described in this study were grown on GaSb substrates in a molecular beam epitaxy (MBE) reactor equipped with valved cracker sources for both As and Sb. Following thermal oxide removal at 540°C, a 200nm GaSb smoothing layer was grown. The substrate temperature was then adjusted for the As2 etch process (if needed) and the GaSb surface was exposed to a controlled As2 flux. The beam flux monitor equivalent pressures (BFM) for As2 were in the range of 7E-7 to 1E-5 Torr and the exposure time was varied from 60s to 600s. The As2 etch was followed by a 300s Sb soak to aid the formation of nanostructures. In samples for structural measurements, the growth was terminated at this point. For optical measurements, a 4 nm GaSb layer sandwiched in between Al0.5Ga0.5Sb barrier layers was etched using As2. Cross-sectional transmission electron microscopy (TEM) and energy dispersive x-ray analysis (EDX) were performed to analyze the dimensions and compositions of the nanostructures. Areal density and structural properties were measured using atomic force microscopy (AFM). Cryogenic photoluminescence (PL) measurement efforts are ongoing and will also be presented.

The samples described in this study were grown on GaSb substrates in a molecular beam epitaxy (MBE) reactor equipped with valved cracker sources for both As and Sb. Following thermal oxide removal at 540°C, a 200nm GaSb smoothing layer was grown. The substrate temperature was then adjusted for the As2 etch process (if needed) and the GaSb surface was exposed to a controlled As2 flux. The beam flux monitor equivalent pressures (BFM) for As2 were in the range of 7E-7 to 1E-5 Torr and the exposure time was varied from 60s to 600s. The As2 etch was followed by a 300s Sb soak to aid the formation of nanostructures. In samples for structural measurements, the growth was terminated at this point. For optical measurements, a 4 nm GaSb layer sandwiched in between Al0.5Ga0.5Sb barrier layers was etched using As2. Cross-sectional transmission electron microscopy (TEM) and energy dispersive x-ray analysis (EDX) were performed to analyze the dimensions and compositions of the nanostructures. Areal density and structural properties were measured using atomic force microscopy (AFM). Cryogenic photoluminescence (PL) measurement efforts are ongoing and will also be presented.

The samples described in this study were grown on GaSb substrates in a molecular beam epitaxy (MBE) reactor equipped with valved cracker sources for both As and Sb. Following thermal oxide removal at 540°C, a 200nm GaSb smoothing layer was grown. The substrate temperature was then adjusted for the As2 etch process (if needed) and the GaSb surface was exposed to a controlled As2 flux. The beam flux monitor equivalent pressures (BFM) for As2 were in the range of 7E-7 to 1E-5 Torr and the exposure time was varied from 60s to 600s. The As2 etch was followed by a 300s Sb soak to aid the formation of nanostructures. In samples for structural measurements, the growth was terminated at this point. For optical measurements, a 4 nm GaSb layer sandwiched in between Al0.5Ga0.5Sb barrier layers was etched using As2. Cross-sectional transmission electron microscopy (TEM) and energy dispersive x-ray analysis (EDX) were performed to analyze the dimensions and compositions of the nanostructures. Areal density and structural properties were measured using atomic force microscopy (AFM). Cryogenic photoluminescence (PL) measurement efforts are ongoing and will also be presented.
quality of InP quantum dots, understanding the relationship between their structure and optical properties is quite important. In this work, we have achieved high performance InP/ZnS/ZnSe core/shell/shell quantum dot heterostructures using halogen atoms and evaluated their optical properties, morphology, and atomic structure. Various kinds of halogens were added to InP cores, and shell layers were formed in the presence of halogens. Among halogens, Cl and Br increased PLQY to >90%, almost doubled from the halogen-free sample. In addition to that, Cl drastically reduced the FWHM from 37 nm to 31 nm. Cl is commonly used as a surface capping agent to increase PLOY [1]. However, because the addition of Cl after shell formation had little effect on FWHM, there should be a different mechanism. To understand the role of Cl, structural analysis was performed using C-s-corrected scanning transmission electron microscope (STEM). Compared with the non-Cl doped samples, the shape of the Cl added quantum dots was more spherical and their particle size distribution was narrower. This indicates that Cl influences the shell growth dynamics. Atomic-resolution high-angle annular dark field (HAADF)-STEM image revealed that Cl added quantum dots contained stacking faults. Until now, stacking faults were believed to degrade the emission efficiency [2]. However, these results suggested that stacking faults in Cl-added InP quantum dots may not determine their optical properties. [1] D. A. Taylor et al., Chem. Mater. 33, 4399-4407 (2021). [2] E. J. ang et al., ACS Energy Lett. 5, 1316-1327 (2020).

2:30 PM X04 Study of Al2O3:Dielectric on Ga-Assisted MBE Grown GaAs0.75Sb0.25 Nanowires Priyanka Ramaswamy, M. ehu Paraksh, Shisir Devkota, Hranelep K. choor, Kendall D. Hawkins, and Shanthi Iyer; North Carolina A&T State University, United States

III-V semiconductor nanowires (NWs) are being pursued as a potential candidate for next-generation electro-optical devices. They offer unique and superior properties stemming from their anisotropic geometry compared to their bulk counterparts. The self-catalyzed vapor-liquid-solid (VLS) growth mechanism of these nanowires enables high phase purity growth with excellent homogeneity amongst NW ensembles, thus eliminating foreign contamination and induced defects arising from metal-catalyzed growth that has been commonly used until recently. However, the presence of a high density of surface states arising due to the anisotropic NW geometry is detrimental to the efficiency, sensitivity, and speed of these self-catalyzed III-V NW devices. The severity of surface state formation depends on the un-passivated dangling bonds arising from the sharp termination of material growth radially and native oxide formation. These can act as non-radiative recombination centers or surface charge traps, thereby increasing surface scattering leading to decreased carrier mobility and increased density of electronic states within the bandgap, causing Fermi level pinning at the surface. It is known that the Fermi level pinning creates a depletion region on the surface, thus ruling out the effect of native oxides on optical degradation. Further, the Raman characterization observed significant redshifts, peak broadening, and asymmetry for Al2O3 passivated NWs when compared to as-grown NWs, suggesting the presence of point defects on Al2O3 ALD deposition. Hence, the 4K-PL optical degradation observed in both sulfur-treated and untreated Al2O3 passivated NWs samples suggests non-radiative recombination centers arising from complex NW/dielectric interface formation to be the main contributing factor. Reporting of similar PL degradation in GaAs NWs, while enhanced PL intensity in In-based NWs allows us to speculate that non-radiative recombination centers arising from the Al2O3/NW interface states are peculiar to Ga-based III-V NWs only, and surface passivation in GaAs/Sb NWs may also enhance this contribution. Thus, AlD deposited Al2O3 layer is not a good choice for the passivation layer for GaAs/Sb NWs.

Acknowledgments: This work is primarily based upon research supported by the Air Force Office of Scientific Research (AFOSR) under grant number W911NF1910002. The Optical Science Foundation (OSF) also funded a part of this work under grant# 1832117. This work was performed at the JSNN, a member of the Southeastern Nanotechnology Infrastructure Corridor (SENIC) and National Nanotechnology Coordinated Infrastructure (NNCI), which is supported by the National Science Foundation (ECCS-1542174).

2:50 PM X05 (Student) Tuning Selective Narrowband Infrared Absorption Using Coaxial InAs-Ga0.5Sb0.5 Nanowires with Partial Shell Segment Coverage Ali Reza A brand1, Nicklas A nntu2, and Parsian M ohsen1,1,3; Rochester Institute of Technology, United States; 1Bo Akademi University, Finland

Vertical III-V nanowires (NW) arrays with core-shell geometries are promising candidates for infrared (IR) photodetection applications due to their unique optoelectronic properties such as efficient carrier collection, strong light absorption, and high detectivity under room temperature operation. Due to their remarkable ability to accommodate strain relaxation, an unprecedented set of lattice-mismatched material combinations can be realized using coaxial NW geometries with tailored properties. Generally, NWs with large diameters are required for efficient absorption in the IR range. However, increasing the NW diameter results in a loss of spectral range selectivity and an enhancement in dark current due to increase in material volume. Therefore, novel methods for achieving spectrally-selective light absorption while minimizing the collection medium volume and array fill factor are highly desired for applications in NW-based IR photodetectors with low-size, weight, power, and cost (SWaP-C) metrics. Based on simulations performed independently using finite element method (FEM) and rigorous coupled-wave analysis (RCWA) techniques, we demonstrate dramatic tunability of the IR absorption spectrum of coaxially heterostructured NW arrays consisting of InAs core segments that are partially encapsulated by GaAs0.5Sb0.5 shell layers. Embedding the bases of InAs NWs in Au backside contact layers results in periodic evanescent fields between adjacent NWs. The position, spatial extent, and separation of the evanescent modes depend mainly on the NW core segment diameter and wavelength of incident light. We show that otherwise decoupled light in the 2 to 3 μm wavelength range can be selectively absorbed in InAs NW core segments by adding partial GaAs0.5Sb0.5 shell layers with dimensions corresponding to the position and spatial extent of the evanescent fields. The GaAs0.5Sb0.5 layers are transparent at this wavelength range and only act to enhance absorption of otherwise decoupled light. Wavelength-selective absorption is localized to positions along the InAs core
segments where they are partially encapsulated. The absorption wavelength can be manipulated as a function of the partial shell segment position, length, and diameter. Moreover, tunable narrowband selectivity can be controlled by tuning the length of the InAs NW core segment. Such site-specific absorption in InAs NWs can be exploited for enhancement of carrier collection efficiency by positioning active p-n junctions at the predefined locations of GaAs$_2$Sb$_3$-based shell layers. The design approaches highlighted in this work enable novel, low-SWAP-C, NW-based IR photodetector membranes with tunable narrowband selectivity along specific NW locations.

3:10 PM Refreshment Break

3:30 PM X06

(Student) Growth and Transformation of Mixed Valence Manganese Oxides on Epitaxial Graphene-Silicon Carbide Heterostructures

Michael Pedowitz, Daniel Lewis, Sooram Kim and Kevin Daniels; University of Maryland, United States

Mixed valence manganese oxides (MnO$_x$) have attracted significant research interest in recent years due to the easily reversible redox reactions between manganese oxidation states which enable applications in catalysis, energy storage, and gas sensing. Of these mixed-valence manganese oxides, those containing high concentrations of Mn$^{3+}$ atoms have been of particular interest due to the high reactivity of these sites. However, the use of these MnO$_x$ materials has been hampered by their low electrical conductivity ($10^{-10}$-S/cm), which significantly reduces the speed of surface redox reactions. To overcome this challenge, heterostructures have been formed between manganese oxide, and graphene, which seek to couple the high conductivity of graphene to the reactive properties of MnO$_x$ compounds. Currently, these methods are hampered by the use of graphene oxide and reduced graphene oxide, due to the use of harsh oxidizing chemicals, which significantly limits the conductivity enhancements of these heterostructures. In this work, we demonstrate the growth electrochemical growth of layered MnO$_2$ on pristine epitaxial graphene, and its non-destructive transformation to Mn$_2$O$_3$ and Mn$_3$O$_4$ via a simple heat treatment. The electrodeposition was carried out in a three-electrode electrochemical cell with an Ag/AgCl reference electrode, a Pt counter electrode, EG/SiC as the working electrode, and a 100mM manganese acetate solution. The electrodeposition process consisted of three steps, a reduction step, oxidation step, and reduction step, with their potentials determined by cyclic voltammetry. The resulting MnO$_2$ thin films were then annealed in argon and air at 500°C to form Mn$_2$O$_3$ and Mn$_3$O$_4$, respectively. These films were then characterized through Raman spectroscopy, scanning electron microscopy (SEM), and atomic force microscopy (AFM) to determine their crystalline surface morphology. Raman spectroscopy of the three films indicated the initial formation of MnO$_2$ due to the presence of peaks at 640-650 cm$^{-1}$, 575-585 cm$^{-1}$, and 490-510 cm$^{-1}$ (Fig. 1a). The transformation of these films to Mn$_2$O$_3$ and Mn$_3$O$_4$ was also confirmed by the Raman data, with the formation of strong peaks at 650 cm$^{-1}$, and 705 cm$^{-1}$ in the case of Mn$_2$O$_3$ and strong peaks at 650 cm$^{-1}$, 374 cm$^{-1}$, and 320 cm$^{-1}$ for Mn$_3$O$_4$ (Fig. 1b-c). The surface morphology of the films was also revealed through AFM and SEM. The SEM images indicated that the MnO$_2$ was of nanofibrous character, with nanofibers on the order of 100nm thick (Fig. 2a). After transformation to Mn$_2$O$_3$, these nanofibers were replaced with a large plane covered in nanopores, and with transformation to Mn$_3$O$_4$ these were further replaced with nanocubes connected by nanowalls (Fig. 2b-c). The AFM revealed similar information about the morphology. These results suggest that the transformation process had led to an increase in surface roughness of the films (Fig. 4). In addition to our transformations of MnO$_2$ we also attempted to intercalate various metal ions into the layered MnO$_2$ structure (Li, K, Na). Raman analysis of these results (Fig. 4) indicated that we were successful in intercalating some of the ions, specifically Na, as indicated by the changes in the Raman spectra after the reaction. This demonstrates that we can successfully deposit films of MnO$_2$ on conductive EG/SiC, and transform it to alternate bimetallics as well as MnO$_2$ and MnO$_4$, providing a platform for enhanced performance from these materials.


3:50 PM X07

(Student) Enhancement of Visible Photoluminescence Through Atomic Layer Deposition Surface Passivation of Porous Silicon Nanowire Arrays Fabricated by Metal-Assisted Chemical Etching Kyle G. Tezanos and Parsian Moshfeghi; Rochester Institute of Technology, United States

The unique optical response properties of porous silicon nanowires (SiNWs) in the visible range enables potential applications across a variety of energy conversion technologies. While crystalline silicon has an indirect band gap of 1.12 eV and provides only low photoluminescence (PL) quantum yield in the bulk form, porous silicon exhibits strong visible emission at room temperature, attributed to a combination of surface state and quantum confinement effects. In this work, dense arrays of porous SiNWs are fabricated via metal-assisted chemical etching (MA-CEtch) with Au-Pd alloy catalyst layers. Room-temperature PL spectra collected from as-prepared samples show a clear variability in the intensity of the characteristic broad visible emission peak, centered at ~650 nm, as a function of the porous SiNW array volume. The influence of metal oxide surface passivation by atomic layer deposition (ALD) on PL emission wavelength and intensity is investigated. Commonly used ALD materials, including Al$_2$(O$_3$), hafnia (HfO$_2$), and titania (TiO$_2$), are deposited on SiNWs fabricated samples varying in etch depth from 30 to 100 μm. The emission spectra of ALD-passivated SiNW samples are compared to those coated with indium tin oxide (ITO) by sputter deposition. A clear enhancement of PL emission is observed for all ALD-processed samples. The passivation layer thickness is increased from 10 to 50 nm, favoring those passivated with HfO$_2$. The passivation potential of each ALD material is tracked over a 6-month period from the time of deposition and compared. This work highlights the importance of conformal passivation of ultrahigh aspect ratio porous SiNWs and tunability of their optical response properties toward applications in photoelectrochemical water splitting and photovoltaic energy conversion.

4:10 PM X08

Intraband Optical Gain in Colloidal Nanoplates Benjamin Dire Dit; Argonne National Laboratory, United States

Colloidal nanoplatelets show some of the most promising optical gain characteristics of any material. Using a modified quantum fountain design, thresholdless intraband optical gain at near-infrared wavelengths is demonstrated in using colloidal nanoplatelets. This is the first demonstration of unipolar gain in a colloidal system, requiring only electrons in this case. Stimulated emission depends on the thickness of the samples and can be tuned to technologically important wavelengths such as 1.3 and 1.5 μm. The modal gain, gain bandwidth, and gain lifetime of this intraband gain may be manipulated using excitation energy and temperature. Unlike bipolar laser media which competes with non-radiative Auger recombination, intraband stimulated emission must
Granular metals comprise nanoscale metal islands embedded in an insulating matrix. These materials are of great interest both as a platform for studying fundamental electron transport mechanisms and for enabling unique applications. Electron transport studies often feature noble metals (Au, Ag) in silica or yttria-stabilized zirconia (YSZ) matrices. In such materials, the transition from tunneling and hopping transport for low-metal fraction granular metals (dielectric regime) to percolative transport at high metal fractions (metallic regime) has been well-studied. This change in conduction mechanisms manifests as a $10^{-6}$ to $10^{-2}$ increase in DC conductivity as the metal fraction increases, 20% to 80%, for various granular metals [1]. Applications include strain sensors and memory storage with magnetic granular metals exhibiting giant magnetoresistance.

To expand the potential application space of granular metals into high voltage and high current applications, we developed granular metals with Co and Mo islands in silicon nitride and YSZ matrices. These materials were chosen to protect against joule heating causing island coalescence at high current densities. Mo and Co granular metal films with metal fractions 20% to 80% were prepared via rf co-sputtering of the metal and insulator. Electron microscopy images and DC conductivity measurements of these films showed the nanostructures and dielectric-to-metallic transitions characteristic of granular metals. Preliminary tests show breakdown strengths > 100 kV/mm. These Co-SiN and Mo-SiN are the first known granular metals with a silicon nitride insulating matrix. This work complements prior development of Co-Y SZ [2] and expands on limited prior studies of Mo-based granular metals [3].

The conductivity of our granular metal films was moderately sensitive to metal fraction, increasing $10^{-6}$ - $10^{-2}$ times as the metal fraction increased 20-80%. To understand these conductivity trends, we used x-ray photoelectron spectroscopy to evaluate metal/insulator interactions such as surface oxidation of the metal islands and band bending resulting from the work function differences between the metal islands and YSZ matrices. We found that metal/insulator interface interactions, including bonding, alloying, and band-bending, have a pronounced and previously unappreciated impact on granular metal conductivity. We posit that such interfacial interactions underlie conductivity trends in the broader family of granular metals [4].

This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories, a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.

because the bonded β-Ga2O3 substrate was initially ~700 μm thick, the β-Ga2O3 was thinned prior to measuring the thermal boundary conductance of the bonded interface. The β-Ga2O3 thinning and polishing recipes were developed in this study and employed to examine the subsurface lattice damage induced or removed by each thinning and polishing step. For all thinning (grinding and lapping) and polishing steps, ~10 kPa downward pressure and 30 RPM pad rotation speed were used. After bonding to Si, the unbonded backside of the β-Ga2O3 was grinded with 30 μm diamond paste. This resulted in a (001) β-Ga2O3 XRD rocking curve FWHM of ~7° and FW (0.001)M of ~19° after removing ~600 μm of material. After grinding, 5 μm then 1 μm Al2O3 particles were used for lapping. After lapping with 5 μm Al2O3, the rocking curve FWHM and FW (0.001)M decreased to ~40° and ~130°, respectively. 1 μm Al2O3 particles were then used as a finer lapping step, which further reduced the FWHM and FW (0.001)M to ~30° and ~100°. The reduction in rocking curve peak widths (either changing to a softer particle material or smaller size) corresponds to the removal of subsurface lattice damage induced by each previous step. Lastly, 70-nm colloidal silica was used as the final polishing step, which reduced the rocking curve FWHM and FW (0.001)M to 20° and ~40°, respectively. The final polished surface roughness was 0.4 nm. During the lapping and polishing steps, a wedge in the β-Ga2O3 was intentionally induced such that the β-Ga2O3 layer had a thickness gradient ranging from ~2 to ~10 μm. The thickness gradient enables a more reliable extraction of the thermal boundary conductance of the bonded interface using steady-state thermoreflectance. The thermal boundary conductance measurements for these bonded β-Ga2O3 films structures is comparable to our previous work by bonding β-Ga2O3 to 4H-SiC (~6 MW/m²K), and greater than other work reported in the literature that utilized mechanical tape exfoliation methods to bond (100) or (201) β-Ga2O3 to quartz or diamond (8-17 MW/m²K)). The authors would like to acknowledge the support of the Office of Naval Research through a MURI program, grant No. N00014-18-1-2429.

References

2:10 PM Y03
Ionic Exchange in Perovskite Thin Films Using Solid-State Reactions
Martin G. Reyes-Banda, Leunam Fernandez-Izquierdo, Jesus A. Caraveo Frecas, Victor F. and M anuel Quevedo Lopez; The University of Texas at Dallas, United States

One of the most appealing aspects of perovskite materials is that their composition can be tuned to dramatically impact carrier mobility, carrier concentration, bad gap, etc. Their unique composition tuning can enable applications such as solar cells, LEDs, sensors, batteries, transistors, memories, lasers, photodetectors, X-ray, and radiation sensor, among many others. Besides directly impacting device performance, perovskite composition also plays a crucial in the resulting reliability and stability of any of these devices. In this work, a simple solvent-free, versatile, and flexible route for material properties modulation in halide perovskite thin films has been developed using CsPbBr3 thin-films. The method enables composition, morphology and electrical properties control using a solid-state ion-exchange reaction. The presence of PbX2 (X = Cl, Br, I) or Br2 (Br = C6H5+, M n+) vapor. The original CsPbBr3 thin films were grown using close-space sublimation (CSS), and CsPbBr3 crystals obtained by grown by the antisolvent vapor crystallization (AVC) method as the precursor. The resulting CsPbBr3 (Br, X) (PbX2 treated) films maintained an orthorhombic structure with increased in-plane β-Ga2O3 grain growth with grains as large as 25 μm in films as thick as 8 μm. This perovskite annealing process also tune their band gap in the range of 1.7 - 2.9 eV and tailor their transport electronic properties. Exposure to PbX2 (X = Cl, Br, I) vapor for longer annealing durations resulted in higher mobility (~13 cm2/V s) and an increase in carrier concentration (~5x1017 cm−3).

Furthermore, the CsPbBr3 (X) films enabled diodes with very low leakage current (1x10−6 A/mm²), likely due to the large crystalline grains. The diodes were used as radiation detectors, with superior alpha particle sensing from a 210Po source. In addition, preliminary results of B-site ion exchange show blue-shift emission and recrystallization opening a way to control both the composition, optoelectronic and electronic properties of inorganic perovskite thin films while enabling depositing films using a large area compatible methodology.
Quantum cascade lasers (QCLs) are mid-infrared electrically injected lasers that generate photons via electronic transitions between bound levels of coupled quantum well heterostructures. Since the initial demonstration in 1994, QCLs have rapidly matured and are now available commercially. QCL lifetime is a significant consideration in the cost of ownership of one of these devices. Previous studies have predicted device lifetimes exceeding eight-hundred nine thousand hours; however, little attention has been given to predicting premature device failure where the device fails within several hundred hours of operation. Premature device failure presents a significant cost-threat to work where QCLs are integrated into complex systems, and a method to predict this failure would be able to help mitigate this threat. In this paper, we show how an accelerated burn-in process coupled with a support vector machine (SVM), a type of supervised learning algorithm, can be used to predict premature failure of QCLs. We report accurate prediction of premature device failure up to 201 hours prior to the catastrophic failure of a device.

