SYMPOSIUM Z

Structure-Property Relationships of Oxide Surfaces and Interfaces - II

December 2 - 3, 2002

Chairs

Kathleen B. Alexander C. Barry Carter Robin W. Grimes Xiaoqing Q. Pan Thomas Wood

Los Alamos National Laboratory Univ of Minnesota Imperial College Univ of Michigan 3M Company

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* Invited paper

SESSION Z1: Chairs: C. Barry Carter and Robin W. Grimes Monday Morning, December 2, 2002 Independence West (Sheraton)

8:30 AM <u>Z1.1</u>

ATOMIC SCALE MODEL OF THE GRAIN BOUNDARY POTENTIAL IN PEROVSKITE OXIDES. <u>R.F. Klie</u>, Y. Zhu, Brookhaven National Laboratory, Dept. of Applied Science, Upton, NY; N.D. Browning, University of Illinois at Chicago, Department of Physics, Chicago, IL.

8:45 AM <u>Z1.2</u>

AB-INITIO THEORY OF GRAIN-BOUNDARY SEGREGATION IN α -ALUMINA: ATOMISTICS, ENERGETICS, AND ELECTRONIC STRUCTURE. Stefano Fabris and Christian Elsässer, Max-Planck-Institut für Metallforschung, Stuttgart, GERMANY.

9:00 AM <u>*Z1.3</u> SIMULATING OXIDE INTERFACES AND HETEROINTERFACES. John Harding, University College London, Dept of Physics and Astronomy, London, UNITED KINGDOM.

9:30 AM *Z1.4

MASS AND CHARGE TRANSPORT IN OXIDES: THE ROLE OF INTERFACES. Joachim Maier, Max-Planck-Institut für Festkörperforschung, Stuttgart, GERMANY.

10:00 AM BREAK

10:30 AM Z1.5

DENSITY FUNCTIONAL INVESTIGATION OF H₂O ADSORPTION ON THE (110) SURFACE OF RUTILE TiO2. Leonard A. Harris^{a, b} and Andrew A. Quong^b; ^aCornell University, ^bSchool of Chemical and Biomolecular Engineering, Ithaca, NY; ^bLawrence Livermore National Laboratory, Livermore, CA.

10:45 AM Z1.6

SEGREGATION OF YTTRIA TO THE SURFACES OF TETRAGONAL ZIRCONIA. Susan E. Redfern, C.R. Stanek, Robin W. Grimes and Rees D. Rawlings, Dept. of Materials, Imperial College, London, UNITED KINGDOM.

11:00 AM <u>*Z1.7</u> THE ROLE OF BULK DIFFUSION IN THE GROWTH, SMOOTHING, AND RECONSTRUCTION OF THE TITANIUM DIOXIDE SURFACE. K.F. McCarty, J.A. Nobel, and N.C. Bartelt, Sandia National Laboratories, Livermore, CA.

11:30 AM <u>*Z1.8</u>

ACCURATE MEASUREMENTS OF SPACE CHARGE AND

LATTICE DISPLACEMENT OF INTERFACES IN SUPERCONDUCTING OXIDES. M. Schofield, Lijun Wu and Yimei Zhu, Brookhaven National Laboratory, Upton, NY.

SESSION Z2:

Chairs: Kathleen B. Alexander and Robin W. Grimes Monday Afternoon, December 2, 2002 Independence West (Sheraton)

1:30 PM *Z2.1

ATOMIC STRUCTURES OF MIXED IONIC-ELECTRONIC CONDUCTING OXIDE THIN FILMS. S. Stemmer, D.O. Klenov, Univ of California-Santa Barbara, Santa Barbara, CA; W. Donner, A.J. Jacobson, Univ of Houston, Houston, TX.

2:00 PM *Z2.2 SrTiO₃(100)/LaMnO₂)_{2n} (SrMnO₂)_n LAYERED HETERO-STRUCTURES: A COMBINED EELS-TEM STUDY. Jo Verbeeck, Oleg Lebedev, <u>Gustaaf Van Tendeloo</u>, EMAT, University of Antwerp, Antwerp, BELGIUM; Bernard Mercey, CRISMAT, University of Caen, Caen, FRANCE.

2:30 PM <u>Z2.3</u>

ATOMIC-SCALE DELTA DOPING IN STRONTIUM TITANATE. Harold Y. Hwang, Akira