In total, 9 QCLs undergo an accelerated burn-in process. The devices are operated in continuous-wave (CW) mode at 80% of their peak CW optical power at an elevated heat sink of 328K. All the QCLs are from different portions of the same semiconductor wafer that was grown by metal organic chemical vapor deposition. The devices are 5 mm long and have ridge widths that vary from 9 to 12 μm. During the burn-in process, light-current-voltage (LIV) measurements are measured approximately every 2.5 hours. For two of the devices that undergo longer burn-in testing, the interval between measurements varies from 10 to 4 hours. A cross the nine devices, 473 LIV measurements are acquired.

The accelerated aging test consists of two stages. In the first stage, the LIV data from 5 QCLs are used to train the SVM model, and the LIV measurements from the remaining 2 devices are used to test the model. We use different combinations of the devices for training and testing to avoid overfitting to a particular combination of devices, and the parameters of the SVM are optimized over these 10 combinations. In the second stage, all 7 devices from the prior stage are used to train the same SVM model while test dataset consists of 2 new devices.

The model identifies healthy devices with 100% accuracy for every test combination, encompassing over 1300 hours of measurements for the operational devices. Across all measurements, an LIV from an operational device is never labeled as an LIV from a device that will fail prematurely. Additionally, every device that fails during the accelerated burn-in testing has at least one LIV labeled as belonging to a failed device. For many devices, LIV measurements very early in the testing are identified as problematic, which would allow an operator to cease testing well before the actual catastrophic failure of the device. This can be as much as 201 hours before failure. The proposed aging procedure can be integrated into a QCL production pipeline to decrease manufacturing costs and the time required before deployment.

3:10 PM Refreshment Break
packaging techniques to examples of interconnect technologies, all proven reliable at cryogenic temperatures. Electronic packaging techniques demonstrated focus on low temperature flip-chip bonding, compatible with process-sensitive superconducting materials. Additionally, epoxy underfill processes are demonstrated and evaluated with confocal scanning acoustic microscopy. Unique cabling solutions that we have designed and developed that utilize these low temperature electronic packaging techniques are demonstrated. Fabrication processes performed to yield reliable cryogenic cables are detailed and significant material considerations are described. Cables designed are proven reliable at cryogenic temperatures and against multiple thermal cycles (from room temperature, to as low as 4.2 K, returning to room temperature) for DC and RF applications. Dielectrics used in the fabrication of cables were characterized by utilizing superconducting half-wavelength, series microstrip resonators. These resonators facilitated the extraction of parameters such as dielectric constant and loss tangent at GHz frequencies for cryogenic temperatures. Lastly as an extension to electronic packaging techniques, thru-hole processing on molybdenum (a robust low coefficient of thermal expansion material) is demonstrated, specifically comparing the use of nanoscale and femtosecond pulsed laser processing. Molybdenum thermal characteristics performed as low as 2.2 μs with a physical property measurement system are described to augment future cryogenic electronic interconnect simulations. Techniques, processes, and characterizations detailed in this work provide excellent solutions for cryogenic interconnect challenges while creating a framework for forward-looking unique approaches.

4:10 PM Z03
Indium Microbump Interface Evolution with Varying Underbump Metalurgy Stack-Ups Rebecca A. Wheeling; Sandia National Laboratories, United States

Flip chip interconnections using indium have many advantages for high bandwidth applications with large strain between layers and cryogenic operation temperatures. Indium can form a cold weld at room temperature preventing undue stress during the flip chip bonding process. Furthermore, indium is highly ductile even at cryogenic temperatures and thus capable of accommodating strain between CTE mismatched substrates. Despite wide and diverse use, understanding of the reliability of indium microbumps is limited by the complex metallurgy occurring at the indium/under bump metal interface.

Due to the low melting point and high spattering efficiency, it is difficult to obtain cross-sectional images of indium interconnects and thus determine the kinetics of intermetallic formation, qualities important to the reliability of the interconnect. We utilize cryogenic focus ion beam (cryo-FIB) and scanning electron microscopy to determine the kinetics of intermetallic formation. Three kinetic parameters: activation energy, time exponent, and pre-exponential constant are calculated through a multivariable linear analysis of intermetallic thickness as a function of time and temperature. The intermetallic stoichiometries are further validated with x-ray diffraction. Additionally, interfacial evolution will be modeled and correlated to mechanical performance via shear testing.

Three underbump metalurgy stack-ups have been evaluated: 1) Ti/Cu/Ni; 2) Ti/Ni; 3) Ti/Ni/Au. The addition of Au appears to significantly reduce the activation energy for intermetallic growth, compared to only Ti/Ni. The Ti/Ni stack-up is the most stable of these three. However, at elevated temperatures, complete consumption of the indium bump occurs by the Ni-In intermetallic, confirmed by diffraction data. Mechanical performance of the bumps for each stack-up will be reported.

4:30 PM Z04
(Student) UV Curable Ink Composition for Novel Direct Ink Writing Processes Yurt Piraç; Chris Areias, Yibo Li, Andrew M. Luce, Emily Lamport, Oshadha Ranasingha, Susan Tullii, Craig Armiento and Alik Timucin; 1University of Massachusetts Lowell, United States; 2Raytheon, United States

A UV curable dielectric ink composition is presented which enables adaptable and high-resolution direct ink writing for printed electronic applications. The UV curable dielectric ink composition is designed using non-hazardous, commercially available ingredients. Specifically, the ink composition includes bisphenol-A type acrylate and epoxide monomers, a longwave ultraviolet light absorbing Type 1 radical photoinitiator, an ionic liquid to aid in epoxide monomer conversion process, and high aspect ratio boron nitride nanoparticles. The ink manufacturing procedure is devised to require only fundamental lab equipment, without the need for complex reaction conditions or harmful processes. The UV dielectric ink composition is engineered to meet a range of direct ink writing application specific needs. These needs include a tailored rheology, cured film rigidity, dielectric performance, and adhesive ability onto substrates which are central to the printed electronics ecosystem. The versatility of this ink composition is demonstrated through the fabrication of dielectric bridges and interconnects for printed coplanar waveguides, bare die chip integration, and interconnects between printed circuit board regions.

4:50 PM Z05
(Student) Additive Microfabrication of System in Package for Heterogeneous Integration with Semiconductor Dies B hushan Lohani and Robert C Roberts; University of Texas at El Paso, United States

This abstract explores the possibility of employing metal additive microfabrication of system in package (SiP) with inbuilt heat sinks and leadframe consisting of multiple pads for QFN packaging. The SiPs were fabricated using 17-4Ph stainless steel powder employing a relatively less expensive DM LS system. The use of affordable metal additive manufacturing systems is considered by the authors to encourage further research on its applicability towards heterogeneous integration in the semiconductor industries. The International Technology Roadmap for Semiconductors (ITRD) 2012 emphasized on the importance of integration of system on chip (SoC) and SiP. DM LS is one possibility for such heterogeneous integration due to the possibility of customizability as the parts are directly fabricated from a CAD file. DM LS has been considered superior to its plastic or resin-based counterparts in applications where conductive parts with better accuracy and strength are required. All these features make DM LS parts, a possible option for the fabrication of SiP with few functionalities like heat sinks and connectivity. 3D packaging and heat extraction for die is one of the grand challenges of International Roadmap for Devices and Systems (IRDS). In this abstract, different QFN leadframes with and without cooling systems are presented. The original leadframe design with only the pads forms a comparison reference for the remaining three systems. The three systems are: QFN leadframe with microchannel, inlet, and outlet for fluid flow, QFN leadframe with arrays of fins below the die location, and a QFN leadframe with fins along with additional inlet and outlet for optional fluid flow. Figure 1 shows the CAD top views of all four proposed package system. Each package system can hold a lcm by lcm semiconductor die for testing purposes. The microchannels are 500μm square channels whereas the fins are 1000μm in diameter. The affordability comes with the trade-off of resolution and the present DM LS system can faithfully produce the mentioned dimensions with compatible features for the channels and fins.

The first step towards the fabrication of the packages is the CAD design and simulation. The CAD design was then fed to the metal
3D printer, which then sliced the model and created 3D laser part. The fabrication proceeds by melting and fusing a 30μm layer of powder, repeating the process, coating top layers on top of layers, and fusing them together until the final 3D part is built as per the CAD file. EDM wire cutting or grinding of previously created support will be extended. The whole system will then be covered with epoxy and left to cure. The final step will be to grind away the back end of the cured part to remove support metal plate on the bottom of the packaging parts as shown in Figure 3.

Figure 4 shows the separated parts with a spot for semiconductor die to be affixed and various other sub-parts. Figure 5 shows the water (colored for visibility) filled leadframe with microchannel, and the other one with fins, inlet, and outlet is shown in Figure 6. Figure 7 shows the preliminary infra-red image of all four devices heated to 40°C and left to cool down. The devices were in the same order as Figure 4. As per the theoretical idea, fins with channels perform the best followed by the one with microchannel, and the one with only fins based on the time required for them to cool down (a-f in Figure 4). The preliminary result appears promising and the material characterization along with testing is in process. Figure 8 and 9 shows the SEM characterization of build device compared to the design. The variation from the design is very small.

SESSION AA: Plasmon and Surface Phonon Polaritons

Session Chairs: Anthony Hoffman and Milan Palei
Thursday Afternoon, June 30, 2022
Senate Chamber

1:30 PM AA01
(Student) Lateral Permittivity Patterning by Ion Irradiation in CdO Thin Films for Mid-IR Plasmonics
Angele Cieri¹, S M Ingze Hø², Kajsa S. Diaz-Granados³, Joshua Caldwell³ and Jon-Paul Maria³
¹The Pennsylvania State University, United States;
²Vanderbilt University, United States

Donor doped cadmium oxide (CdO) thin films demonstrate excellent optoelectronic properties, further enabled by advanced synthesis techniques such as high-power impulse magnetron sputtering (HIPIMS), which yields high quality crystals with easily controllable transport properties. Tunable carrier concentrations between 10¹⁴-10¹⁷ cm⁻³ while maintaining mobilities between 300-500 cm²/V-s facilitate low-loss plasmon modes spanning the mid-IR. Further, fabricating layered CdO structures with varying thickness and carrier density in each stack has given way to interesting nanophotonic phenomena such as multiple epsilon-near-zero (ENZ) resonances in a single structure, strong coupling between ENZ and surface plasmon polariton modes, and hyperbolic behavior in homoeptaxial structures. By controlling donor dopant levels in individual layers, one can engineer permittivity of a stack in the out-of-plane dimension. Here, we extend this principle to the in-plane dimensions by ion irradiation patterning to locally induce donor defects and achieve lateral permittivity control. Current methods to achieve similar lateral control, e.g., lithographic approaches, require lithographic approaches that almost always introduce physical boundaries, roughness, or interface defect densities that interfere with high fidelity plasmonic modes. Instead, this novel ion irradiation method creates lateral patterns which are free of physical interfaces but exhibit sharp contrast in permittivity. In this presentation, we will demonstrate lateral control of electronic and optical properties in thin film CdO by ion irradiation using patterned hard masks.

1:50 PM AA02
MBE Growth of Delta Doped Si:InAsSb/GaSb HMM and Their Hyperbolic Response
Kurt Eyink, Heather Haugan, Krishnamurthy M allictingam, Derek Bas and Augustine Urbas; Air Force Research Laboratory, United States

Hyperbolic metamaterials have been receiving considerable due to their large density of states, high spontaneous emission rates and tailorable properties. One way of forming these structures is through the combination of a degenerately doped semiconductor and undoped semiconductor to form stacks of these materials. Here the metallic component is the degenerately doped semiconductor and the metallic fraction is fixed from the ratio of the metallic region to the total thickness. We, as well as others, used a doped InAsSb in combination with undoped GaSb. The composition of the InAsSb was lattice matched to the GaSb to allow a wider range of topological structures. We have recently characterized Si:InAsSb/GaSb stacks and have found that the Si:InAsSb structures have the doped charge squeezed into the central region of the InAsSb. We had found that the amount of squeezing was relatively independent of the size of the InAsSb region being consistently in the 3nm range. In this study we first look at the delta doping an Si:InAsSb/GaSb stacks. The constant doping density was similar to the previous study (~2×10¹⁷/cm³). Delta doping was studies as a function of position and amount in the structures and was characterized using HRXRD and spectroscopic ellipsometry. Delta doping was achieve by interrupting the growth while continuing to expose the surface to Si. HRXRD showed that with interruption on the GaSb surface, a large degradation in the quality of the stack occurred. Whereas instrumentation on the InAsSb retained a high quality stack. We further showed this layer could be as thin as a single monolayer thus effectively allowing the delta doping at each interface. Stacks of InAsSb/GaSb with Si delta doping at both edges of the InAsSb as well as constant doping throughout the structure were formed and subsequently characterized with spectroscopic ellipsometry. We found contrary to the constant doped structures which contained a single peak in the spectroscopic ellipsometry response these structures contained two peaks. This peaks presence of these peaks will be discussed in terms of doping as well as potential quantum transitions in the structure.

2:10 PM AA03
(Student) Understanding Organ Pipe Resonances in SPHP Trenches for Spectroscopic Sensing
Esfidani M osayeh, Vazhefi M ayar, and Thomas G Folland; The University of Iowa, United States

Surface plasmon polaritons (SPPs) and surface phonon polaritons (SHPs) modes form when light interacts with the surface of materials with a negative dielectric function. They have attracted much attention due to their ability to confine light to deeply subwavelength dimensions which can enable significantly enhanced interaction with nanoscale systems. Understanding the design principles for excitation of SPP modes in the mid infrared (MIR) will make them more relevant for applications including optical modulators, photodetectors, and sensor technologies. For instance, using surface enhancement infrared absorption (SEIRA) one can create high sensitivity molecular sensors. In SEIRA a SPP is used to enhance the optical absorption of the molecule. However, to design an effective SEIRA sensor it is critical to carefully optimize the coupling between free space light, the SPP mode, and the molecule, to get a large change in signal when operated. Given that SEIRA is a resonant process, which is dependent on the interaction between numerous geometric parameters of the SPP resonator, designing an efficient and low-cost biosensor is very time consuming. Therefore, understanding
the design of resonant structures is crucial to improve the enhancement. In our work, we investigate periodic trenches etched into a silicon carbide surface. Resonances in this structure form between the walls of the trenches, and form a vertical standing wave which, analogous to resonances in an organ pipe. We develop a model based on considering the structures as finite length metal-insulator-metal (MIM) waveguide to investigate the frequency of modes and optimize the height and pitch of the structure for the purpose of sensing. Attention will be focused on various heights and trench widths that are important for realizing a sensor. Numerical simulations are compared between using two different approaches—numerical solutions to maxwells equations computed using full wave simulations and a simplified analytical model implemented in MATLAB based on S-matrix formalism and cavity model. The measured SPHP modes of standing wave in different mode with various height and gaps of both methods are compared, and we find the simplified analytical model is well capable of calculating the reflection and quality factor for MIM waveguide. Our results are general, and can be applied to any types of rectangular MIM waveguides to achieve an optimal design, notably for the comparison of different sensor geometries and materials.

2:30 PM AA04

(Student) Physical Vapor Transport Growth of α-MoO₃ Sheets for Hypersonic Thermal Transport via Hyperbolic Phonon Polaritons Ryan Spangler, Angela Cleri, Josh Nordlander, Katja S. Diaz-Granados, Daniel Hirt, John Tomko, Patrick Hopkins, Joshua Caldwell and Jon-Paul M. aria; \The Pennsylvania State University, United States; V anderbilt University, United States; \University of Virginia, United States

For high-frequency and high-power electronics, especially those that rely on low-thermal conductivity semiconductors, advanced thermal management is critical in improving device performance and lifetime. In recent years, van der Waals materials such as h-BN and α-MoO₃ have been identified as natural platforms for hosting low loss, highly confined hyperbolic phonon polaritons (HPHPs). These quasi-photons of coupled oscillations of light and heat result from extreme anisotropy of the dielectric function, where the in-plane and out-of-plane dielectric permittivity have opposite signs. Furthermore, in α-MoO₃, the in-plane components also exhibit hyperbolic dispersion in some spectral regions; in this way, the propagation of HPHPs can be restricted to a single crystal direction. These rays may permit delocalized heating, where energy absorbed by a hyperbolic material may travel ballistically at hypersonic velocities, even against a thermal gradient, before thermalizing. In this work, single crystals of α-MoO₃ have been synthesized using a physical vapor transport technique, which has been identified as an effective approach for the growth of these materials. We have achieved α-MoO₃ growth oriented with the b-axis perpendicular to the substrate and with low out-of-plane mosaicity, eliminating the tendency of the crystals to grow in other orientations which would limit applicability in devices. We present structural, microscopic, and optical data characterizing the formation of α-MoO₃ crystals on various substrates for the purpose of investigating hyperbolic phonon polariton behavior.

2:50 PM AA05

(Student) Control of Thermal Transport at Ultrahigh Temperatures by Immiscible Oxide Heterostructures Sean M. CSherry, Matthew Webb, Jonathan Kaufman, Zhihao Deng, Ali Davoodabadi, Tao Ma, Emmanouil Kioupiakis, Keivan Esfarjani, John T. Heron, and Andrej Lenert; University of Michigan-Ann Arbor, United States; University of Virginia, United States; University of M.ichigan-Ann Arbor, United States

Degradation of materials under harsh, high-temperature conditions is one of the grand challenges of high-performance energy conversion. Current approaches make use of refractory materials that do not possess ideal properties but are resistant to decomposition by heat. To suppress undesired thermal transport, multiple refractory materials are shaped and arranged with varying degrees of complexity, ranging from multilayers to plasmonic arrays and 3D photonic crystals. Ultimately these structures progress toward more thermodynamically favorable configurations and result in intermixing, reaction or new phase formation, and coarsening. This severely limits their performance in extreme conditions. Here, we introduce the concept of using immiscible refractory oxides with high crystallinity as building blocks of functional ultrahigh-temperature materials. We demonstrate epitaxial oxide heterostructures made from perovskite 

BaZr₀.₅Hf₀.₅O₃ (BZHO) and rocksalt MgO as a photonic crystal (PhC) that can suppress undesired thermal emission at a desired cutoff wavelength. The PhC is implemented as surface filter to suppress mid-infrared thermal emission from the best intrinsic, spectrally selective emitter operating at 1350°C in air. The heterostructure exhibits coherent atomic registry that retains clearly separate refractive index mismatched layers without interface coarsening, interdiffusion, phase change, or decomposition up to at least 1100°C in dry air. The use of dissimilar crystal structures, with low lattice and thermal expansion mismatch, allows for high crystallinity superlattices with interlayer immiscibility at high temperatures. The understanding gained from this study can be used to develop thermal barrier coatings and selective emitters that are resistant to instabilities in air. Beyond BZHO/MgO, we computationally identify ~10² potential oxide pairings that fit our design criteria, demonstrating the vast potential of this approach.

3:10 PM Refreshment Break

3:30 PM AA06

Plasmon-Enhanced Distributed Bragg Reflectors Aaron M. Muohowski, M. organ Berghold and Daniel Wasserman; The University of Texas at Austin, United States

Distributed Bragg reflectors (DBRs), comprising quarter wavelength pairs of low and high refractive index layers, are a key element of modern photononic architectures, with applications ranging from vertical-cavity surface emitting lasers, to resonant cavity photo- and light-emitting diodes, to Fabry-Perot reflection modulators, to high-q cavities for single photon emission. While DBRs are commonplace in mature visible and near-infrared wavelength systems, the quarter-wavelength thicknesses of the constituent layers becomes increasingly problematic at the longer wavelengths of the mid-infrared spectral region. As a result, III-V resonant cavity photonic devices often employ A1AsSb/GaSb DBRs with mirror thicknesses approaching 10 μm, despite the comparatively high refractive index contrast of 0.6 between A1AsSb and GaSb [1]. Such thick mirrors significantly increase fabrication complexity and decrease the yield of the resulting devices, to the point where mid-infrared resonant cavity photonics are largely untenable. Critically, DBR thicknesses for a given reflectance can be reduced by increasing the refractive index contrast of the constituent layers. Various avenues towards increasing index contrast have been explored and have been explored, including oxide [2] and air-gap DBRs [3] at shorter wavelengths, as well as heteroepitaxial integration of high-contrast materials [4]—each with their own additional degree of complexity over conventional epitaxial DBRs. The free electron response of highly-doped semiconductors has long been known to reduce the refractive index. Indeed, this exact mechanism has been exploited as plasmon-enhanced waveguides for quantum cascade lasers [5]. Here, we explore the application of highly-doped semiconductors as low index layers within DBRs. Simulations for DBRs over a range of design wavelengths and achievable doping densities are used to illustrate the unique features of plasmon-enhanced DBRs and examine the interplay between free-carrier losses, stop band width, and maximum
reflectance. Finally, we realize a plasmon-enhanced DBR using highly-doped InAsSb lattice-matched to GaSb with a design wavelength of 4.3 µm that is 43% thinner than an AIAsh-GaSb DBR with equivalent reflectance. In contrast to other low-index epitaxial DBR technologies, this marked reduction in mirror thickness requires no additional ex situ fabrication or heteroepitaxy outside of a conventional material system.

References

3:50 PM AA07
(Student) All-Epitaxial Ultra-Thin Long-Wave Infrared Plasmonic Detectors Morgen Berghold1, Priyanka Petluri1, Aaron J. M. Muhowski1, Leeland J. Nordim2, and Daniel Wasserman1,2
1The University of Texas at Austin, United States; 2Stanford University, United States

The desire to confine light into sub-diffraction volumes for optoelectronic device applications has long driven interest in the field of plasmonics. Strong subwavelength confinement can be achieved by leveraging modes, supported at metal/dielectric interfaces, such as the surface plasmon-polariton (SPP) or the localized surface plasmon (LSP). Devices using these modes often operate in the visible or near IR wavelength ranges where noble metals such as Au and Ag can function as the plasmonic material. Unfortunately, with rising wavelength these metals behave increasingly like perfect electrical conductors—precluding them from supporting highly confined plasmonic modes [1] at long wavelengths. Fortunately, other classes of plasmonic media, such as transparent conducting oxides [2] and highly doped semiconductors [3] can be used as tunable plasmonic media in the mid-infrared (mid-IR). Furthermore, highly doped semiconductors can be grown by molecular beam epitaxy (MBE), thus their optical properties can be tightly controlled and they can be monolithically integrated with mid-IR optoelectronic device architectures with relative ease.

One such device architecture is the nBn detector, which is comprised of an (n-doped) absorber-conduction band barrier-(n-doped) thin epitaxial contact region, design. Ultra-thin plasmonic detectors [4] leveraging nBn device architectures, which exhibit markedly lower dark current than their conventional counterparts, use a commensurately thinner contact region. In this regime, metal diffusion becomes increasingly problematic and can effectively short out the device, particularly when the fabrication processes require high temperatures. Likewise, the metallic grating, which provides momentum matching of the SPP to free space, can serve as a problematic source of diffusion. One method to mitigate metal diffusion would be to replace the grating layer with a highly doped semiconductor, eliminating metal diffusion from the grating and providing additional space for the metal contact to diffuse without the associated risk of device failure.

In this work we demonstrate a type-II superlattice nBn detector with epilaxial gratings. A 750 nm thick silicon doped (n∗∗∗) InAs/InAsSb T2SL grown lattice matched to the GaSb substrate serves as a plasmonic semiconductor backplane. On top of this highly-doped material is a 311 nm InAs/InAsSb long-wave infrared (LWIR) T2SL absorber followed by a 146 nm A1A Sb barrier then a 46 nm LWIR T2SL top contact layer. The top layer consists of 127 nm of the same highly doped InAs/InAsSb T2SL that forms the plasmonic backplane. A finite growth this layer is lithographically patterned and wet etched into square patch antennas with a 1.5 µm width and 3.0 µm period that allow coupling into the SPP modes at the T2SL layer. A lithography and wet etch process is then used to fabricate electrically isolated mesa and top and bottom contacts are deposited. A after fabrication the detectors are mounted in a cryostat where spectral response, responsivity, and IV measurements are performed. External quantum efficiency (EQE) is then calculated from the spectral response and responsivity. The detector EQE peaks at 9 µm with a magnitude of 34% in an active region with thickness λ/29.

5 From V. A. Podolskiy’s research group, see http://viktorm-podolskiy-research.wiki.uml.edu/RCWA.

4:10 PM AA08
(Student) ErAs:InGaAsIBAs for 1.55 µm-pumped Terahertz Photoconductive Switches Wilder Acuna, Joseph P. Avenoso, James Bork, Lars Gundlach and Joshua Zide; University of Delaware, United States

We present our latest work on the molecular beam epitaxy growth of ErAs nanoparticles embedded within an InP-based (InGaAsIBAs), (InAlIBAs),, digital alloy for use in photoconductive (PC) switches for terahertz (THz) sources and detectors. A high-performance PC switch requires specific properties in the active layer: specifically, ErAs (InGaAsIBAs), (InAlIBAs), (hereinafter: ErAs:InGaAsIBAs) must have a short carrier lifetime, high dark resistivity, and high carrier mobility. In addition, a semiconductor working at a 1550 nm pumping wavelength is highly desirable due to the many advantages of compact, fiber-based components in the setup. For these desired properties, ErAs:InGaAsIBAs offers some advantages; ErAs nanoparticles pin the Fermi level and act as efficient carrier capture traps, decreasing the carrier lifetime to sub-picosecond values [1]. On the other hand, the InGaAsIBAs matrix gives enough degrees of freedom to engineer the band alignment to the pinned Fermi level, thereby increasing the dark resistance while having a bandgap below 0.8 eV. To quantify these properties, we characterized the materials with several techniques. High-resolution X-ray diffraction (HR-XRD) is used to determine material quality and an approximation of the bismuth incorporation. Spectrophotometry allows the measurement of the bandgap in the material. Hall effect measurements can be used to determine dark resistance, carrier concentration, and mobility. In the same way, optical-pump THz-probe spectroscopy provides the carrier dynamics in the structure. Finally, we present our progress on both measurement of material quality and also direct testing of PC switches properties in fabricated devices. [1] Appl. Phys. Lett. 75, 3548 (1999).

4:30 PM AA09
Plasmon-Phonon-Intersubband Transition Interactions at THz Frequency in a Bi2Se3 -GaAs Heterostructures Quang To, Zhengianye Wang1, Quoc Dao H2, Ruiqi Hu3, Garrett Bryant3, Anderson Janotti1, Joshua Zide1, Stephanie Law1 and Matthew Dubey1
1University of Delaware, United States; 2National Institute of Standards and Technology, United States

In this work we probe theoretically strong coupling at THz frequency in a system consisting of Bi2Se3 and AlGaAs/GaAs quantum wells, focusing on the creation of new hybrid excitation modes, namely Dirac plasmon phonon intersubband transition (DBT) polaritons. Rabi splitting arising from the interactions among the THz excitations in the system shows features of strong coupling which can be experimentally observable. Our calculations based on scattering matrix method reveal that the Rabi splitting...
Topological insulators (TIs) are materials whose bulk band gap is crossed by conducting surface states. The electrons that reside in these surface states are massless and obey time-reversal symmetry due to the large spin-orbit coupling in the system that prohibits backscattering. Bi$_2$Se$_3$ is a widely-studied 3D TI with a single Dirac cone at the $\Gamma$ point. Plasmons are the collective oscillation of the free electrons in a system. Plasmons excited on the surface states of a TI are called Dirac plasmon polaritons (DPPs) and their resonance frequencies lie in the terahertz (THz) range of the optical spectrum. The THz is an important frequency range for many practical applications as many molecules have absorption resonances in this range which can be used for gas sensing and monitoring, pharmaceutical testing, and so on. In this paper, we will explore in-plane plasmon coupling between TI nanostructures for future applications in THz plasmonic or metasurface devices. In TI films where the film thickness is much smaller than the wavelength of the light, DPPs are excited on both top and bottom surfaces simultaneously. They then couple to each other through their evanescent electric fields. This results in the two coupled DPP modes: the acoustic and the optical mode. Due to the momentum mismatch between the photon and the plasmon, it is not possible to excite plasmons by directly shining light on the sample. Patterning the film into stripes of width ($W$) adds the momentum of $n\cdot\pi/W$ to the incoming photons to overcome the momentum mismatch required for the excitation of plasmons. Researchers have mapped the DPP dispersion by changing the stripe width and thickness of samples. Although it helped us to understand the basic physics of DPPs, a clear idea of how these plasmons couple to each other in the plane was still missing. We started by growing eight 50 nm Bi$_2$Se$_3$ thin films on sapphire (0001) substrates using molecular beam epitaxy. From room temperature hall measurement, we get the sheet density of $2.46\times10^{15}$ cm$^{-2}$. As mentioned earlier, plasmons cannot be excited directly in the TI films, therefore we etched all films into stripes of width 2.5 μm with variable gap lengths ranging from 0.3 μm to 7.5 μm using electron beam lithography. Then we measured the transmission through the samples both in transverse electric (TE) mode and transverse magnetic (TM) mode using the room temperature Fourier transform infrared spectroscopy. Plasmon modes can be excited only in TM mode as a standing wave. The extinction spectra for all samples were calculated using $E=1 - T(o)/T(o,e)$, where $E$ is extinction, $T(o)$ is the transmission through bare sapphire and $T(o,e)$ is the transmission through the sample. The TE extinction spectra of all samples looked similar with two distinct phonon modes $\alpha$ and $\beta$ around 2 THz and 3.9 THz. For TM extinction curves instead of distinct phonon peaks, we observed a broader asymmetric peak around 3 THz that blue shifted with the increase in gap size. It indicates the excitation of plasmons and that couple to the phonons. We therefore modeled our data using a double Fano-type interaction model to extract the plasmon frequency. We observed an increase in the plasmon frequency with increasing gap size indicating in-plane coupling from the plasmons. We were able to fit the data with an exponential decay curve which is consistent with dipole-dipole coupling. We demonstrated that the in-plane coupling becomes negligible when the lattice constant exceeds 2.8 times the stripe width. This result is comparable to the studies on the in-plane plasmon coupling of metallic nanoparticles. In summary, this work helped to explore and understand the nature of in-plane plasmon coupling in TIs and can be useful in designing TI-based metasurfaces to manipulate THz light.

**SESSION BB: Electrochemical Energy Storage and Conversion**

**Session Chairs: J. Young-Hyun Kim and Edward Yu**

**Thursday Afternoon, June 30, 2022**

**Cartoon Room #1**

**1:30 PM B801**

(Student) High Performance Wafer-Scale Metal-Insulator-Semiconductor Photoanodes for Solar-Driven Water Splitting

Soonil Lee and Edward T. Yu; The University of Texas at Austin, United States

Solar-driven water splitting offers a promising and environmentally friendly route for conversion of renewable solar energy to hydrogen gas that can serve as a transportable fuel, chemical feedstock, or energy storage medium. Various semiconductor materials have been studied for use as the light absorption layer in photoelectrochemical (PEC) cells designed to execute reduction and/or oxidation of water to create hydrogen and oxygen molecules, respectively. Among those materials, Si as the light absorber in PEC cells is especially attractive due to its moderate bandgap, high charge mobility, diffusion length, cost efficiency, and scalability in manufacturing. To improve the stability of Si-based PEC cells in operation, metal-insulator-semiconductor (MIS) structures have been widely used for high-performance Si-based photoanodes and photocathodes. For photoanodes, a metal catalyst improves the oxygen evolution reaction (OER) kinetics and the insulating layer protects the Si surface from corrosion. Typically in such structures, the photogenerated charges must be extracted through the insulating layer via tunneling so that a very thin insulating layer is required for efficient operation. However, a thick insulating layer is desirable for long-term stability. Therefore, optimizing the insulating layer thickness is important for both stable and efficient Si-based MIS photoanodes. In this work, we employ a simple and highly scalable method to fabricate high performance Si-based MIS photoanodes with localized conduction paths through the thick SiO$_2$ insulating layers and demonstrate its application to the fabrication of wafer-scale photoanodes. The localized conduction path enables low-resistance charge extraction even through thick insulating layers, and this approach has been shown in our previous work to yield photoanodes with excellent stability. In addition, we demonstrate a two-step NiNiFe electrodeposition process to create efficient OER catalysts. The NiNiFe catalyst layers increase Schottky barriers between Si and metal catalyst and lower the photoanode onset potential, improving applied bias photon conversion efficiency (ABPE) by a factor of more than two compared to a Ni catalyst, to 2.36. The fabricated wafer-scale photoanodes show low onset potential 0.9 V vs. NHE and saturation current density of 25 mA/cm$^2$ under outdoor solar illumination. Excellent device stability is also achieved. Similar approaches are also under development for wafer-scale fabrication of Si-based MIS photocathodes for the hydrogen evolution reaction (HER) in solar water splitting.
A major challenge in the field of solid oxide fuel cell development is the long-term durability of system and cell components. Last decades, a huge number of long-term durability tests have been carried out on SOFC materials and complete systems, aiming at extreme low degradation rate over the required life expectancy of at least 5 years. Even though an extensive degradation mechanism resulting in the severe failure of the cell components has been revealed. Herein, we introduced a highly robust GDC buffer layer that completely overwhelms the interdiffusion of cell components during high-temperature operation. This buffer layer is fabricated via a multi-layer green film lamination approach, in which the NiO-YSZ, NiO-ScCeSZ, ScCeSZ, and GDC green films were co-laminated by warm iso-static pressing and co-sintered. This green film lamination process improved the interfacial connectivity and packing density of both ScCeSZ and GDC layers. Thus, the interdiffusion between the cathode to the electrolyte is efficiently suppressed during high-temperature operation. The multi-layer anode supported cell exhibited a very low degradation rate of 0.1%/kh, which fulfills the critical life expectancy benchmark for the commercialization of technology. This work presents a facile, cost-effective, scalable, and reproducible technique for mass production of highly reliable and robust anode-supported SOFC.

**2:10 PM BB03**

**PIFM (Photo Induced Force Microscopy) Based Nanoscale IR Spectroscopy and Imaging in Energy Research**

Song Xu and Derek Nowak; Molecular Vista, United States

Correlating spatial chemical information with the morphology of closely packed nanostructures remains a challenge for the scientific community. For example, supramolecular self-assembly, which provides a powerful and low-cost way to create nanoscale patterns and engineered nanostructures, is not easily interrogated in real space via existing nondestructive techniques based on optics or electrons. A novel scanning probe technique called infrared photoinduced force microscopy (IR PIFM) directly measures the photoinduced polarizability of the sample in the near field by detecting the time-integrated force between the tip and the sample. By imaging at multiple IR wavelengths corresponding to absorption peaks of different chemical species, PIFM has demonstrated the ability to spatially map nm-scale patterns of the individual chemical components of two different types of self-assembled block copolymer films. With chemical-specific nanometer-scale imaging, PIFM provides a powerful new analytical method for deepening our understanding of nanomaterials.

We will discuss three topics that demonstrate the application potential of PIFM application in energy research:

1. Nanometer resolution chemical analysis of a solar cell material, the ternary cation halide Cs$_x$FA$_{1-x}$MA$_{0.2}$Pb$_{1.8}$Bi$_{0.2}$I$_{3}$ (Cs-FAMA), based perovskite solar cell.
2. PIFM chemical imaging of a low cost high performance polymer solar cells with donor poly[(thiophene-alt-(6,7-difluoro-2-(2-hexyldecyloxy) quinoxaline)] (PTQ10).
3. PIFM chemical imaging of lithium-ion migration during the charging process. We observed the high resolution mapping of delithiation process.

**2:30 PM BB04**

**Student** Porous Current Collector Network Materials for High-load Li-Ion Battery Cathodes

Michael Lee, Navin Verma, Lalith Rao, Christopher Brooks, Jay Sayre, Hanna Cho and Jung Hyun Kim; The Ohio State University, United States; Honda R&D Americas, LLC, United States

The demand for Lithium Ion Batteries (LIBs) in the energy, transportation, and consumer sectors has led to widespread investigation of approaches for increasing the energy density and rate performance of batteries. In order to overcome the rate limitations of ionic diffusion, production batteries are limited to relatively thin layers of active material in both electrodes (100um). This structure, when layered, results in a high volume and mass of passive material in the battery cell and offers the potential for energy density and performance increases if the electrode porosity and ionic resistivity can be adequately reduced. To this end, many groups have proposed 3D electrode materials structured by a variety of methods, from laser ablation to freeze casting, but none have proven economical and scalable enough for widespread implementation. To this end, we have investigated the performance of a porous aluminum current collector material which enables new 3D electrode geometries to be fabricated without these specialized methods. We began with the hypothesis that the use of a porous aluminum material could improve electrode performance in two ways. First, the experimental current collector would create an unbroken electrically conductive network of aluminum strands spanning the full thickness of the electrode, improving the electrical conductivity to a degree impossible in traditional electrodes of the same thickness. Second, we hypothesized that cracking and delamination behaviors which were found to hurt the performance of traditional thick electrodes would align with the strands of current collectors in the porous electrodes, enhancing the ionic conductivity. We informed these hypotheses with parameters based on physics-based computational modelling, allowing us to select behavior-optimized electrode characteristics.

We fabricated a series of electrodes using Lithium Iron Phosphate (LiFePO$_4$) as an active material and 95% porous aluminum from the Sumitomo Electric Industries’ “Celmet” line as a current collector, and measured the effects of composition, mass loading, degree of calendaring, and other key parameters on cell performance at variable rates of both charge and discharge. We found that, controlling for other electrode parameters, our electrodes could achieve up to 6 times the active material loading of traditional thin electrodes while performing comparatively well when discharged at C-rates beyond 1C. We also observed favorable electrode cycle life. To support this understanding, we comprehensively characterized the material structure and compositional heterogeneity before and after testing via SEM, XRD, and other methods. Our findings indicate that, based on electrode performance and manufacturing accessibility, 3D thick electrodes manufactured by this method have the potential to significantly improve battery energy density.

**2:50 PM BB05**

**Student** Strategy to Passivate High-Voltage Spinel Cathode-Electrolyte Interfaces (CEI) in Li-ion Batteries

Xinwei jiao, Megen Thompson, Neel K. Kriener, Jay Sayre and Jung Hyun Kim; The Ohio State University, United States; Nexus, United States

The LiNi$_{0.5}$Mn$_{1.5}$O$_4$ (LNMO) spinel cathode has been extensively researched as a promising candidate for next-generation Li-ion batteries owing to its high operating voltage (~ 4.7 V vs Li) and high...
specific energy (650 Wh/kg). In addition to this, its cobalt-free composition and excellent rate capability due to three-dimensional Li+ diffusion makes it particularly attractive for a wide range of applications. However, the high operating voltage in full-cells (LNMO Graphite) triggers unwanted parasitic reactions at the electrode/electrolyte interface which lead to active Li+ consumption and consequent capacity fading. Elemental substitution of Ni/Mn is a very actively pursued strategy to alleviate the capacity fading. In particular, Ti-substitution for Mn in LiNi0.5Mn0.5Ti1-xO2 (LNMT) has improved the full-cell performances as evidenced by (i) higher capacity retention and Coulombic efficiency and (ii) lower oxidative reaction and self-discharge rates. The primary improvement mechanism of the Ti-substitution in LNMT is a formation of Ti-enriched passivation layer at the expense of initial Mn-dissolution at the cathode-electrolyte interface (CEI). Once generating the passivation layer, further Mn-dissolution became suppressed. Despite these results, carbon conductor (Super P) inside cathode still actively oxidizes the electrolyte due to its good electrical conductivity and large surface areas.

In this regard, we adopted advanced binders to passivate the carbon conductors for the LNMT cathodes. Polyvinylidene fluoride (PVdF) has been used as the binder in cathodes due to its electrochemical stability. However, PVdF does not offer the effective passivation of carbon conductors, while suffering from mediocre adhesion strength and raising environmental concerns by using N-M ethyl-2-pyrrolidone (NMP), a toxic organic solvent. Studies have shown that advanced aqueous binder chemistries can be used to create an effective passivating layer at the cathode-electrolyte interface, improve adhesion strength and eliminate the use of toxic organic solvents. Among them, lithium polycrylate (LiPAA) has demonstrated positive multifunctions such as proton scavenging, donating Li+ and effective passivation of both carbon and active material particles. Our full-cell testing data showed that the LiPAA binder in LNMT cathodes delivered an improved cycle life and a lower cell impedance compared to those of PVdF binder in LNMT cathodes. To better understand the characteristics of the CEI passivation on the LiPAA and LNMT cathodes, we will discuss about the various surface analyses of the fresh and aged electrodes using XPS, Raman, and HR-TEM.

3:10 PM Refreshment Break

3:30 PM BB06

(Student) Study of V205/LiPON Interface Using Depth-Resolved Cathodoluminescence Spectroscopy Pablo Rosas Martinez1, Zachary Levy1, Victoria Ferrari3, Mitchell Walker2, David Stewart1 and Leonard J. Brillison2, 1The Ohio State University, United States; 2University of M aryland, United States; 3Northwestern University, United States

Lithiated V205 has shown great potential as a candidate cathode material for solid-state batteries. Usually, LiPON is a common choice of a solid electrolyte due to its stability in a large voltage window and it can be manufactured using different systems such as ALD and rf-sputtering. In order to improve the applications of solid-state batteries, it is important to understand the process of lithiation that occurs when the battery is cycled. While cycling the battery system, the V205/ LiPON battery system lithiates. With enough lithiation, the battery may undergo an irreversible phase change and can degrade over time. Pure V205 has been shown to have several characteristic emissions, such as 1.8eV/2.0eV, 2.7, 3.0, 3.3, 3.7, and 4.0 eV[1]. The 1.8eV/2.0eV is called the split-off band, which corresponds to the V3d3z/2 -2p2x/2p2y states. The “split-off” part signifies a gap in the density of states between the two peaks (1.8/2 eV) and the V3d t2g conduction bands [1]. As V205 is lithiated, the split-off band decreases, most likely due to lattice distortion as V205 undergoes a phase change. In order to conduct this experiment, multiple thin films of V205/LiPON were sent to us by Dr. David Stewart and his graduate student Victoria Ferrari. These thin films were made by both co-sputtering V205 and Li2O, and then sputtering LiPON on top, and by electrochemically cycling V205 under LiPON, in order to achieve different levels of lithiated V205/LiPON. X-ray Photoemission Spectroscopy (XPS) was also conducted on pure lithiated V205 versus depth to track the lithiation throughout V205. We then proceeded to use Depth-Resolved Cathodoluminescence Spectroscopy (DRCLS) to study the band structure of various amounts of cyclized V205/LiPON. Using Monte Carlo simulations to extract the maximum penetration depth of secondary electrons at a particular beam energy, we can precisely observe different characteristic emissions of V205/LiPON at various depths.

3:50 PM BB07

(Student) Comparing Performance Enhancement by Different Carbon Additives for Si Anodes in Lithium-Ion Batteries Jun Wei Yag, Jung Hyun Kim and Hanna Cho; The Ohio State University, United States

In recent years, following the increasing demand for Lithium-ion (Li-ion) batteries with higher energy density, interest in Si-based anodes has soared. Si-based anode holds superior theoretical capacity (4200mAh/g) when compared to traditional graphite anodes (372mAh/g). However, Si-based anode suffers from large volume change and poor electronic conductivity. To resolve the former issue, Si nanopowder has been used because nano-sized Si experiences faster relaxation of mechanical stress caused by the volume expansion. To address the latter issue, we investigated the effect of carbon conducting additives on the electrochemical performance of Si anodes.

The baseline Si-anode is made using conductive carbon black (Super P Li™) which consists of ~50 nm scale carbon particles. To enhance carbon network and improve the electron transport within the anode microstructure, we employed carbon nanotubes (CNT) from Alidrich and carbon nanofibers (CNF) from Alidrich. CNF’s specification is 100 nm in diameter and 20-200 micro m in length, while CNT’s specification is 6 - 13 nm in diameter and 2.5 - 20 micro m in length. Although adopting the CNF or CNT in Si anode would not be a new approach, there is lack of systematic work to compare and understand the mechanisms in which CNF and CNT improve the performance of Si anodes.

In this work, different percentages of CNF and CNF (calculated based on total weight of conductive carbon content) were added to Si-anodes. Understanding of the performance difference is done by examining electrochemical performances and microstructure. Surface morphology of the anodes before and after cycle aging is
studied with the help of scanning electron microscopy (SEM). The results revealed significantly different quality of coated anode surfaces; 5wt% of CNT and above suffers from the poor surface coating, whereas CNF maintained good quality coating throughout. For electrochemical characterization, galvanostatic cycling, electrochemical impedance spectroscopy (EIS), and fast charging/discharge capability tests were performed. Data analysis showed that CNT and CNF both, helped improved the capacity retention and fast charge/discharge capability, albeit to different extend. Linking this to EIS results, reveals that the improvement seen are from lower early cycle change transfer impedance and lower late cycle loss of contact impedance. When comparing between anodes with CNT and CNF, it is revealed that performance of anode with CNT is sporadic, which could stem from the inconsistency in surface coating seen in SEM images. However, anodes with CNF followed a predictable trend of higher CNF content equaling better performance. Overall, this work proofs that both materials provide different level of improvement to the cell performance, with CNF showing larger improvement in performance. Future work can be aimed investigating origin of the bad surface coating seen in Si anode with CNT and experimenting on different types of CNT, such as single walled, multi walled and double walled to further understand the contribution of conductive additive on the performance of Si anode.

4:10 PM BB08
(Student) Enabling High-Rate Long-Life Span Lithium-Sulfur Batteries via Stereolithography Technique and Oxidative Chemical Vapor Deposition
Yuxuan Zhang, Han Wook Song and Sungwan Lee
Purdue University, United States; Korea Research Institute of Standards and Science, Korea (the Republic of)
Enhancing battery energy storage capability and reducing the cost per average energy capacity is urgent to satisfy the increasing energy demand in modern society. The lithium-sulfur (Li-S) battery is especially attractive because of its high theoretical specific energy (around 2600 W h kg⁻¹), low cost, and low toxicity. Despite these advantages, the practical utilization of lithium-sulfur (Li-S) batteries to date has been hindered by a series of obstacles, including low active material loading, shuttle effects, and sluggish sulfur conversion kinetics. The traditional 2D planar thick electrode is considered as a general approach to enhance the mass loading of the Li-S battery. However, the longer diffusion length of lithium ions, which results in high tortuosity in the compact stacking thick electrode, decreases the penetrability and the ability of the electrolyte into the entire cathode. An attempt to induce catalysts in the cathode was made to promote sulfur conversion kinetic conditions, catalysts based on transition metals suffered from the low electronic conductivity and some elements (i.e.: Co, Mn) may even absorb and restrict polysulfides for further reaction.
To mitigate the issues listed above, herein we propose a novel sulfur cathode design strategy enabled by additive manufacturing and oxidative chemical vapor deposition (oCVD). Specifically, the cathode is designed to have a hierarchical hollow structure via a stereolithography technique to increase sulfur usage. Microchannels are constructed on the tailored sulfur cathode to further fortify the wettability of the electrolyte. The as-printed cathode is then sintered at 700 °C in a N₂ atmosphere in order to generate a carbon skeleton (i.e.: carbonization of resin) with intrinsic carbon defects. The intrinsic carbon defects are expected to create favorable sulfur conversion conditions with sufficient electronic conductivity. In this study, the oCVD technique is leveraged to produce a conformal coating layer to eliminate shuttle effects. Identified by scanning electron microscopy and energy-dispersive x-ray spectroscopy mapping characterizations, the oCVD PEDOT is not only covered on the surface of the cathode but also the inner surface of the microchannels. High resolution x-ray photoelectron spectroscopy analyses (C 1s and S 2p orbitals) between pristine and modified sample demonstrate that the high concentration of the defects have been produced on the sulfur matrix after sintering and posttreatment. In-operando XRD diffractograms show that the Li-S is generated in the oCVD PEDOT-coated sample during the charge and discharge process even with a high current density, confirming an eminent sulfur conversion kinetic condition. In addition, ICP-OES results of lithium metal anode at different states of charge (SoC) verify that the shuttle effects are excellently restricted by oCVD PEDOT. Overall, the high mass loading (> 5 mg cm⁻²) with an elevated sulfur utilization ratio, accelerated reaction kinetics, and stabilized electrochemical process have been achieved on the sulfur cathode by implementing this innovative cathode design strategy. The results of this study demonstrate significant promises of employing pure sulfur powder with high electrochemical performance and suggest a pathway to the higher energy and power density battery.

4:30 PM BB09
(Student) Optimization of Li₂B₂O₅ Interlayer for Garnet-Based All-Solid-State Lithium Metal Batteries
Zhenghuan Tang; The Ohio State University, United States
Recently Solid-State Battery has received increased attention as the next generation energy storage device due to its high energy density, improved safety, and thermal stability. Among various types of solid electrolytes (SE), lithium (Li)-stuffed garnet-type Li₁ₓLi₄ₓTa₂O₇ (LLZT) delivered high Li ion conductivity (~10⁻⁴ S/cm) and wide electrochemical stability window. Despite such promising ionic conductivity, there are few technical challenges that prevent the implementation of LLZT in practical battery cells. First, LLZT suffers from a high interfacial resistance due to its poor wettability in contact with Li metal anode. Second, LLZT suffers from Li-dendrite penetration through grain boundaries during cycling. It was reported that grain boundaries have high electrical and low ionic conductivities which favors Li-ions and electrons to nucleate and form Li metal. Additionally, poor wetting between Li-anode and LLZT causes partial contacting at the Li/SE interface. In result, contacting area at the interface are limited to several small hot spots. Therefore, current is focused on those small spots and more Li nucleate and deposit at these hot spots during cycling, which eventually aggravates Li penetration into SE. M any strategies such as element doping, in-situ Solid Electrolyte Interface formation, and interlayer engineering have been proposed to improve the issues. In our study, we chose to apply an amorphous glass coating layer between Li-anode and LLZT because of its simple processibility, and potentials towards industrial manufacturing. Preparation of the amorphous glass layer coating onto the LLZT pellet requires melting the glass by heating above its melting temperature followed by fast cooling. Therefore, melting temperature of the coating layer(< 1000°C) is be one of the important criteria because we want to avoid unwanted reactions at
the interface and maintain mechanical integrity of the cell at heat
treatment temperature. In addition, the coating layer should have a
moderate ionic conductivity (>10⁻⁴ S/cm) which does not sacrifice
the overall conductivity. Various materials have been proposed,
and we have selected the materials to LiBO₂ (LBO) due to its low
melting point (~700°C), good stability between Li metal and LLZT,
and moderate ionic conductivity (~10⁻⁴ S/cm). In the study, we
systematically controlled the critical parameters such as heating
rate, cooling rate, slurry composition, heat treatment temperature,
and heat treatment duration to improve coating quality. During
optimization process, we found that good coating quality required:
slow heating rate, low binder content in the slurry, moderate
cooling rate, heat treatment temperature and duration. Using the
optimized coating condition, we managed to obtain an 8-μm LBO
coating layer without cracks or pinholes. After coating the interlayer, we fabricated Li symmetric Swagelok cells using the
LBO-coated LLZT for electrochemical characterization and
uncoated LLZT for reference. Based on our Electrochemical
Impedance Spectroscopy (EIS) results, LBO coated symmetric cell
managed to reduce the interfacial resistance from 6000 to 400 Ω
cm². Secondly, we conducted a Critical Current Density (CCD)
test to study the tolerance against Li-dendrite penetration. LBO-
coated LLZT reached 0.4 nmA/cm² while bare LLZT only reached
0.1 mA/cm². Finally, we performed a cycling test which we
plate/strip the symmetric cells under 0.1 mA/cm² with a capacity of
0.05 mAh/cm². The bare LLZT cell failed after 10 cycles, but the
LBO-coated cell managed to stay operating without shortage for
93 cycles. Our optimization steps could be a useful guideline for
future researchers if they plan to apply coating using similar
method even with other materials. Furthermore, our results showed
a proof of concept that our optimized LBO amorphous glass
interlayer significantly improves LLZT performance by
suppressing Li dendrite growth and improving interfacial wetting.

4:50 PM BB10
(Late News) Rapid Thermochemical Solvent-Free Synthesis of
Crystalline Metal Borides and Their Investigation as Water
Splitting Electrocatalysts E dward Gillan; University of Iowa,
United States

Metal borides are often refractory solids that are produced from
higher energy process such as arc melting and high temperature
sustained heating. Elemental boron is itself a refractory solid and is
often used as a starting material. Solution precipitation routes can
form amorphous, structurally ill-defined metal borides that require
annealing to crystallize them. Transition-metal borides have very
long history as refractory materials and often are electrically
conducting. In recent years, metal non-oxides have been
tensively investigated as electroactive heterogeneous catalysts
and metal borides are beginning to find interest as water splitting
electrochemistry (hydrogen evolution and oxygen evolution
reactions, HER and OER). To better investigate the possible value
of refractory metal borides in electrocatalysis, it is useful to
develop facile and rapid synthetic strategies that can produce well-
deﬁned crystalline metal borides and composite structures. This
Late News presentation will describe our recent success using
reactive M@B₂ and Mg/B powder mixtures to rapidly reduce and
react with a series of anhydrous early and late metal halides to
produce crystalline metal borides in seconds (e.g., TiB₂, ZrB₂,
CoB, and NiB). Notably, these syntheses are oxygen and hydrogen
free and produces several hundred milligrams of product for
analysis and electrocatalysis investigations. The tunability and
thermochemistry of these exothermic and solvent-free solid-state
metathesis (SSM) reactions will be described. In some cases, it is
possible to mix multiple precursors together to form composite
structures such as TiB₂/TiN and TiB₂/CoB materials. Several
crystalline metal borides were investigated as HER and OER
electrocatalysts in acidic and basic solutions. In some cases, earth
abundant metal borides show appreciable HER and OER activities
in pure form and composite structures.

5:10 PM BB11
(Late News) Atomistic Simulations of Reaction Kinetics at
Electrochemical Interface Y uanyue Liu; University of Texas at
Austin, United States

Electrochemistry at solid-water interface lies at the center of many
technologies to address energy and environment challenges.
However, there is a general lack of kinetic information (e.g.
activation energy) at atomic scale, especially for electrochemical
steps. One of the major challenges is the lack of computational
methods to effectively simulate the electrochemical kinetics at
solid-water interface. Here we present an effective first-principles
model, and use it to elucidate the atomic mechanisms of single
metal atom in graphene for carbon dioxide reduction and oxygen
reduction reactions [1,2,3]. This method enables us to explain the
puzzling experiments that cannot be explained by conventional
models focusing on thermodynamics.

10.1021/jacs.1c02186
10.1021/jacs.9b13872
10.1021/jacs.8b03002
Piezoresistive Sensing PAAMPSA/PANI/PA Polymer Complex (Student, Late News) Effects of Small Molecule Dopants in neuromorphic computing applications.

Penners2,1, Katherine Webb3,1, Sarah Veres1, Gina Lusvardi1, Sofia Luna1, George Chen1 and Evan Wujcik1; 1The University of Alabama, United States; 2New Mexico Institute of Mining and Technology, United States; 3University of Florida, United States

Our electrochemical random access memory (ECRAM cells show promising as an analog resistive synapse for future in-memory and analog state retention at elevated temperatures. ECRAM is highly linear and symmetric switching with very low read and write currents (<100 nA), and endurance of 300 million read/write cycles.

To create a more predictable analog resistive memory, we incorporated a yttria-stabilized zirconia (YSZ) solid electrolyte sandwiched between the two MIECs like TiO2-x and WO3-x. During the writing, the solid electrolyte blocks direct electronic current and joule heating; instead, only electrochemical currents are allowed to move oxygen vacancies between the MIECs. The oxygen vacancy concentration in the MIEC is used to store analog resistance states. This developing device type is projected to outperform traditional memory devices in the visible-light wavelength range was greater than 90%.

The thickness of the RS layer and the sputtering conditions of the IGZO RRAM were modified to tailor the property of the RS layer. A SiO2 inserting layer can offer extra difficulty meeting the requirements of future data storage device design the TE material's diffusion capabilities to the RS layer and restrict the efficiency of traditional computer designs. Due to memory technology limitation.

In conclusion, transparent IGZO-based RRAMs have been created. Top electrode materials. For our IGZO layer, the best ratio of O2/Ar sputter gas, its electrical properties can be easily tuned. The IGZO atoms. More importantly, by controlling the oxygen ratio in the sputter gas, its high transparency and high atomic diffusion property of oxygen atoms. The IGZO switching layer because of its high transparency and high atomic diffusion property of oxygen atoms. The IGZO switching layer attracts great attention for the RRAM switching layer.

Indium gallium zinc oxide (IGZO) has been applied to the thin-film transistor (TFT), thus, it is very attractive for In-Memory Computing

Nonvolatile Analog Electrochemical Random Access Memory

8:20 AM

FRIDAY ORAL PRESENTATIONS
8:20 AM CC01
Nonvolatile Analog E electrochemical Random Access M emory for In-Memory Computing
Yiya Li1; University of Michigan, United States

In-memory computing using analog resistive memory can significantly reduce energy and latency in data-intensive tasks like machine learning. Resistive random access memory (RRAM) stores resistances states through the motion of oxygen vacancies in mixed ionic and electronic conductors (MIEC), whereby the oxygen vacancies act as electron donors. Existing resistive memory suffers from memory retention and stochastic switching due to the creation of a nanosized 1D conducting filament. As a result, filament-based RRAM has struggled with reliable analog switching.

To create a more predictable analog resistive memory, we incorporated an yttria-stabilized zirconia (YSZ) solid electrolyte sandwiched between the two MIECs like TiO2-x and WO3-x. During writing, the solid electrolyte blocks direct electronic current and joule heating; instead, only electrochemical currents are allowed to move oxygen vacancies between the MIECs. The oxygen vacancy concentration in the MIEC is used to store analog resistance states. Our electrochemical random access memory (ECRAM) cells show highly linear and symmetric switching with very low read and write currents (<100 nA), and endurance of 300 million read/write cycles. Moreover, our ECRAM cells show long-term nonvolatile analog state retention at elevated temperatures. ECRAM is highly promising as an analog resistive synapse for future in-memory and neuromorphic computing applications.

8:40 AM CC02
(Student, Late News) Effects of Small Molecule Dopants in Piezoresistive Sensing PAAm/PSA/PANI/PA Polymer Complex
Colton Duprey1, Hadi Rouhi1, Elham Ghalavand1, Nicole Penners1,2, Katherine Webb1,2, Sarah Veres1, Gina Lusvardi1, Sofia Luna1, George Chen1 and Evan Wujcik1; 1The University of Alabama, United States; 2New Mexico Institute of Mining and Technology, United States; 3University of Florida, United States

As wearable electronics increase in popularity, it becomes evident that a sensitive, flexible, comfortable, and biologically compatible material is required to make an optimal wearable biosensor. As a result, polymeric piezoresistive sensors show great promise in movement monitoring and biosensing. Their polymer composition provides flexibility and stretchability which allows for unique sensor applications where traditional metallic sensors are too brittle and rigid. The polymer complex to be used as a strain sensor is composed of a templating poly(3-acrylamido-2-methyl-1- propane sulfonic acid), polyaniline, and a small molecule dopant, originally phytic acid. By substituting the small molecule dopant for various other small molecule acids, the impacts the various dopants have on the strain sensor’s conductivity, mechanical properties, and piezoresistive sensitivity can be studied. Typically, small molecule dopants that increase conductivity decrease stretchability and mechanical stability, which stems from more acidic dopants being able to protonate and facilitate ion transport throughout the sensor. On the opposite hand, functional groups with increased hydrogen bonding tend to increase mechanical properties, as well as allow for autonomous self-healing. By increasing our understanding of the impact these various dopants have on the properties of the strain sensor, we can tailor the usage of these small molecule dopants as we try to increase the sensitivity and conductivity of our sensor for usage in biosensing and kinesiological monitoring applications.

9:00 AM CC03
(Student) Influence of Oxygen Vacancy and Top E electrode on Switching Behavior of InGaZnO Based Resistive Random Access M emory
Fei Qin1, Han Wook Song2 and Sunghwan Lee1; 1Purdue University, United States; 2Korea Research Institute of Standards and Science, Korea (the Republic of)

Biomimetic synaptic processes, which are imitated by functional memory devices in the computer industry, are a key focus of artificial intelligence (AI) research. It is critical to develop a memory technology that is compatible with Brain-Inspired Computing in order to eliminate the von Neumann bottleneck that restricts the efficiency of traditional computer designs. Due to restrictions such as high operation voltage, poor retention capacity, and high power consumption, silicon-based flash memory, which restricts the efficiency of traditional computer designs, is being replaced by neuromorphic computing. Resistive random-access memory (RRAM) has sparked intense investigation because of its simple two-terminal structure: two electrodes and a switching layer. RRAM has a resistive switching phenomenon which is a cycling behavior between the high resistance state and the low resistance state. This developing device type is projected to outperform traditional memory devices. Indium gallium zinc oxide (IGZO) has attracted great attention for the RRAM switching layer because of its high transparency and high atomic diffusion property of oxygen atoms. Moreover, by controlling the oxygen ratio in the sputter gas, its electrical properties can be easily tuned. The IGZO has been applied to the thin-film transistor (TFT), thus, it is very promising to integrate RRAM with TFT.

In this work, we proposed IGZO-based RRAMs. ITO was chosen as the bottom electrode towards achieving a fully transparent memristor. As for the IGZO switching layer, we varied the O2/Ar ratio during the deposition to modify the oxygen vacancy of IGZO. Through the XPS measurement, we confirmed that the higher O2/Ar ratio can lower the oxygen vacancy concentration and lower the ratio. We also chose ITO as the top electrode, and also, for the comparison, two active metals copper and silver were tested for the top electrode materials. For our IGZO layer, the best ratio of O2:Ar is the middle value. And copper top electrode device has the most stable cycling switching and the silver one is perfect for large memory window, however, it encounters a stability issue. The optical transmission examination was performed using a UV-Vis spectrometer, and the average transmittance of the complete devices in the visible-light wavelength range was greater than 90%, indicating good transparency. 50nm, 100nm, and 150nm RS layers of IGZO RRAM were produced to explore the thickness dependency on the characteristics of the RS layer. Also, because the oxygen vacancy concentration influences the RS and RRAM performance, the oxygen partial pressure during IGZO sputtering was modified to maximize the property. Electrode selection is critical and can have a significant influence on the device’s overall performance. As a result, Cu TE was chosen for our second type of device because Cu ion diffusion can aid in the development of conductive filaments (CF). Finally, between the TE and RS layers, a 5 nm SiO2 barrier layer was used to limit Cu penetration into the RS layer. Simultaneously, this SiO2 inserting layer can offer extra interfacial series resistance in the device, lowering the off current and, as a result, improving the on/off ratio and overall performance.

In conclusion, transparent IGZO-based RRAMs have been created. The thickness of the RS layer and the sputtering conditions of the RS layer were modified to tailor the property of the RS layer. A series of TE materials and a barrier layer were incorporated into an IGZO-based RRAM and the performance was evaluated in order to design the TE material’s diffusion capabilities to the RS layer and the BE. Our positive findings show that IGZO is a potential material for RRAM applications and overcoming the existing memory technology limitation.
M emistor, which simply consists of a switching layer inserted between two electrodes, is one of the most strong candidates to become a device-platform for imitating the principal characteristics of the biological neural network due to its nonlinear and dynamic electrical characteristics depending on the history of applied electrical programming [1-3]. In this study, we fabricated a SiO$_x$ nanorod memristor using E-beam evaporator with glancing angle deposition at the wafer-scale and utilized the device as an artificial neuron for probabilistic computing applications [4]. Notably, the SiO$_x$ nanorod structure provides the random distribution of multiple nanopores all across the active area, capable of forming a multitude of Si filaments at many SiO$_x$ nanorod edges after the electromigration process. This can facilitate probabilistic switching that can mimic integrate-and-fire signaling and the stochastic dynamics of biological neurons with very high dynamic range (~$-5.15 \times 10^9$) [4].

Different probabilistic activation (ProbAct) functions in a sigmoid form are implemented, showing its controllability with low variation by manufacturing and electrical programming schemes. Then, as a proof of concept, based on the suggested memristive neuron, we demonstrated the self-resting neural operation with local circuit configuration and electrical programming schemes. Then, taken all together, our study shows the availability of the designed SiO$_x$ nanorod memristive neuron for probabilistic neural networks that can be efficiently used for a variety of uncertainty quantification problems.

References


hardware vision platform for designing next-generation machine intelligent systems.

10:40 AM CC07
(Student) Spike-Timing Based Adaptive Photo Encoder Considering Monolayer MoS2-Based Memtransistors
Dipanjan Sen, Shiva S. Radhakrishnan, Shakya Chakraborti, M. ayukhi Das, Thomas Schranghamer, Amritanand Sebastian and Saptarshi Das; The Pennsylvania State University, United States

Bio-inspired devices and systems have effectively showed its potential in the current era of neuromorphic chips. Moreover, it has also depicted the capability to bridge the gap between natural and artificial intelligence. It must be highlighted that imitating the functionalities of a brain paves the way for smart computing with an intent to solve complex problems. In this context, the spiking neural network’s (SNNs) have captured a lot of attention as it mimics the processing of information with minimum energy consumption and faster inference. Note that, the SNNs tend to convert the external stimuli into corresponding spike trains by exploiting someafferent neurons. Here, we have designed and fabricated an optoelectronic integrated circuit comprising of 21 memtransistors based on monolayer MoS2 for spike-timing dependent photo encoding in a neural network to that, we have demonstrated that the different intensities can be efficiently encoded into spike trains, where the time to the first spike determines the strength of the visual stimuli, i.e., higher illumination intensity generates earlier spikes and vice versa. Furthermore, the non-volatile storage and electrical programming capability of the photo sensitive memtransistors enables the encoder for photo encoding with controlled adaptivity that allows accelerated spike trains under low light condition and delayed spike trains under higher illumination intensities, respectively. Therefore, it can be inferred that our demonstration of the spike-timing based photo encoder exploiting the 2D memtransistors can be transformative for cutting-edge neuromorphic applications.

11:00 AM CC08
(Students) Ultralow-Power Photoactivated Spiking Silicon Neurons
Ragib Ahsan, Hyun Uk Chae and Rehan Kapadia; University of Southern California, United States

Human brains can perform complex computations with an unparalleled power efficiency that exceeds state-of-the-art digital computers by ~100,000 times. The spiking neurons in the brain are instrumental to achieving such extraordinary efficiency. There has been a great amount of effort put into emulating the spiking behavior of spiking neurons recently thanks to the emergence of phase-change alloys. We have performed atomic layer epitaxy of amorphous GeTe and polycrystalline TiN samples also dropped by scanning electron microscopy even after 500 cycles, and the samples remained insulating when four-point probe measurements were performed. Conversely, continuous Sb2Te3 film growth was observed after 500 cycles on amorphous GeTe with 3d5/2 core levels near 527 eV and 572 eV, respectively. Compared to Sb2Te3 reference spectra, the ratio of intensities also matches the expected stoichiometry. Moreover, the sheet resistance of amorphous GeTe and polycrystalline TiN samples also dropped noticeably. We will further consider atomic layer epitaxy of Sb2Te3 in upcoming experiments. The authors are grateful to ONR N0014-18-12511 for support and Penn State’s 2DCC through DM R-1539916 for epitaxial substrates.

11:20 AM CC09
Atomic Layer Deposition of Antimony(III) Telluride
James C. Carter, Ian Campbell, Ama Agyapong and Suzanne E. Mohney; The Pennsylvania State University, United States

Antimony(III) telluride has a layered structure with van der Waals bonds between Te atoms in adjacent quintuple layers. It is interesting as a topological insulator and because it is a component of phase-change alloys. We have performed atomic layer deposition of Sb2Te3 using bis(trimethylsilyl)tellurium and antimony(III) ethoxide, which are previously reported precursors.1 Bis(trimethylsilyl)tellurium was also used in some experiments. In this work, we studied growth on a variety of substrates using different surface preparations. Growth of a continuous layer with few cycles is highly dependent on the starting surface. On SiO2, incompletely coalesced islands were observed by scanning electron microscopy even after 500 cycles, and the samples remained insulating when four-point probe measurements were performed. Conversely, continuous Sb2Te3 film growth was observed after 500 cycles on amorphous GeTe, single-crystal Bi2Te3, and polycrystalline TiN films, only when subjected in situ to a remote Ar plasma before growth. X-ray photoelectron spectroscopy confirmed the presence of Sb and Te with 3d5/2 core levels near 527 eV and 572 eV, respectively.

12:50 AM CC10
(Students) Electrochemical Additive Manufacturing Producing Composite Materials for Electronics
Onsdoveren F. Demisse, Pawan Tyagi and Eva M utunga; University of the District of Columbia, United States

Due to tremendous potential to deliver unique features, not attainable by traditional manufacturing methods, 3D printed
electronics have caught the interest of industry and researchers in recent years. This new technology has the potential to revolutionize electronics device design and manufacturing methods. 3D printing involving porous conducting materials, composite materials with metal and polymer components, and microscopic particles encapsulated in copper like thin films can lead to new set of materials. Although multi-material additive manufacturing has advanced significantly in recent years, little progress has been made in the additive manufacturing of hybrid components. Here we discuss a low temperature 3D hybrid material printing method that can yield novel composite materials for futuristic computer hardware. We investigated electrochemical additive manufacturing(ECAM) method. The basic working principle of the ECAM machine we are developing is based on the transport of metal particles from ionic solution to the substrate covered with microscopic metallic powder. Metallic powder is dispersed on the substrate by a custom designed nozzle that serves two purposes: (a) control the metal particle dispersion rate on to the substrate, and (b) serve as the counter electrode to provide bonding between metal powders via electrodeposition. For example, ECAM can disperse ~10-50 µm nickel powder and produce copper thin film coating among particles. This approach creates a multi material composite at fast rate. A vast range of materials are possible via ECAM that can be tested for variety of computer heat control systems and other applications. These materials can also produce radiation and electro-magnetic protection casings for the application of computer hardware in challenging environments.

SESSION DD: Group III-Nitrides—Contacts and Novel Devices
Session Chair: Christian Wetzel
Friday Morning, July 1, 2022
Great Hall Meeting Room 3

8:20 AM DD01
(Student) Role of Point Defects and Compensation in the Formation of Ohmic Contacts to Mg-Doped GaN Cristyan E. Quiñones García1, Pegah Bagheri1, J Hyun Kim2, Dolar Kachharya3, Ronny Kirste2, Pramod Reddy2, Seiji Mita2, Erhard Kohn2, Ramón Collazo2 and Zlatko Sitar1,2; 1North Carolina State University, United States; 2A grit M Aterials, United States

In order to obtain low resistance ohmic contacts to p-type semiconductors, large ionized acceptor densities are required. This is difficult to achieve in GaN, as increasing the acceptor M concentration past a certain point (called the “knee behavior”) induces the formation of compensating point defects which reduce the net ionized charge, N+n. This is known as self-compensation and is usually attributed to the formation of charged nitrogen vacancies (VN), which act as donor-like defects. Therefore, in order to understand the formation of and achieve ohmic contacts to p-type GaN, a thorough understanding and control over the formation of compensating point defects in the high doping regime is necessary. In this work we demonstrate that improved ohmic contacts to p-type GaN can be achieved by suppressing the formation of VN via systematic chemical potential control (CPC) based point defect control. Accordingly, Mg-doped GaN samples were grown with V/III ratios varying from 200 to 8000 by increasing ammonia flow. By growing with higher V/III ratios through higher ammonia partial pressures, we provide nitrogen-richer conditions and consequently increase the chemical potential of nitrogen, and the formation energy of VN. This reduces VN incorporation and shifts the onset of the self-compensation towards higher Mg concentrations as evidenced via photoluminescence (PL) measurements.

Transmission line model (TLM) was used to analyze Ni/Au contacts to p-type GaN grown under these high V/III ratios. The specific contact resistance and threshold voltages were accordingly extracted using a method for analyzing non-ohmic contacts described by Sarkar et al. The alloyed contacts to samples grown at high V/III consistently showed lower contact resistance and threshold voltages with increasing Mg concentration. In fact, contacts with a threshold voltage of ~0 V were only obtained for samples grown with large V/III ratios, suggesting that the suppression of VN formation is necessary. Finally, we demonstrate that by growing a thin, heavily doped (|Mg| > 8x10^19 cm^-3) GaN layer with VN control on a more lightly doped (|Mg|~2x10^19 cm^-3) p-GaN layer, better ohmic contacts are achieved. Using reactive-ion etching (RIE) to expose the lower layer, TLM measurements were performed on both as grown and etched surfaces. The extracted threshold voltages and specific contact resistances on each of the individual layers clearly demonstrate that improved ohmic contacts are achieved by incorporating the heavily Mg-doped, VN controlled GaN layer. Potential application of these contacts to UV optoelectronics devices will be discussed.

References

8:40 AM DD02
Effect of Rhenium Layer Thickness and Annealing Temperature on the Surface Microstructure of Re-Al-Ni-Au Based Ohmic Contacts on n-Type GaN Amit P. Shah, Bhagyashri Chakile, Vivas Mathe and Arvind Bhattacharya; Tata Institute of Fundamental Research, India

Low specific contact resistivity ohmic contacts (ρ<10^6 Ω-cm^-2) with thermal and chemical stability play an important role in III-nitrides based optoelectronic, high temperature and high frequency devices. A Ti/Ai/Ni/Au based multilayer metallization is the most commonly used scheme and requires high temperatures (>800°C) to form reliable ohmic contacts. High temperature annealing can result in intermixing in the multi-quantum-well layers and introduce additional defects. There are very few reports on the microstructure analysis of the ohmic contacts formed on n-GaN substrates.[1]

Low specific contact resistivity ohmic contacts (ρ<5x10^5 Ω-cm^-2) were formed on n-GaN using Re-Al-Ni-Au based multilayer metallization [2]. In this work, we report the effect of rhenium (Re) layer thickness and annealing temperature on the microstructure of such Re-Al-Ni-Au based contacts. Several samples with Re thicknesses (10, 30, 60 nm) were prepared and annealed at 550°C, 650°C and 750°C temperatures. The resistivity was estimated using C-TLM measurements while AFM, GIXRD and SEM equipped with EDS were used to analyze the chemical composition and microstructure characteristics of the ohmic contacts.

For the sample with Re~30 nm thickness annealed at 650°C, 40 µm x 40 µm AFM scans show numerous islands with sizes up to 3 µm and average height of ~400-450 nm, much higher than the original metal stack thickness of 290 nm (Re, Al, Ni and Au~30, 100, 60 and 100 nm respectively). The RMS roughness is ~90 nm. We surmise that the islands are formed due to segregation of the metals.

For the sample with Re~30 nm thickness annealed at 650°C, the GIXRD profile shows several diffraction peaks corresponding to known inter-metallic phases of alloys of the Re-Al, Re-Ni-Al and Al-Au systems, indicating that there is a considerable intermixing of the metal layers. The diffraction peaks observed are mainly from different phases such as ReNiAl1, AlRe, AlAu and AlAu. We observe the same phases in other samples with different rhenium thickness and annealed at different temperatures. We believe that these inter-metallic phases are responsible for the lowering of the barrier height ΦB, and hence the reduction of
contact resistance. We have not observed any peak related to the phase AlAlu, which seems to be responsible for the lateral flow of the metal.

Energy dispersive spectroscopy (EDS) maps of the elements – rhenium, aluminium, nickel and gold – present in the metal stack were obtained to evaluate the spatial elemental distribution over the contact area. For the sample with Re–30 nm thickness annealed at 650°C, the SEM image of the annealed metal contact shows three distinct regions; region-A: dark isolated rectangular agglomerates, region-B: white layer surrounding the agglomerates and region-C: grey colored background. From the corresponding EDS chemical analysis for Re, Al, Ni and Au respectively, we observe that during annealing near the temperature where Al becomes liquid (660°C), the Al starts forming droplets which dissolves Ni to form crystalline Ni-Al alloy agglomerates (region-A). Due to migration of the agglomerates on the surface and coalescence, we get various sizes of isolated agglomerates distributed over the surface. The top Au layer cracks and accumulate around these agglomerates to form Al-Au alloy (region-B). The background consists of all the four metals (region-C). The contrast seen in the Re signal is likely to be influenced by the uneven thickness of the overlying agglomerates and the Al-Au alloy. The RMS roughness increase with temperature can be attributed to the formation, migration and coalescence of Ni-Al agglomerates.

References:

9:00 AM DD03
Development of Low Resistance Ohmic Contacts with Bilayer NiAl/Doped ZnO Thin Films to p-Type GaN

The fabrication of low-resistance and thermally stable Ohmic contacts is essential for the fabrication of reliable GaN power devices. In the particular case of the p-type GaN, a thin NiAl bilayer is commonly used for Ohmic contacts. However, Au metal contacts are quite expensive, incompatible with the complementary metal-oxide-semiconductor (CMOS) foundries and also have poor thermal stability. Thus, seeking an alternative that is affordable and thermally stable is crucial. In the present study, we investigate Au-free Ohmic contact formation on p-type GaN using a bilayer NiAl-doped ZnO (AZO) thin film. The Ni/AZO thin films were prepared by thermal evaporation and radio frequency (RF) magnetron sputtering, respectively. Careful studies were focused on identifying the role of process parameters such as layer thicknesses and annealing parameters: time, temperature and atmosphere in order to obtain an excellent Ohmic contact on p-GaN. Interestingly, structural, morphological and electrical properties of the Ni/AZO contacts deposited on the p-type GaN layer were analyzed in detail using X-ray diffraction (XRD), transmission electron microscopy (TEM) as well as circular transfer length model (c-TLM) techniques, respectively. Our results show that the contact resistance can be significantly reduced using an AZO/Ni bilayer with a suitable rapid thermal process. We demonstrate that specific contact resistance for AZO/Ni on p-GaN can reach a lowest value of 1.85×10^4 Ω·cm^2 for a sample annealed at 500°C in air ambient for 5 min with a 5 nm Ni layer. These results present also methods for improving the electrical properties of the contacts to p-GaN. Our work demonstrate that the bilayer Ni/AZO contact could be a suitable scheme for efficient GaN power diodes.

9:20 AM DD04
(Student, Late News) HTOL Reliability of Novel Re-GaN Schottky Diodes
Nathaniel O'Real, A. Alex Mollina-2, Guillermo Passrobles-1, Alexander Mundi-2, Burnel Clemmer-1, Matthew A. Porter-1, Christopher M artino-1, Todd R. Weatherford-2 and Suzanne M.ohnney-3

Vertical power devices fabricated on native bulk GaN substrates have demonstrated performance comparable to SiC power devices in recent research. While continuing improvements have been achieved in substrate quality and device performance characteristics, little research has been carried out on the reliability of metal-semiconductor interfaces under the levels of high current stress expected in power device operation. This work examines the reliability of Re-GaN Schottky interfaces under high current stress. Research on thermal stability of Re-GaN Schottky contacts through thermal annealing studies has shown that the barrier height of the contact is not reduced by annealing conditions up to 600 C, in contrast to more commonly used Pd-GaN contacts which degrade significantly in barrier height after similar thermal conditions. This stability makes Re-GaN a prime candidate for a Schottky contact with high stability under high current stress conditions, under which self-heating at the junction is expected to be significant. To carry out experimental studies, n-type GaN epitaxial layers were grown via MOCVD to a doping level of 2×10^{16} cm^-3 and a thickness of 11 um atop a n+ doped bulk GaN substrate. Re Schottky diodes were fabricated via e-beam deposition of Re followed by electroplating with 1 um of Au. Die were singulated and packaged on DBC Al₂O₃ ceramic substrates for testing. Testing under high temperature operating life (HTOL) conditions was performed using a novel automated stress-measure-stress system enabling time dependent measurements of the diode characteristics via IVT characterization. Devices were initially stressed under a time-dependent step-stress regime, in which the stress current density was stepped from 950 A/cm^2 to 2000 A/cm^2 in 150 A/cm^2 steps, and held at the stress current at each step for 6 hours and a package temperature of 30°C. Step-stress testing showed that the barrier height of the Schottky contacts remained stable with less than 1% degradation up to a stress current density of 1600 A/cm^2, after which the barrier height degraded quickly by over 10% from a maximum of 0.8 V. The ideality factor of the diode also degraded by 13% to a maximum of 1.3 above this stress current. Constant stress-measure-stress HTOL testing was also performed at current densities of 1500 A/cm^2, 1600 A/cm^2, 1700 A/cm^2, 1800 A/cm^2 and 2000 A/cm^2 at fixed package temperatures for a stress period of over 90 hours. The contact barrier height was found to remain stable for 1500-1700 A/cm^2 tests, while degrading by 16% and 11% for the 1800 A/cm^2 test. It was found that the degradation rate was not constant but changed rapidly at a time dependent upon the magnitude of the current density. There is also a degree of variation among the devices leading to these rates nonuniformly increasing. Subsequent tests will include HTOL testing on similarly fabricated Pd-GaN diodes as a basis for comparison. Based upon these results, Re-GaN Schottky contacts show promising stability under high current density stress conditions and are a prime candidate for Schottky contacts in large area vertical GaN power devices.

9:40 AM DD05
(Student, Late News) N-Polar GaN HEMTs with ALD HfO; as Gate Dielectric
Subhajit Mohanty1, Zhe Ashley Jian1, Z. Z. Shangyian, K. P. Namikkali, K. M. Almaha, S. U. K. A. Abor, United States; 2Naval Postgraduate School, United States; 3Avionics and H. M. A. Abor, United States

High power efficiency over wide range of frequency range has established GaN-based high electron mobility transistors (HEMTs) as-de-facto standard for RF power amplifiers in radars and high
frequency applications [1]. N-polar GaN has a natural back-barrier which offers several advantages over Ga-polar counterpart such as better 2DEG confinement, improved ohmic contact, output resistance and pinch-off characteristics [2]. Moreover, the frequency of operation can be increased by reducing gate length which can be suppressed by inserting a thick insulator layer between channel and gate metal. High-k dielectrics such as HfO2 with thick dielectric can be deposited without altering the gate capacitance. In this work, we demonstrate an N-polar HEMT with regrown contacts and implanted mesa isolation which exhibits low leakage and DC-RF dispersion. MOCVD-grown N-polar GaN HEMT structure commercially available from Transphorm Inc., was used for this study [3]. SiO2 and Al2O3 were used as the hard mask and etch stop to define the regrown area and a UID-GaN/m2 GaN was regrown in source/drain regions to minimize ohmic contact resistance. Device isolation was achieved by ion implantation with Aluminum to form high-resistive region between devices. Then, the sample underwent a sequence of wet cleaning, UV-ozone conditioning and in-situ ALD plasma treatment prior to deposition of thermal ALD HfO2. HfO2 was removed under the contact area using a BCl3-based dry etch and a hydrochloric acid wet etch was performed immediately before 30/200 nm of Ti/Au deposition by electron-beam evaporation. A very low M-etal-to-GaN contact resistance of 0.1 Ω-mm was measured from un-passivated Transfer Length Method (TLM) with sheet resistance (Rsh) of 292 Ω/sq. Finally, 30/420 nm of Ti/Au optical gate and contact pads were patterned via liftoff followed by 120 nm PECVD SiN passivation. A combination of a capacitance-voltage (C-V) measurement and gated TLMs (GTLMs) on passivated structure exhibited a 2DEG density of 1.38 × 10¹³ cm⁻² which increased to 200 nA/mm with an increase in VGD = 2 × 50 μm, L = 500 μm, Lgs = 400 nm, Ldo = 2.4 μm. The output characteristics demonstrated a maximum fT of 1.02 A/mm and an ON-resistance (ROH) of 1.26 Ω-mm at VGS = 0 V. The transfer characteristics showed a peak trans-conductance (gm) of 254 mS/mm, pinch-off voltage (Vp) of -7.3 V and a subthreshold swing of 135.7 mV/dec at VDS = 3 V. The device exhibited an OFF-state current of 1.5 × 10⁻¹⁵ A/mm at VDS = 3 V with Ion/OFF = 7.6 × 10⁹. The gate leakage current was very low (~10 nA/mm) which increases to 200 nA/mm with an increase in VDS = 15 V. The device exhibited decent DC-RF dispersion indicating the presence of surface traps between gate-drain region. The small-signal RF results were obtained using a Keysight N5247B network analyzer analyzer calibrated to the probe tips via a Short-Open-Load-Thru (SOLT) calibration method from an off-wafer impedance substrate standard. The device demonstrated a peak fT = 19.1 GHz (f1/f10% = 9.55 GHz) at VDS = 10 V and VGS = -3 V and a peak fmax = 69.5 GHz at VGS = 11V and VDS = -4V. HfO2 gate metal is effective in suppressing the gate leakage which shows promise for ultra-thin channel high-aspect ratio HEMT devices for high frequency applications. [1] U. K. Mishra et al., Proc. IEEE, vol. 96, no. 2, pp. 287–305, Feb. 2008. [2] M. H. Wong et al., Semicond. Sci. Technol., vol. 28, no. 7, p. 074009, Jul. 2013. [3] D. Bisi et al., 2021 IEEE 8th Workshop on Wide Bandgap Power Devices and Applications (WIPDA), 2021, pp. 250–254. 10:20 AM DD06 (Student) N-Polar GaN Photocathodes Stabilized with h-BN Emma Brooks1, Vincent E. Meyers2, Benjamin M. Ewen3, L. D. Bell1 and Fatemeh (Shadi) Shahedipour-Sandvik1; 1SUNY Polytechnic Institute, United States; 2Case California Institute of Technology, United States III-nitride photocathode detectors provide picosecond response, low noise, single photon detection across a broad spectrum spanning from IR to UV wavelengths. N-polar III-nitride photocathodes have shown particular promise in simulation as well as experiment due to positive surface charge produced by the structure depleting and polarization. However, the N-polar surface is challenged by a thicker native oxide, and N-polar photocathodes must be etched using HCl to remove this oxide prior to measurement or packaging. Surface encapsulation with 2D materials has previously been proposed for alkali photocathodes. 2D materials are advantageous as they are molecularly impermeable, allowing surface stabilization without detrimental widening of the surface potential well. Simulations of Cs2Sb photocathodes with BN suggest improved quantum efficiency due to the smaller work function of BN compared to the Cs2Sb bulk. Surface stabilization with 2D materials have also been shown experimentally with graphene coatings on K, C, Sb, and Cu photocathodes. A monolayer hexagonal (h-)BN surface stabilization of N-polar GaN photocathodes is reported here for the first time. N-polar GaN photocathodes consisting of 450 nm p-GaN/10 nm u-GaN cap were grown via metal organic chemical vapor deposition (MOCVD). The photocathode was cleaned in HCl to remove surface oxide and contaminants immediately prior to placement of monolayer h-BN on the surface through a wet transfer process. A control sample of N-polar GaN photocathode with h-BN stabilizing layer was studied, also utilizing HCl cleaning prior to photoemission measurement. The control sample exhibited a quantum efficiency of 1.9% at 6 eV incident photon energy. For similar N-polar GaN photocathodes, QEs decay in efficiency due to air exposure almost immediately following HCl cleaning, with a percent change of ~96% after 10 days to ~0.15%. The photocathode terminated with h-BN exhibited a maximum QE of 0.4% at 6 eV photon energy, due to the addition of the h-BN layer. While the initial maximum QE is lower, the QE decay is markedly slower, with a percent change of ~50% after 10 days in air—an improvement in the degradation rate by a factor of ~125. The decreased QE of h-BN capped photocathode after air exposure may be the result of incomplete coverage or damage to the h-BN layer. X-ray photoelectron spectroscopy shows lower coverage of oxygen and carbon on the h-BN sample after air exposure, compared to the bare GaN photocathode sample. This result shows proof of concept for stabilizing N-polar III-nitride photocathodes with 2D h-BN. Development of the wet transfer process of h-BN to N-polar GaN photocathodes will also be discussed. 10:40 AM DD07 (Student) Pulsed-Mode M O C V D Growth of ZnSn(Ga)N2 and Determination of the Valence Band Offset with GaN Kaśian Zhang1, Chenxi Hu2, A F M Anhar Uddin Bhuian3, Menglin Zhu4, Vijay G. Thirupakuzi Vangipuram1, M D Rezaul Karim1, Betharya H. Jayatunga2, Jinwoo Hwang4, K athleen Kash5, and Hongping Zhao1; 1The Ohio State University, United States; 2Case Western Reserve University, United States Orthorhombic ZnSnN2 is analogous to wurtzite GaN, with a doubled unit cell and cation sites replaced by Zn and Sn. Cation-disordered ZnSnN2 exhibits wurtzite symmetry. Both phases can in principle be integrated with III-nitride heterostructures. The concept of type-II InGaN-ZnSnN2 quantum wells (QW's) was proposed as an active region for high-efficiency amber light emitting diodes (LED's) [1]. To achieve the predicted performance, high quality ZnSnN2, and ZnSnN2-InGaN heterostructures must be
developed. However, efforts on the growth of ZnSnN₂ by MOCVD are still very limited. Our previous studies have shown that the MOCVD growth window of ZnSnN₂, particularly temperature, is limited, and Sn droplets form readily at the higher growth temperatures.

In this work, pulsed-mode MOCVD growth of ZnSnGaN₂ on GaN-on-sapphire templates was investigated. DEZn, TM Sn, TM Ga and ammonia were used as the precursors for Zn, Sn, Ga and N, respectively. Unintentionally doped GaN (uGaN) regrowth at 975 °C and a chamber pressure of 200 Torr was done prior to the ZnSnGaN₂ growth. For the ZnSnGaN₂ growth, the TM Ga and NH₃ molar flow rates were 90.6 μmol/min and 178 μmol/min, respectively, the reactor pressure was 500 Torr, and growth temperature varied from 560 °C to 580 °C. The DEZn, TM Sn and NH₃ molar flow rates were 36.6 μmol/min, 36.5 μmol/min and 201 μmol/min, respectively. It was found that GaN was unintentionally incorporated into the films, which were intended to be pure ZnSnN₂.

For the TM Sn pulsed-mode growth, the TEM Sn flow was pulsed periodically while the flow rates of DEZn and NH₃ were kept constant, as shown in Figure 1. While the DEZn and NH₃ were kept at constant flow rates, the TM Sn flow rate was controlled with t_on (flowing to chamber) and t_off (bypass) for each pulsing cycle (1 min). The authors noted that the pulsed-growth mode allowed the expansion of the MOCVD growth window of ZnSnGaN₂ towards higher temperatures while avoiding the formation of Sn droplets. It was also found that a GaN regrowth layer inserted prior to the pulsed-mode growth had substantial impact on improving the ZnSnGaN₂ crystalline quality. The pulsed-mode growth was optimized by tuning the TM Sn pulsing rate to 15 sec on, 45 sec off (Fig. 2). At 580 °C, a ZnSnGaN₂ film with a stoichiometric Zn/Sn ratio and a 50% alloy with GaN was grown. X-ray photoemission spectroscopy (XPS) measurements showed the valence band offset of 0.97 eV at the ZnSnGaN₂/GaN heterointerface, in line with the theoretical prediction (Fig. 3) [2]. In summary, pulsed-mode MOCVD growth of ZnSnGaN₂ on a GaN template was investigated. Results from this study will motivate applications of ZnSnGaN₂ and III-N heterostructures for device designs, with the potential to address some of the key challenges facing III-nitride-based electronic and optoelectronic devices today.

Acknowledgments: The authors acknowledge funding support from the U.S. Department of Energy (DE-EE0008718).

References

11:00 AM DD08
Novel Treatment of Raman and Photoluminescence Spectroscopy Analysis for Assessment of Electrical Characteristics of Mg Implanted-Annealed GaN Elaheh Kheirandish1, Vincent E. M eyers2, Emma Rocca3, Benjamin McEwen3, Mike Shevelev2, Vlad Skylar2 and Fatemeh (Shadi) Shahedipour-Sandvik1, SUNY Polytechnic Institute, United States; Gyrotron Technology Inc, United States

For its advanced electronic and optical characteristics including a direct tunable bandgap, high critical electric field and high electron mobility, GaN has proven to be a promising material for advanced high power electronics, optoelectronics, sensors and RF technologies. Development and characterization of uniform, high conductivity p-type GaN either by Mg implantation or selective area growth are essential to the advancement of next generation high power electronics and optoelectronics. [1-2]

In polar semiconductors, the coupling between the Raman active longitudinal optical (LO) phonon modes and plasma oscillations of the free carrier gas results in the emergence of the Raman active coupled phonon-Plasmon LPP modes. [3] The energy exchange between the carrier relaxation and transport is related to the LPP. [8] Therefore, the shift and change in the width of LPP permits interrogation of some electrical parameters of the material. [4-9, 8]

Prior analysis of the upper LPP mode, LPP⁺ mode, for n-type GaSb, ZnO and GaN have provided reasonable estimations of carrier concentration and mobility close to experimental values using Hall measurement. However, evaluation of the electronic properties of p-GaN through examination of LPP⁺ mode has been unsuccessful due to the highly damped Plasmon in the material. [8-10]

In this study, photoluminescence (PL) and Raman spectroscopy were used to evaluate the carrier concentration and Plasmon damping constant, and correlation of these with optical properties of Mg+N co-implanted GaN, before and after high temperature annealing, using various techniques including gyrotron microwave annealing. Metal organic chemical vapor deposition (MOCVD) grown unintentionally doped GaN (u-GaN) was grown on n⁺-HVPE GaN and is co-implanted with 10¹⁹ cm⁻³ Mg+N ions to 250 nm depth, capped with AlN, and annealed in N₂ at 1000 °C for 30 minutes. A neutralization was performed at temperatures roughly at 1350, 1400 and 1450 °C peak temperatures. The AlN cap layer was etched away after the annealing process prior to PL and Raman spectroscopy. A quality assessment parameter ΔLPP⁺ ranging from 10⁻¹⁻¹⁰⁻¹ cm² was defined for quantitative study. ΔLPP⁺ is defined by the relative shift of the LPP⁺ frequency and by its FWHM. Using this parameter, we demonstrate that there is a correlation between this parameter and the PL intensity ratio of UV to GL2 defect bands. This parameter qualitatively relates to the Mg dopant activation efficiency, reduction of the optically active Vₓ, and the presence of p-type doped or semi-insulating implanted regions on the u-GaN/n⁺-HVPE templates. The hole concentration estimation of the p-GaN layers is assessed to be in the range of 10¹⁶⁻¹⁰¹⁸ cm⁻³ for different annealing conditions. This study could offer a nondestructive, contactless, optical method for evaluation of the electronic and optoelectronic quality of p-type GaN in the p-n structure.

Acknowledgement
This work was funded by a grant from ARPA-E PNDIODES program, Grant No. DE-FOA-001691 under the direction of Dr. Isik C. Kizilyalli.

References
2. V. M eyers et al., J. Appl. Phys. 130, 085704 (2021)
Liquid Metal Printing of High Mobility 2D In\textsubscript{2}O\textsubscript{3} for Flexible Electronics

Park and William Wong; University of Waterloo, Canada

Transparent conducting oxides’ exceptional optoelectronic properties make them promising materials for driving emerging sensing, neuromorphic computing, and virtual reality applications. The high performance of oxide semiconductors can be unlocked by a sintering process converting the ink into a conductive film. This is simultaneously achieved through various printing methods where a final pattern of different transistors (TFTs) is deposited. Unlike vacuum-deposited bulk Ag films, solution-processed Ag nanoparticles (NPs) may be deposited and patterned on a substrate. The printed ink was sintered with different temperatures (T\textsubscript{Ag}) from 90 °C to 240 °C in 30 °C steps. Using these conditions, a bottom-gate TFT structure was fabricated by inkjet-printing of regioregular poly[3-hexylthiophene-2,5-diyl] (P3HT, Ossila) as the active layer with printed Ag source and drain (S/D) electrodes (using a Microfab printhead on the Ceradrop printer). The devices had a 30 μm and 850 μm channel length and width, respectively.

Current-voltage (I-V) measurements of the fabricated TFTs showed good switching behavior. The transfer characteristics in the saturation regime (V\textsubscript{DS} = 30 V) shows that the on-current level increased with increasing Ag NP T\textsubscript{Ag}. The extracted saturation field-effect mobility (\mu\text{sat}) increased from 8 × 10\textsuperscript{4} cm\textsuperscript{2}/Vs to 2.3 × 10\textsuperscript{5} cm\textsuperscript{2}/Vs with T\textsubscript{Ag} = 210 °C. It was observed that while the sheet resistance of the printed Ag NP increased with increasing annealing temperature, at T\textsubscript{Ag} > 180 °C, the sheet resistance did not change significantly, but the TFT \mu\text{sat} increased by about a factor of two. To investigate the origin of this effect, scanning electron microscopy (SEM) was used to characterize the structure and morphology of the sintered Ag. From the SEM characterization, the diameter of Ag NPs was ~30 nm prior to annealing. After a T\textsubscript{Ag} = 150 °C, the printed Ag nanoparticles were observed to form a porous film with a high density of void structures. At T\textsubscript{Ag} = 180 °C, most of the Ag NPs merged together with neighboring NPs forming a more continuous film. At T\textsubscript{Ag} = 210 °C, the structure transformed into large clusters of a few hundred nanometers, with noticeable voids between the clusters. Based on four-point probe measurements, the sheet resistance remained constant between T\textsubscript{Ag} = 180 and 210 °C. Further investigation of the P3HT formation on the Ag electrodes showed the P3HT structure improved on the Ag electrodes annealed at higher T\textsubscript{Ag}. Atomic force microscopy (AFM) revealed the polymer film surface morphology and structure were dependent on the annealed Ag NP electrodes. The surface morphology of the P3HT film was found to change with the Ag surface roughness when large continuous Ag clusters resulted in smoother P3HT films. The smoother P3HT morphology on these S/D regions correlated to T\textsubscript{Ag} between 150 °C to 210 °C. The change in the structural characteristics of the polymer matrix may provide the thin-film semiconductor with better crystallinity, enhancing the electrical contact between the semiconductor and Ag electrode. Verification of this hypothesis was examined by extracting the contact resistance for the different annealing conditions using the Y-function method and the I-V data in a linear regime. The calculated contact resistance (R\textsubscript{c}) values were 1.83, 0.75, and 0.38 MΩ cm for devices annealed at T\textsubscript{Ag} = 150, 180, and 210 °C, respectively. Finally, we will describe approaches to further minimize the R\textsubscript{c} of the inkjet-printed OTFT and optimize the printed Ag film to enhance device performance.
devices must be enclosed by a material that blocks RF waves while allowing the transmission of IR radiation. Transparent conducting oxides (TCOs), metal meshes, and 2D materials have been proposed and investigated to implement IR-transparent shields of electromagnetic interference (EMI). However, a material with minimum trade-off between shielding effectiveness, optical transmittance, scalability, and durability is elusive. Here, we show that single-crystalline semiconductor nanomembranes (NM s) are viable candidates for shielding IR devices from EMI as they provide sufficiently high shielding effectiveness, high optical transmittance, and bending durability. Our experimental work encompasses fabrication of large-area, degenerately doped semiconductor NM s, characterization of the conductivity and IR transmittance of the NM, and measurements of the NM shield effectiveness at radio frequencies. Thickness, doping level, chemical and physical structure of the surface can be varied with a high degree of control. We have grown a 200 nm-thick GaAs NM onto an undoped AlGaAs sacrificial layer/semi-insulating (001) GaAs substrate. Silicon impurities were introduced in the NM during epitaxial growth to achieve a nominal doping level of 1x10^19 cm^-3. We have fabricated van der Pauw test devices and measured a conductivity of 1.15 x 10^4 S/m for the as-grown NM. The calculated shield effectiveness of the GaAs NM is based on the measured conductivity and is as high as 42 dB at 42 GHz. Next, the GaAs NMs are released from the substrate surface via selective removal of the AlGaAs sacrificial layer. Freestanding NM s are transferred to optically transparent substrates (e.g., flexible Kapton films) to characterize IR transmittance and shielding effectiveness. Measurements are ongoing. This research was supported by an appointment to the Intelligence Community Postdoctoral Research Program administered by Oak Ridge Institute for Science and Education (ORISE) through an interagency agreement between the U.S. Department of Energy and the Office of the Director of National Intelligence (ODNI). This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science by Los Alamos National Laboratory (Contract 89233218CNA000001) and Sandia National Laboratories (Contract DE-NA-0003525).

9:20 AM EE04
(Student) Substrate-Free Organic Electrochemical Transistors Based on Ionic Liquid Crystal Elastomer Pushpa R. Raudel1, Chatthuranga Prageeth Hemantara Rajapaksha1, Panambara M udyanasele sinheth G. Kodikara2, Drona Dahal2, Thiloka M adhumane D. Dassanyake M udyanasele3, V ikash Kaphe3, Bjorn Lussem2 and A ntal J akli2,1; 1Kent State University, United States; 2University of Bamberg, Germany

Organic electrochemical transistors (OECTs) have attracted great attention since their discovery in 1984 due to their flexibility and biocompatibility. Although an intense focus has been put on the design of new organic semiconductors, fewer efforts are directed towards the development of optimized electrolytes. However, the electrolyte is an integral part of OECTs and strongly influences the transient responses of these devices. Also, best performing OECTs currently use liquid electrolytes, but there is a growing need for solid electrolytes, as they can be easily integrated into wearable devices. Here, we demonstrate that ionic-liquid crystal elastomers can be used as solid electrolytes of flexible, substrate-free organic electrochemical transistors. We introduce the alignment of the director of the liquid crystal elastomers as a new parameter to tune performance and improve both steady state and transient responses. The normalized maximum transconductance $g_{m,w}$ of the most sensitive iLCE was found to be the highest (7 S m^-1) among all solid-state-based OECTs.

Acknowledgements: This research was supported by the National Science Foundation under grant DMR-1904167 and ECCS 1750011.

References:

9:40 AM EE05
Exploration of New Classes of Solution-Processed High-K Dielectric Materials for Low-Power Electronics Shaida Faraji1,2, Navid M ohammadian3, M. Seneke4, Karim Dallio5, Karem Khiron6 and Leszek A. M ajewski7; 1Istanbul Technical University, Turkey; 2The University of Manchester, United Kingdom; 3Gaston Berger University, Senegal; 4University of Gabès, Tunisia

Organic thin-film transistors (OTFTs) have gained significant attention due to their attractive features, such as low process temperatures, mechanical flexibility, light weight, large-area production and compatibility with all kinds (rigid and flexible) of substrates. For several decades, remarkable advances in development of new semiconducting materials and novel fabrication techniques have resulted in charge carrier mobility of OTFTs to drastically surpass 1 cm²/Vs. Inevitable scaling down of electronic components to few nanometres and growing demand for low-cost flexible electronic circuits have made development of new classes of high-throughput solution-processable materials processable from solution in ambient conditions with good mechanical strength highly desirable. Now with the promising emergence of green electronics to reduce e-waste, environmentally friendly, biodegradable and biocompatible materials and processes have attracted significant attention to realise ecological and recyclable electronic devices. Green electronics aims to manufacture devices in an environmentally friendly and sustainable way. The involved electronic materials are naturally occurring and non-toxic and can be processed using simple, low energy deposition processes and fabrication techniques.

Traditional solution-processed polymers used in the semiconductor industry are generally low-k dielectrics which hinders integration of OTFTs in practical applications, for instance in wearable/portable sensors for health monitoring, due to their relatively high operating voltages (≥ 3 V). To enable operation of OTFTs at substantially low voltage (1 to 3 V), while maintaining high output current, thin but robust layer(s) of high capacitance gate dielectric is required. For the past decade, we have progressively explored and developed new classes of solution-processed, high-k naturally occurring or ‘man-made’ organic, inorganic and inorganic-organic hybrid dielectric materials for applications in low-power and recyclable electronic devices and circuits. We successfully fabricated low voltage (< 3 V) OTFTs in high yields using novel, solution processed high-k nanocomposite low-k polymer bilayer gate dielectric. Different nanocomposite suspensions of barium strontium titanate (BST) and barium zirconate (BZ) nanoparticles dispersed separately in poly(vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP) and cyanoethyl cellulose (CEC) polymer matrices were prepared to form high-k nanocomposite layers. Following successful demonstration of solution-processed OTFTs operating at 1 V using ultra-thin (~4 nm), self-assembled monolayer (SAM) modified aluminium oxide (Al2O3) layers as the gate dielectric, we also reported fabrication of ultralow voltage OTFTs with SAM-modified ultra-thin (~7 nm) tantalum pentoxide (Ta2O5) as the gate dielectric. Most recently, our work was focused on using natural occurring water-processed materials such as almond gum, gum Arabic and Aloe Vera as the gate dielectric in low-voltage OTFTs. Amond gum and gum Arabic are both natural, biodegradable insulator materials that can be directly collected from almond trees and used without any further purification. Moreover, the compelling properties of these gums, such as water solubility, ease of processing, good insulation, low leakage current and good film quality. Such dielectric layers displayed a high capacitance per unit area and low leakage current density below. The corresponding
almond and Arabic gum OTFTs showed relatively large carrier mobilities at low voltages (<3 V). Using such naturally occurring materials paves the way towards green manufacturing of the next generation of electronic devices. This work is aimed at reviewing various high-k dielectric materials, focusing on green materials, for low power electronics.

10:00 AM Refreshment Break

10:20 AM EE06
(Student) Bandlike and Polaronic Charge Transport in Organic Crystals from First-Principles Benjamin K. Chang, Jin-Jian Zhou, Nien-En Lee and Marco Bernardi; California Institute of Technology, United States

Predicting charge transport in organic molecular crystals (OMCs) is challenging due to their complex crystal structure and electronic properties. In this talk, we will present two first-principles frameworks to accurately predict the charge carrier mobilities in OMCs. The first is the Boltzmann transport equation (BTE) with ab initio e-ph interactions, which describes the bandlike transport regime in OMCs. [1]. We will show BTE calculations of hole mobilities in various molecular systems, and examine the effect of strain on charge transport. The second approach calculates the e-ph coupling using the cumulant plus Green-Kubo (CK) [2,3], which addresses the regime where the e-ph interactions are of intermediate strength and the charge carriers form polarons. We will present our recent CK calculations of electron mobilities and electron spectral functions in OMCs. Both our BTE and CK approaches provide mobilities in very good agreement with experiments, for a wide temperature range. These broadly applicable methods advance the understanding of charge transport in organic semiconductors.


10:40 AM EE07
PIFM – Nanoscale Chemical Mapping and Spectroscopy via AFM-IR for Ultrathin Organic Films Padraig O’Reilly, Derek Nowak and Song Xu; Molecular Vista, United States

Real-space imaging and identification of chemical components in multi-component systems with nanometer scale spatial resolution remains a challenge for the nano and molecular electronics community. In this talk, we introduce a new nanoscale and non-destructive chemical imaging technique called photo-induced force microscopy (PIFM) where the dipole-dipole force due to optical response of the sample is measured by an atomic force microscope (AFM) along with the standard AFM topography [1]. PIFM can be coupled with a tunable infrared (IR) light source to probe the IR absorption of various organic and inorganic materials and identify the chemical components in multi-component systems. Once controlled, measurement of the IR response provides chemical sensitivity of the sample. PIFM is surface sensitive due to the short interaction range of the measured dipole-dipole force and the single-molecule-level of chemical sensitivity and ~5 nm spatial resolution, making it an ideal tool for characterizing thin films and devices of organic and inorganic materials; monolayer of organic/inorganic constituents, contaminants, and residues can be clearly and uniquely visualized for failure analysis and process development of biosensors and organic/molecular devices. The capabilities of PIFM will be highlighted by presenting data on area selective deposition, which features self-assembled monolayer (SAM) of organic materials as well as ultrathin dielectrics grown via atomic layer deposition (ALD). PIFM provides a powerful new analytical method for deepening our understanding of nanomaterials and facilitating technological applications of such materials.

COF/Monolayer TMD Heterostructures


This material is based upon work supported by the National Science Foundation under Grant No. NSF CMMI-1727572.

blue color purity.

In this study, a pinhole-free PFO thin film with significant beta-phase content (21%) was achieved via RIR-MAPLE with deep molecular beam epitaxy on n-type (001)-oriented Ga2O3 layers. Capacitance-voltage (CV) measurements for all three temperatures investigated here showed low hysteresis and frequency dispersion. The hard irreversible breakdown voltage (< 1453V), whereas the 400°C and 500°C had much lower average breakdown voltage (< 1183V). The 300°C MOS capacitor showed the lowest average leakage current <100nA/cm², suggesting their promise for gate or field plate dielectric applications.

Ronan Curran, Nidhin Kurian Kalarickal, Chandan Joishi, Andreas Fiedler, Joe F. McGlone, A shok V. Dheenan, Steven A. Ringel and Siddharth Rajan; The Ohio State University, United States

β-Ga2O3 is a promising material for high power devices due to its high theoretical breakdown field of 8MV/cm and availability of bulk substrates. In order to take full advantage of the potential of this material, synthesis and properties of dielectric-semiconductor interfaces is critical. Dielectric-semiconductor interfaces are needed to sustain electric fields that are significantly higher than previous Si or GaN devices, while maintaining low leakage current and controlled interface traps and charge. For this purpose, Al2O3 grown by different methods such as ALD [1], MOVCD [2] have been explored in this material. This work focuses on the synthesis and electronic properties of Al2O3 deposited using plasma-assisted molecular beam epitaxy on n-type (001)-oriented Ga2O3 layers. Al2O3/β-Ga2O3 metal-oxide-semiconductor capacitors with high reverse breakdown voltage up to 1843V (breakdown field strength of 5.1 MV/cm).

MOSCAPs were further stressed to high reverse bias till they breakdown. The 300°C MOS capacitor showed the lowest average breakdown voltage (< 1453V), whereas the 400°C and 500°C had higher breakdown voltage of 1843 V and 1720 V respectively. The corresponding parallel plate electric field in gallium oxide found to be 4.54MV/cm, 3.05 MV/cm and 4.95 MV/cm for 300°C, 400°C, and 500°C samples respectively. The hard irreversible breakdown occurred at the edge of the MOSCAP pads, suggesting that edge termination could help to achieve better performance. The forward studies demonstrate a microwave power dependent electronic coupling of the inorganic and organic materials in these highly tunable hybrid materials.

REFERENCES

The system of gallium oxide has attracted worldwide attention for its potential for next-generation power electronics. Beyond the intrinsic limit of $\beta$-Ga$_2$O$_3$, alloying the material with Al can effectively widen its bandgap and opens the possibility for high-performance heterostructure device applications. Although common extrinsic dopant elements (e.g. Si and Sn) in gallium oxide are predicted to be shallow donors in Al-alloyed gallium oxide, studies have shown degraded film quality and/or poor dopant incorporation in as-grown Si-doped $\beta$-Al$_{1-x}$Ga$_x$O$_3$ films. To resolve this problem, here we report a method for doping Al$_2$O$_3$ via Si-ion implantation and demonstrate its application for forming ohmic contacts on $\beta$-Al$_{1-x}$Ga$_x$O$_3$.

Device fabrication started with multiple Si-implantations which were carried out at room temperature to form a -80-nm-deep box-profile in Al$_2$O$_3$ epitaxial film followed by a post-implant anneal process in a non-oxidizing environment. The projected Si box-concentration ranges from $3 \times 10^{19}$ cm$^{-3}$ to $9 \times 10^{18}$ cm$^{-3}$. Circular transmission line method (CTLM) device structures were then defined with evaporated 20-nm Ti/80-nm Au metal stack and lift-off process. To ensure the metallization is in direct contact with the heavily doped implanted Al$_2$O$_3$ region, a 80-nm Ti$_2$O$_3$ based reactive-ion-etch recess was applied prior to metallization. Post-metallization rapid-thermal-anneal (RTA) was performed at 470°C for 1 min in N$_2$ to improve ohmic contact performance. Electrical testing and material characterizations (XRD, AFM, SIMS, and S/TEM) were carried out afterward to examine the fabricated devices.

Samples were patterned for linear and circular transfer length method (LTLM/CTLM) structures as well as van der Pauw (VdP) testing structures for selective ion implantation. Si, Ge, and Sn ions were selectively implanted in order to achieve an approximately 100 nm implant box profile at $3 \times 10^{19}$ cm$^{-3}$ dopant concentration for a total dose of 3.3e14 cm$^{-2}$. Rapid thermal annealing (RTA) at 925°C for 30 min in N$_2$ was performed to activate the implanted ions and remove implant damage. The LTLM and VdP structures were further isolated by a 150 nm BCl$_3$ reactive ion etch at 800 W. Evaporated Ti/Au ohmic contacts were deposited and an standard ohmic contact anneal was performed. LTLM and CTLM measurements demonstrated ohmic contacts between the Ti/Au metal stack and GO with a contact resistance ($R_{c}$) of 1.2 $\Omega$mm and 2.3 $\Omega$mm for the Si and Sn implanted samples, respectively. Room temperature (RT) and temperature dependent Hall effect measurements were performed to extract the sheet carrier concentration ($n_s$), sheet resistance ($R_{s}$), and mobility ($\mu$). VdP structures received ion implants at various locations within the structure to confirm if the implanted donors could overcompensate for the N-doped CBL. Hall structures that did not receive implantation of the active region between the ohmic contacts could not be measured due to excessive resistance demonstrating retention of N doped film resistivity. The Hall measurements showed a net free carrier concentration ($N_s$), less than $10^{14}$ cm$^{-3}$. Lateral Schottky barrier diode structures on the HVPE films resulted in breakdown voltages exceeding 2 kV [5].

REFERENCES

Photocurrent measurements of the highly resistive non-implanted V defect structures were performed using an above bandgap UV light with a power of 217 μW. A low dark current was measured ranging from 1-100 pA and photocurrent ranging from 1-100 nA.

The authors would like to acknowledge the support from the Office of Naval Research through a MURI program, grant No. N00014-13-1-0686 (CAIF) and from the OSD/SEP program, grant No. N00014-13-1-0134 (Students). This technique was also employed to remove the subsurface damage for substrates that were initially polished using >1 kPa pressure of only 1 kPa in order to produce a smooth (0.6 nm r.m.s. roughness) surfaces. We have also demonstrated smooth surfaces under such conditions but with significant levels of subsurface damage. The removal rate for the 1 kPa process is ~0.4 μm/hr which is also suitable for CMP for wafer bonding β-Ga2O3 and for assessing the thermal transport characteristics of damaged vs pristine β-Ga2O3 surfaces.

References:
Surface phonon polaritons, light-matter coupled waves at the interface between a dielectric and a polar crystal, have recently attracted much attention as a versatile tool for low-loss nanophotonic applications in a range spanning from mid- to far-infrared. These modes can exist inside the Reststrahlenband, i.e. the region included between the two resonance frequencies of optical phonons (LO and TO) with a negative dielectric permittivity. In particular, materials featuring high optical anisotropy have been shown to support a hyperbolic response that results in hyperbolic polaritons with highly directional propagation and extremely large momenta, enabling the compression of light to deeply sub-wavelength scales. Typically, volume-confined hyperbolic modes in thin films of hexagonal or orthorhombic crystals have been observed, with only few demonstrations of in-plane-hyperbolic surface waves on anisotropic bulk crystal surfaces.\(^3\)

In our contribution, we demonstrate the emergence of a new type of hyperbolic surface waves with broken symmetry of the in-plane-hyperbolic propagation that exist at surface of the even lower symmetry monoclinic crystal beta-gallium oxide (bGO).\(^1\) We directly compare our observations with the higher symmetry hyperbolic surface phonon polaritons on alpha-quartz (αQ). We show that shear phenomena in the dielectric response of the monoclinic system are directly linked to the symmetry breaking, leading to a new polariton class which we call hyperbolic shear polaritons (HShPs). These modes emerge in low-symmetry monoclinic (and triclinic) crystals whose dielectric permittivity tensor cannot be diagonalized, due to the presence of multiple oscillators with non-orthogonal relative orientations contributing to the optical response.

We experimentally demonstrate HShPs in bGO using the Otto-type prism coupling experiments, by mapping out the azimuthal polariton dispersion. Further, we extract the in-plane hyperbolic dispersion at several wavenumbers, by following the frequency momentum dispersion at many azimuth angles. This allows us to reveal the main novel features of HShPs, that is, the continuous evolution of its propagation direction with frequency and asymmetric responses.

Hyperbolic shear polaritons complement previous observations of hyperbolic phonon polaritons in higher symmetry systems. The shear phenomena observed here may provide new opportunities for topological photonics. We anticipate that our results on HShPs will not only offer additional design options for nanophotonic applications, but will additionally greatly expand on the material base for such devices.

References

Beta gallium oxide (bGO) presents great potential for next generation power and RF devices in no small part due to the large area, high quality, melt grown, bulk substrates available, something lacking in alternatives such as gallium nitride, aluminum nitride, and diamond. While bulk crystal growth is essential, so too is growth of high quality and exceedingly phase-pure single crystal epitaxial structures. Among growth techniques, molecular beam epitaxy (MBE) and metalorganic chemical vapor deposition (MOCVD) are common with differing tradeoffs in purity, crystal structure, and defect populations. MBE films are typically grown at more moderate temperatures which can benefit purity at the expense of a greatly reduced growth rate as well as reduced atomic mobility for crystal refinement. Here, we focus on the effects of high temperature annealing on the quality and defect structure of a 500nm thick MBE bGO film grown on an O10 bulk substrate. Specifically, we target annealing near typical MOCVD growth regimes at 1000°C by both RTA and moderate pressure (~30 bar) annealing in nitrogen, as well as rapid heating and cooling pulses (max ~300 K/s) at moderate pressures via multicycle rapid thermal annealing (MRTA) to access intermediate (~1450°C) and high temperature (1600°C) states near the melting point (~1725°C) with rapid quenching to assess the high temperature state. Samples were probed by Nomarski imaging, Raman scattering, X-ray diffraction, positron annihilation spectroscopy (PAS), and Rutherford backscattering spectroscopy with channeling (RBS/c).

M acrostically, bare films annealed at low and moderate temperatures were unchanged while annealing near the melting point yielded surface reconstruction and features parallel to [001]. Suppression of surface reconstruction was achieved using a 100nm PECVD SiO2 cap during annealing. Phononic behavior was not greatly affected as measured by Raman shift and peak width, and only minor deviations in intensity ratios were notable which could be attributed to spatial anisotropy or slight deviations in substrate rotation during acquisition. High-resolution X-ray diffraction indicates consistent quality of films and substrates with no deleterious effects after quenching from any anneal condition.

At the atomic scale, PAS measures defect populations by the annihilation lifetime of injected positrons. Energy dependent PAS was obtained for all conditions yielding S and W parameters as a function of depth. This data was fit to a three layer model to capture surface mediated artifacts, a true film population (~500nm), and the bulk substrate population. Measurements on virgin material shows a greater S parameter of the MBE film and surface relative to the substrate indicating the expected greater defect concentration from the low film growth temperature. Upon annealing, the MBE film defect populations are significantly affected by both the sample temperature and presence of the cap while the bulk material defect population was relatively unaffected by any anneal condition. Film defect populations were indeed even improved upon beyond the population of the bulk substrate as indicated by the reduced S-parameter. Furthermore, plots of S vs W show a linear trend for both the MBE film and substrate for all samples indicating a similar defect or defect complex dominating the PAS signal for all films and substrates.
Photoluminescence (PL) has been under intense scrutiny in an attempt to define the mechanisms that generate the emissions in gallium oxide (Ga$_2$O$_3$). In general, PL spectra is used to characterize the defects leading to radiative recombination processes within a specific material. In this regard, the PL spectra for β-Ga$_2$O$_3$ has generally been deconvoluted in three emission peaks: UV, blue, and green. However, peak shapes from any point defect are expected to require more than a single Gaussian for a complex crystal structure like β-Ga$_2$O$_3$, possibly having an asymmetric shape and requiring a more complex model, which takes into consideration the vibrational broadening of the PL spectrum due to electron-phonon coupling. The sum of many phonon replicas makes it challenging to fit the spectra uniquely.

A dosing energy level broadening from disorder or extended defects makes deconvolution of the β-Ga$_2$O$_3$ PL spectrum even more difficult. As such, there is little chance of being able to spectroscopically discern different types of defects in β-Ga$_2$O$_3$ from luminescence as any defect considered can result in a very wide luminescence band, even near 0 K Kelvin. This has resulted in an intense debate in defining the defects and phenomenological explanations of electronic processes that cause these particular emissions. In these debates, point defects have been the only explored and discussed potential source for the visible PL emission in β-Ga$_2$O$_3$. But, as far as can be determined, no previous works in the literature have discussed whether extended defects affect PL.

Here, a systematic PL study on three series of β-Ga$_2$O$_3$/aluminum gallium oxide films and bulk single crystals is performed. The first series includes three film samples with varying Si-doping: UID ($-10^{18}$ cm$^{-3}$), $-10^{19}$ cm$^{-3}$, and $-10^{20}$ cm$^{-3}$. All samples in the series are (010) oriented Si-doped β-Ga$_2$O$_3$ film grown on Fe-doped β-Ga$_2$O$_3$. The second series contains three samples and compares (-201) β-Ga$_2$O$_3$. This series includes a bulk crystal of (-201) UID β-Ga$_2$O$_3$, a (-201) UID β-Ga$_2$O$_3$ film grown on Fe-doped β-Ga$_2$O$_3$, and a (-201) UID β-Ga$_2$O$_3$ film grown on sapphire. The last series compares (010) oriented (Al$_{1-x}$Ga$_x$)$_2$O$_3$ films, i.e., A GO of varying Al concentrations (0%, 10%, and 25%), grown on Fe-doped β-Ga$_2$O$_3$. These are compared to a (100) oriented bulk 10% A GO (β-Al$_{1-x}$Ga$_x$)$_2$O$_3$ crystal. A second part of the series compares (-201) oriented 0%, 2%, 10%, and 28% A GO films grown on sapphire. The Si-doped series yields homogeneous crystalline films with a low density of extended defects [1] and a dominant UV emission in PL. In the (-201) series, the bulk (-201) β-Ga$_2$O$_3$ sample also shows a dominant UV emission. On the other hand, Heteroepitaxial and homoepitaxial (-201) β-Ga$_2$O$_3$ films show consistent PL features with dominant blue emission. The (-201) films’ poor quality [2, 3] is likely the reason for this shift in the dominant emission, as observed when comparing UID films grown on (010) and (-201) bulk β-Ga$_2$O$_3$ crystals with comparable growth conditions. The A GO series shows consistent blue centered PL with no UV emission for both homoepitaxial and heteroepitaxial A GO samples. The A GO films show extended defects throughout a poor-quality film revealed using transmission electron microscopy (TEM) on the 25% A GO grown on (010) bulk β-Ga$_2$O$_3$ crystal.

Lastly, representative samples chosen from all three series were compared and it is shown that extended defects have an essential role in the PL emission of β-Ga$_2$O$_3$ and A GO films. Homogeneous films with no extended defects or stacking faults and bulk crystals will yield a UV dominant PL emission. Samples of poor film quality that have stacking faults and extended defects will have a dominant blue PL emission.
Alloying $\beta$-Ga$_2$O$_3$ with Al$_2$O$_3$ to create (Al$_x$Ga$_{1-x}$)$_2$O$_3$ enables ultra-wide band gap material deep into the UV. Here, photoluminescence (PL) spectra of $\beta^+$-doped Cr$^{3+}$ in $\beta$-Ga$_2$O$_3$ and (Al$_{0.1}$Ga$_{0.9}$)$_2$O$_3$, denoted $\beta\text{-}(\text{Al}_{0.1}\text{Ga}_{0.9})\text{O}_3$ or AGO. Temperature dependent PL properties were studied for Cr$^{3+}$ in AGO and $\beta$-Ga$_2$O$_3$ from 285 to 16 K. For $\beta$-Ga$_2$O$_3$, at room temperature, the red-line emission doublet $R_1$ and $R_2$ occurs at 696 nm (1.78 eV) and 690 nm (1.80 eV) respectively along with a broad emission band at 709 nm (1.75 eV). The $R_1$ line is approximately 1 nm higher for AGO compared to that of $\beta$-Ga$_2$O$_3$. For both AGO and $\beta$-Ga$_2$O$_3$ the $R_1$ line increases in intensity with decreasing temperature. This can be explained by the thermal depopulation effect of the $R_1$ state, which occurs with increasing temperature. The $R_1$ and $R_2$ lines of both materials were observed to blue-shift with decreasing temperature. Additional emission lines emerge at lower temperatures, with $\beta$-Ga$_2$O$_3$ showing more peaks than AGO. $R_1$ and $R_2$ peak parameters such as energy, intensity, width, and splitting were studied as a function of temperature, with significant differences between the two materials.

SESSION GG: Epitaxial Growth on Patterned Substrates

Session Chair: Minjoo Lee and Kyle M. Nichols

Friday Morning, July 1, 2022

Cartoon Room #1

8:20 AM GG01

(Student) Selective Area Epitaxy by MBE for Self-Alignment III-V Devices

Alec M. Skipper, Andrew Jones, Morgan Bergthold, Aaron J. M. Uhlowski, Ashlee Garcia, Daniel J. Ironside, Daniel Wasseman, Joe Campbell, and Seth R. Bank

University of Texas at Austin, United States; University of Virginia, United States

Semiconductor devices have historically been processed with growth first, followed by metal and dielectric deposition, patterning, and etching. However, careful process control is required to reduce undesirable recombination and dark current at device surfaces. Commonly used III-V materials experience Fermi level pinning at the semiconductor/air interface [1], leading to undesirable device characteristics such as elevated dark currents arising from etch residue, sidewall damage, and oxidation [2-4]. As a result, great care must be taken to choose the correct etch chemistry and surface passivation must be performed quickly before harmful oxides form on the etched sidewalls. Additional process steps are required to mitigate these effects, complicating the manufacturing process and reducing device yield/performace. By contrast, devices created by selective area growth present a possible solution to these issues by bypassing the need for challenging alignment and surface treatment steps [5]. Selective area growth utilizes a template on the surface of the sample to define the device regions. Unlike self-assembled quantum dots and nanowires, selective area growth allows complete control over the size, placement, and distribution of the grown nanostructures by simple photolithography. Furthermore, since the device structure is created in situ during growth under ultra-high vacuum, there is no risk of oxidation and the sidewalls can be nearly atomically smooth. We present self-aligned devices passivated in vacuo by selective area molecular beam epitaxy growth. Silicon dioxide was deposited on III-V wafers and windows were etched to the substrate in the shape of the desired devices. Periodic supply epitaxy (PSE) was then used to selectively grow the device layer structures in the windows. PSE utilizes interruptions in the group-III flux and high growth temperatures to enhance desorption and diffusion on the silicon dioxide surface, ensuring growth only occurs in regions seeded from the substrate [6]. This results in the device structure growing within the window that naturally conforms to the dielectric sidewall. Furthermore, this semiconductor-dielectric interface is formed in vacuo, meaning there is no risk of creating unstable III-V oxides. As a prototype, an InAs tunnel diode was grown by selective area epitaxy and compared to a conventionally fabricated diode with the same layer structure. Comparable current-voltage characteristics were observed from the two devices, suggesting that the PSE growth process does not negatively impact electrical characteristics. Investigation of dark current and photoluminescence is underway and will be reported at the conference.

This research was partially supported by Lockheed Martin and the National Science Foundation through the Center for Dynamics and Control of Materials: an NSF MRI SEC under Cooperative Agreement No. DM R-1720595, as well as DM R-1839175, CCF-1833435, and ECCS-1926187.

efficient. However, optical output is limited compared to regrown devices.

While epitaxial regrowth is optimal for device performance, it introduces new complexity due to infilling of the PC and because obtaining a clean regrowth surface is challenging. To optimize pre-regrowth chemical treatment and identify the maximum tolerable temperatures for in-situ thermal cleaning. Secondly, for PCSEL design, it is important to match the resonance of the PC cavity to the photoluminescence of the active region. Relevant parameters include PC lattice structure, lattice period, void shape, PC fill factor, and the relative indices of refraction of PC materials. To control PC resonance, the influence of regrowth void morphology is investigated and compared. In this study, a PC region is patterned over a range of 8 exposure doses to vary printed void radii. The voids are then measured by SEM before and after regrowth and compared. This study demonstrates that pre-regrowth void radius influences growth direction, i.e. growth at the sidewalls or at the bottom of the void, and allows us to engineer pre-regrowth voids to produce the desired post-regrowth morphology. Regrown PCSEL devices are fabricated by optical pumping and electrical injection.

In addition to PCSEL fabrication by regrowth methods, non-regrowth methods are explored. Non-regrowth is advantageous because it significantly reduces fabrication time, enabling researchers to make quick empirical studies of photonic crystal designs. Additionally, it bypasses the complicated regrowth step and the high temperature exposure associated with it. This can be particularly important for quantum dot devices as high temperatures can blue shift their emission. However, relative to regrowth, the optical output of these devices is limited. Non-regrowth fabrication typically consists of a single axial growth with a bottom contact layer, bottom cladding, active region, top cladding, and top contact layer. The epitaxial structure is patterned by electron beam lithography and ICP etch. A SiN aperture is formed by lift-off and chemical vapor deposition (CVD). Indium tin oxide (ITO) is deposited by sputtering as a transparent conductive material to make electrical contact with the PCSEL surface. Non-regrowth PCSELs are fabricated for electrical injection and compared to edge-emitters from the same epitaxial structure.

In conclusion, orientation-aligned InP mesas were integrated on Si and TLP grown InP on SiO2. It indicates the much lower contribution of trap-assisted non-radiation recombination and lower defect density. At the GaAs/InP and Si interface, various thread defects and stacking faults can be observed from the TEM images, some of which propagate to the surface of the GaAs/InP layer, but are terminated at the interface. However, InP by TLP strictly followed the MOCVD grown InP lattice structure, and none of the point defects, stacking fault, or twinning boundaries were observed in this region.

Crystaline orientation was determined by electron backscatter diffraction (EBSD) and transmission Kikuchi diffraction (TKD). As demonstrated in Figure 4 (a) and (b), a representative area of TLP mesas showed identical <100> out-of-plane orientation with the MOCVD GaAs/InP substrate across the whole sample. A much lower number of twinning boundaries were observed from the raw crystal orientation map compared with the map from InP on SiO2. The inverse pole figure by TKD from the cross-section lamella of the sample allowed the detailed orientation and texture study with higher resolution (~40 nm in this measurement). The three-directional crystal orientation map in Figure 4 (d) to (f) confirmed the ideal orientation-alignment of InP by TLP growth in this new approach.

In conclusion, orientation-aligned InP mesas were integrated on Si wafer with TLP growth technique and demonstrated superior structural and optoelectronic properties. It paved the pathway toward scalable 3D high-quality III-V semiconductor-based devices on Si.
epitaxy (PSE), a method to inhibit polycrystalline deposition by cycling group III deposition under a constant group V flux.  Combining high growth temperatures and low growth rates, PSE enables SAE by mitigating the nucleation of poly-GaAs through increased Ga adatom diffusion to seeding windows and desorption off the mask.  While an all-MBE approach has been demonstrated to achieve selective growth of features ~2µm wide and ~300nm tall, applications requiring larger features such as mid- and long-wave infrared high-contrast photonics and aspect ratio trapping of threading dislocations for metamorphic growth, are limited by nucleation of polycrystalline semiconductor on the amorphous surface due to low adatom surface diffusion.  To expand the accessible applications, a numerical 1D model was developed to describe PSE selectivity by fitting adsorption, desorption, and diffusion constants to GaAs growth on SiO2 films at 650°C with a growth rate of 0.7Å/s and a 65x As4/Ga ratio.  The model (1) identifies selective growth regimes to clarify their underlying mechanisms and (2) allows optimized growth conditions to be determined for a given SiO2 pattern.  Two growth regimes were identified: desorption- and diffusion-limited.  The desorption-limited regime relies only on thermal desorption off the mask to achieve selectivity and therefore is feature-independent.  The remainder of the space is diffusion-limited in which sufficient III adatom diffusion off the mask is required to achieve selectivity.  Desorption-based selectivity can be achieved with a PSE cycle, the fraction of time the group III shutter is open, under 18% based on the model.  This regime was verified experimentally with scanning electron microscopy.  No polycrystal formation on the mask surface after 100nm of GaAs growth with a 10% cycle on a SiO2 film and SiO2 gratings spaced 1µm apart with varied widths from 1 to 10µm indicates that the GaAs layer is feature-independent.  Experiments to further extend achievable mask height using a feature-independent growth regime and investigate the physical limit of diffusion-based growth for high aspect ratio features are underway and will be reported at the conference.


This research was partly done at the Texas Nanofabrication Facility (NSF grant NNCI-205227) and was supported by Lockheed Martin and NSF via the UT CDCM: an NSF MRSEC under Cooperative Agreement DMR-1720595, as well as CCF-1838435 and DMR-1839175.

SESSION HH: Lattice Mismatched Epitaxial Growth

Session Chairs: Minjoo Lee and Kyle M.Nicholas
Friday Morning, July 1, 2022
Cartoon Room #1

10:20 AM HH01
two-photon absorption for wavelengths >1.1 μm, (3) large refractive index (~3.1-3.4), (4) relatively wide bandwidth of 2.26 eV for visible wavelengths >0.55 μm, and (5) non-centrosymmetric crystal structure. GaP-on-insulator (GaPOI) fabricated by wafer bonding and etch-back has recently been proposed as a novel platform for integrated nonlinear photonics. An alternative integration method would be to grow GaP directly on the silicon-on-insulator (SOI) wafers that are commonly used in Si photonics foundries, followed by selective Si removal using XeF₂ to form suspended GaP structures. In this work, we describe the effects of molecular beam epitaxy (MBE) growth parameters on the structural properties of GaP on SOI. By studying the impact of V/III ratio on Ga-induced pitting, surface roughness, and anti-phase boundary (APB) formation, we achieved epitaxial GaP on SOI films with root-mean-square (RMS) surface roughness of ~1 nm.

GaP was grown by MBE on SOI wafer pieces (SEH America) over a substrate temperature (Tsub) of 535-580°C and V/III of 5-10. We consider formation of anti-phase boundaries (APBs) to be unavoidable in these layers, since commercially available SOI wafers are manufactured with an exact (001) surface orientation. While APBs are unacceptable in minority carrier optoelectronic devices, their effect may be less severe in the passive photonics structures targeted here. Before growth, SOI substrates were precleaned with piranha and diluted HF to remove organic residues and oxides. After deoxidation in the growth chamber at Tsub = 800°C for 20 min, 220 nm of GaP was directly grown at 0.5 μm/hr. Symmetric (004) omega-2theta high-resolution XRD scans confirmed the epitaxial relationship between GaP and SOI, with the appearance of Pendellösung fringes indicating a smooth interface. The surface morphology and roughness of samples were investigated by Nomarski microscopy, SEM, and AFM.

All GaP on SOI samples exhibit pits with a density of 10⁷-10⁸ cm⁻². Tilted-view SEM image showed that pits on the GaP surface originated from damage at the Si surface, most likely due to Ga-induced melt-back etching at the beginning of growth. Accordingly, the sample grown with the lowest V/III ratio (5) exhibits the highest pit density of 8.7x10⁷ cm⁻². Lower substrate temperature or higher V/III ratio decreased the pit density by ~10⁻², presumably due to reduced Ga clustering.

V/III ratio is also a critical factor to obtain a smooth surface in the regions away from pits, and samples grown with V/III=6.0-7.5 showed ~1.5-2.0 nm RMS surface roughness than one with V/III=5.5. To balance the contradictory effects of V/III ratio on pit density and surface smoothness, we employed a two-step growth using a high V/III ratio (10) for the first 20 nm of growth and a low V/III ratio (5) for the remaining 200 nm. The sample grown using this two-step growth process exhibited RMS roughness of 1.29 nm; for context, high-quality, relaxed GaP grown on GaP/Si templates from NAsP GmbH typically exhibit roughness of 0.6-2.1 nm. Interestingly, the low RMS roughness of the two-step growth sample was also accompanied by a lower APB density. In conclusion, by understanding the strong effect of V/III ratio on surface morphology, we showed epitaxial GaP on SOI with ~1 nm RMS roughness. SOI wafers are widespread in Si photonics foundries, and the addition of GaP to the palette of available materials could enable new applications such as integrated visible and non-linear photonics.

**10:40 AM HH02**

(Student) Monolithic III-V Growth Directly on Metal for Device Application

Hyun Uk Chae and Rehan Kapadia; USC, United States

Direct growth of III-V crystalline on top of metal has been desired to design electrically tunable photonics devices to utilize the metal layer as an electrical contact and bottom reflector. Devices such as metal-insulator-metal (MIM) resonator can be achieved by using this approach. Here in this work, we have demonstrated indium arsenide (InAs) directly grown on metal to build a platform for the device application. Indium arsenide was selected among other III-V semiconductors for growth demonstration thanks to their low bandgap and high electron mobility, which has high potential to achieve the fast dynamic change in refractive index for the photonics devices. The growth was carried at growth temperature of 300°C by low temperature templated liquid phase (LT-TLP) growth. Unlike our previous grown templates on top of amorphous substrates, it is noteworthy that the size of the grown InAs area is over >80 μm domain size with various InAs thickness (from ~100 nm up to μm scale) by tuning the initial indium template thickness. Thickness of the InAs was verified by using Fourier Transform Infrared Spectroscopy (FT-IR) and focused ion beam (FIB). This approach enables us to control the size and thickness of the grown crystalline, potentially can be used to grow single crystalline size up to mm scale by optimizing the growth conditions and processes, opening the new door to realize the large scale III-V growth on metal for device applications.

**11:00 AM HH03**

(Student) Integrating GaSb-Based Infrared Detectors with Si Substrates via Interfacial Misfit Arrays

Trent Garrett; Madison Drake¹, Pooja D. Reddy², Kunal Mukherjee², Shimmon Maimon³, and Paul Simmonds³,⁴,⁵; Boise State University, United States; ²Stanford University, United States; ³NetZVision LLC, United States

With applications from night vision and aerial target acquisition, to space telescope operation, infrared (IR) detectors are of great interest to the defense and scientific communities alike. The functionality of these detectors hinges on achieving a high signal-to-noise ratio so that weak signals can still be resolved. Of the many designs for IR detectors, the nBn device has emerged as a leading choice. As the name suggests, nBn detectors comprise an n-type absorber layer, an electron-blocking barrier, and an n-type contact layer. This simple, yet effective, design prevents the collection of majority carriers (electrons), while allowing minority carriers (holes) to flow freely to the collector [1].

nBn-based IR detectors are typically grown on GaSb, which marks perhaps their biggest disadvantage. GaSb substrates are expensive and only widely available up to 4” diameter formats, placing a limit on high volume manufacturing. Successfully integrating III-V based nBn detectors with Si substrates would overcome these wafer cost and size constraints. However, this approach comes with its own set of challenges, primarily due to the large lattice mismatch between GaSb and Si. Direct deposition of GaSb onto Si typically results in the formation of large 3D islands that prevent planar growth, as well as the formation of a high density of threading dislocations and other defects that help to relieve the strain [2]. These threading dislocations mean that an nBn detector grown above this interface will suffer from poor performance. We are therefore adopting the use of interfacial misfit (IMF) arrays to manage the heterointerface between the III-V epi-layers grown by molecular beam epitaxy (MBE) on Si substrates. IMF Fs consist
of the spontaneous formation of a 2D array of 90° dislocations that lie in the plane of the heterointerface. Unlike 60° threading dislocations, 90° dislocations do not migrate vertically to affect layers grown above. IMFs have been shown to relieve close to 100% of the strain right at the interface, enabling the growth of smooth, high-quality material above [3].

For the specific case of III-Sb materials grown on Si substrates, previous studies have shown that thin layers of AlSb are critical for producing the aforementioned IMF arrays. Compared with the growth of GaSb directly on Si, GaSb deposited onto an AlSb/Si IMF heterostructure has dramatically improved material quality and lower threading dislocation density (TDD) [4]. To ensure the growth of GaSb-on-Si virtual substrates with the highest possible quality for subsequent n-bn growth, perfecting the growth of this AlSb/Si IMF layer is fundamentally important. We will discuss how choices regarding AlSb growth initiation, Si substrate temperature, annealing strategies, AlSb thickness, and AlSb growth rate affect the quality of GaSb overlayers. By optimizing these MBE growth conditions, initial results suggest that we can grow GaSb layers with quality comparable to the current state-of-the-art, which provides us with a valuable reference point from which to make further improvements. Next steps to further enhance material quality will include the use of dopant species, such as Be, to reduce dislocation mobility via solid solution strengthening. We will also investigate the use of dislocation filtering superlattices above the IMF to induce dislocation annihilation and further reduce TDD in n-bn devices grown on these GaSb-on-Si templates.

This work is supported by the Office of Naval Research through grant N00014-21-1-2445.

References:

11:20 AM HH04
(Student) Heteroepitaxy of GaSb on GaAs(111)A Substrates for Electron Transport Studies Madison D. Drake, Trent Garrett and Paul Simmonds; Boise State University, United States

III-V semiconductors grown by molecular beam epitaxy (MBE) on (111) surfaces have some interesting electronic properties. For certain materials with a (111)-orientation, the Γ- and L-valleys are reasonably close in energy. This means that it may be possible to take advantage of electron conduction in the L- and Γ-valleys at the same time, allowing us to overcome the so-called “density-of-states bottleneck,” and enable transistors with large drive currents [1]. We are eager to investigate this phenomenon in GaSb- and InAs-based 2D electron gases for which the electron effective masses are low.

However, growth of materials with a (111) orientation is typically more challenging than on traditional (001) surfaces. The MBE conditions needed to grow high quality material are often poorly understood [2]. We began by exploring InAs/GaSb quantum well (QW) structures, [3] grown directly on GaSb(111)A substrates. We will show that low growth rates under very high group V overpressures produce good GaSb homoepitaxy and InAs heteroepitaxy, as characterized by XRD and AFM. However, although we have been able to identify MBE conditions that lead to the growth of smooth, high-quality material, GaSb(111)A substrates are extremely expensive, as well as being intrinsically n-type, which complicates the carrier transport measurements in which we are interested. If we could instead grow our GaSb-based QW structures on cheaper, non-conductive GaAs(111)A substrates, we could overcome these issues. The challenge is the large lattice mismatch between GaSb and GaAs, which typically results in strain-driven crystallographic disorder at the heterointerface and poor material quality.

One technique that has shown promise in circumventing these problems on (001) surfaces is the use of interfacial misfit arrays (IMFs). Under specific molecular beam epitaxy (MBE) conditions it is possible to produce an array of 90° dislocations that lie in the GaSb/GaAs(001) heterointerface. These dislocations efficiently relieve the strain between the two materials without generating the high density of threading dislocations that one would ordinarily expect. As a result, it is possible to grow high quality materials and active device structures above these IMF-based heterointerfaces.

We will discuss our attempts to extend a modified version of this IMF technique to (111) surfaces in order to grow our InAs/GaSb QWs grown on GaAs(111)A substrates. So far, this work has produced GaSb grown on GaAs(111)A with a full-width-half-maximum (FWHM) XRD peak value of 270° for GaSb/GaAs(001) grown via an IMF approach, other groups have reported FWHM values of 240° [4]. We hope to reach similar values after further optimization. We will show how various MBE parameters such as growth temperature, Sb overpressure, GaSb growth initiation and GaSb growth rate affect IMF formation. As a result, we hope to report initial electron transport measurements from InAs/GaSb QWs grown on GaAs(001) and (111) substrates via this IMF technique.

References:

11:40 AM HH05
(Student) High Mobility n and p Pseudomorphic Channels Grown on Interfacial Misfit Dislocation Assisted Growth on GaSb/GaAs Fatih F. Ince1, Alexander T. Newell1,2, Kevin J. Reilly1, Subhashree Seth1, Thomas J. Rotter1, Ahmad Mansoori1, Darryl Shima1, Preston T. Webst2, Erin Vaughan2 and Ganesh Balakrishnan1; 1The University of New Mexico, United States; 2Air Force Research Laboratory, United States

The majority of the antimonide devices are grown on GaSb substrates. These include detectors, lasers, thermophotovoltaic devices and transistors. However, the ability to grow such devices on a GaAs substrate could have significant benefits, including larger substrate sizes, semi-insulating substrates and reduced surface defect density. A added factor is the economics of growing on GaAs which is a much more established substrate technology and costs considerably less when compared to GaSb. The interfacial misfit dislocation growth mode allows us to realize high quality metamorphic GaSb on GaAs.[1] This growth mode is superior to other metamorphic approaches such as step graded buffers due to the spontaneous relaxation of the GaSb layer on the GaAs substrate thus resulting in significant reduction in buffer
thickness. It has resulted in ~10^8 dislocations/cm^2 with instantaneous relaxation for 0.5 µm of GaSb grown on GaAs. This is achieved by the formation of a highly periodic misfit dislocation array between the GaSb and GaAs layers that almost fully accommodates the mismatch. Several publications by various authors have shown cross-section transmission electron micrograph (X-TEM) analysis and selective area diffraction analysis of the growth, showing complete and spontaneous relaxation of the GaSb epilayers.[1, 2]

Despite over a decade of work on such IMF growths of GaSb on GaAs, there is the issue of residual threading dislocations. The residual dislocations are formed during the coalescence of fully relaxed GaSb islands during the initial stages of GaSb growth on GaAs. The islands themselves are formed with a periodic misfit dislocation network, however when individual islands coalesce, these networks merge but are not in registry with each other. This leads to the formation of 60° misfit dislocations at the points of coalescence which subsequently threads into the GaSb epilayer and results in the aforementioned residual threading dislocations. With thicker growths, the dislocation density can be reduced to the high 10^7 dislocations/cm^2 range, however any further progress is difficult.

In this work we include AlSb based defect filter layers immediately after the GaSb/GaAs interface to bend residual dislocations. The mismatch between AlSb (a_o AlSb = 6.13 Å) and GaSb (a_o GaSb = 6.09 Å) results in compressive strain at the growth interface which causes the dislocations to bend at this interface. The bent dislocations at the AlSb/GaSb interface form a secondary network that appear as a mesh in plan view transmission electron micrographs. The dislocations interact with each other, resulting in significant annihilation and a much reduced threading dislocation density of ~10^7 dislocations/cm^2. The presentation will provide an extensive TEM based analysis of the GaSb/GaAs misfit dislocation interface and the plan view analysis of dislocation annihilation in AlSb/GaSb defect filter layers.

Finally, we will demonstrate the growth of InAs n-channels and InGaSb p-channels on these GaSb/GaAs growths. The purpose of the study is to investigate the mobility of these channels with varied threading dislocation density. A baseline for the study is established by growing the structures on an AlSb buffer on GaSb. While this is not lattice matched, the mismatch is minimum and should result in ~5 x 10^5 dislocations/cm^2. We then demonstrate similar channels on GaSb on GaAs grown using the IMF layer with ~5 x 10^6 dislocations/cm^2. Finally, with different defect layer designs, we will also be able to show the channels on GaSb with dislocation densities ranging from 5 x 10^6 to 5 x 10^7 dislocations/cm^2. This allows us to study the effect of dislocation densities on n and p channel mobility across four orders of magnitude. The MBE growth of the structures is completed and the hall measurements on the samples is completed for most of the structures at this point.
Yin, Xue, W02
Yingling, Yaroslava, EE09
Yoo, Jae Hyuck, H04
Yu, Caroline, PS08
Yu, Edward, BB, BB01
Yvon, Arnaud, DD03

Z
Zabetakis, Daniel, G06
Zainuddin, Shaik, U05
Zhang, Bin, PS45
Zhang, Buang, EE09
Zhang, Chengyang, P04
Zhang, Huairuo, G03, S04
Zhang, Kaitian, DD07
Zhang, Kun, PS02
Zhang, Peng, S02
Zhang, Qihua, W02
Zhang, Yiewei, L01
Zhang, Yuhao, D05, FF03
Zhang, Yuxuan, H04, O06, BB08
Zhang, Zexuan, H10
Zhao, Boyang, M02, S03
Zhao, Hongping, H04, L04, L05, L08, O06, DD07
Zhao, Huan, S03
Zhao, Songrui, W02
Zheng, Hanyu, K01
Zheng, Yikai, CC06
Zhou, Jin-Jian, P09, EE06
Zhou, Weidong, GG02
Zhou, Wenyi, U01, U02
Zhou, You, K01
Zhu, Menglin, U02, DD07
Zhu, Shengnan, B02
Zhukovskyi, Maksym, P07
Zide, Joshua, S04, T, AA08, AA09
Zou, Ke, S01
Zuo, Peng, E02
## EMC 2022 Program Grid

Registration is located First Floor, Great Hall Foyer

<table>
<thead>
<tr>
<th>Rooms</th>
<th>Wednesday AM</th>
<th>Wednesday PM</th>
<th>Thursday AM</th>
<th>Thursday PM</th>
<th>Friday AM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Great Hall Foyer, 1st floor</td>
<td>EMC Registration: 7:30 am - 5:00 pm</td>
<td>EMC Registration: 8:00 am - 5:00 pm</td>
<td>EMC Registration: 8:00 am - 12:00 pm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Performance Hall 1st floor</td>
<td>AM Break: 9:20 am - 10:00 am&lt;br&gt;Exhibit Hours: 9:00 am - 12:00 pm&lt;br&gt;1:30 pm - 4:00 pm&lt;br&gt;6:00 pm - 8:00 pm&lt;br&gt;PM Break: 3:10 pm - 3:30 pm</td>
<td>AM Break: 10:00 am - 10:20 am&lt;br&gt;Exhibit Hours: 9:00 am - 12:00 pm&lt;br&gt;1:30 pm - 4:00 pm&lt;br&gt;PM Break: 3:10 pm - 3:30 pm</td>
<td></td>
<td>AM Break: 10:00 am - 10:20 am</td>
<td></td>
</tr>
<tr>
<td>Great Hall Meeting Room 1 &amp; 2 1st floor</td>
<td>AM Break: 9:20 am - 10:00 am&lt;br&gt;Exhibit Hours: 9:00 am - 12:00 pm&lt;br&gt;1:30 pm - 4:00 pm&lt;br&gt;6:00 pm - 8:00 pm&lt;br&gt;PM Break: 3:10 pm - 3:30 pm</td>
<td>AM Break: 10:00 am - 10:20 am&lt;br&gt;Exhibit Hours: 9:00 am - 12:00 pm&lt;br&gt;1:30 pm - 4:00 pm&lt;br&gt;PM Break: 3:10 pm - 3:30 pm</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Great Hall Meeting Room 3 1st floor</td>
<td>AM Break: 9:20 am - 10:00 am&lt;br&gt;Exhibit Hours: 9:00 am - 12:00 pm&lt;br&gt;1:30 pm - 4:00 pm&lt;br&gt;6:00 pm - 8:00 pm&lt;br&gt;PM Break: 3:10 pm - 3:30 pm</td>
<td>AM Break: 10:00 am - 10:20 am&lt;br&gt;Exhibit Hours: 9:00 am - 12:00 pm&lt;br&gt;1:30 pm - 4:00 pm&lt;br&gt;PM Break: 3:10 pm - 3:30 pm</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>U.S. Bank Conference Theater 1st floor</td>
<td>AM Break: 9:20 am - 10:00 am&lt;br&gt;Exhibit Hours: 9:00 am - 12:00 pm&lt;br&gt;1:30 pm - 4:00 pm&lt;br&gt;6:00 pm - 8:00 pm&lt;br&gt;PM Break: 3:10 pm - 3:30 pm</td>
<td>AM Break: 10:00 am - 10:20 am&lt;br&gt;Exhibit Hours: 9:00 am - 12:00 pm&lt;br&gt;1:30 pm - 4:00 pm&lt;br&gt;PM Break: 3:10 pm - 3:30 pm</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ohio Staters Inc. Founders Room 2nd floor</td>
<td>AM Break: 9:20 am - 10:00 am&lt;br&gt;Exhibit Hours: 9:00 am - 12:00 pm&lt;br&gt;1:30 pm - 4:00 pm&lt;br&gt;6:00 pm - 8:00 pm&lt;br&gt;PM Break: 3:10 pm - 3:30 pm</td>
<td>AM Break: 10:00 am - 10:20 am&lt;br&gt;Exhibit Hours: 9:00 am - 12:00 pm&lt;br&gt;1:30 pm - 4:00 pm&lt;br&gt;PM Break: 3:10 pm - 3:30 pm</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ohio Staters Inc. Traditions Room 2nd floor</td>
<td>AM Break: 9:20 am - 10:00 am&lt;br&gt;Exhibit Hours: 9:00 am - 12:00 pm&lt;br&gt;1:30 pm - 4:00 pm&lt;br&gt;6:00 pm - 8:00 pm&lt;br&gt;PM Break: 3:10 pm - 3:30 pm</td>
<td>AM Break: 10:00 am - 10:20 am&lt;br&gt;Exhibit Hours: 9:00 am - 12:00 pm&lt;br&gt;1:30 pm - 4:00 pm&lt;br&gt;PM Break: 3:10 pm - 3:30 pm</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Senate Chamber 2nd floor</td>
<td>AM Break: 9:20 am - 10:00 am&lt;br&gt;Exhibit Hours: 9:00 am - 12:00 pm&lt;br&gt;1:30 pm - 4:00 pm&lt;br&gt;6:00 pm - 8:00 pm&lt;br&gt;PM Break: 3:10 pm - 3:30 pm</td>
<td>AM Break: 10:00 am - 10:20 am&lt;br&gt;Exhibit Hours: 9:00 am - 12:00 pm&lt;br&gt;1:30 pm - 4:00 pm&lt;br&gt;PM Break: 3:10 pm - 3:30 pm</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cartoon Room 1 3rd floor</td>
<td>AM Break: 9:20 am - 10:00 am&lt;br&gt;Exhibit Hours: 9:00 am - 12:00 pm&lt;br&gt;1:30 pm - 4:00 pm&lt;br&gt;6:00 pm - 8:00 pm&lt;br&gt;PM Break: 3:10 pm - 3:30 pm</td>
<td>AM Break: 10:00 am - 10:20 am&lt;br&gt;Exhibit Hours: 9:00 am - 12:00 pm&lt;br&gt;1:30 pm - 4:00 pm&lt;br&gt;PM Break: 3:10 pm - 3:30 pm</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Rosa M. Alabouni Room 3rd floor</td>
<td>AM Break: 9:20 am - 10:00 am&lt;br&gt;Exhibit Hours: 9:00 am - 12:00 pm&lt;br&gt;1:30 pm - 4:00 pm&lt;br&gt;6:00 pm - 8:00 pm&lt;br&gt;PM Break: 3:10 pm - 3:30 pm</td>
<td>AM Break: 10:00 am - 10:20 am&lt;br&gt;Exhibit Hours: 9:00 am - 12:00 pm&lt;br&gt;1:30 pm - 4:00 pm&lt;br&gt;PM Break: 3:10 pm - 3:30 pm</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Archie M. Griffin East Ballroom 2nd floor</td>
<td>AM Break: 9:20 am - 10:00 am&lt;br&gt;Exhibit Hours: 9:00 am - 12:00 pm&lt;br&gt;1:30 pm - 4:00 pm&lt;br&gt;6:00 pm - 8:00 pm&lt;br&gt;PM Break: 3:10 pm - 3:30 pm</td>
<td>AM Break: 10:00 am - 10:20 am&lt;br&gt;Exhibit Hours: 9:00 am - 12:00 pm&lt;br&gt;1:30 pm - 4:00 pm&lt;br&gt;PM Break: 3:10 pm - 3:30 pm</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Poster Reception:** 6:00 pm - 8:00 pm

**Conference Dinner Reception:** 6:00 pm - 8:00 pm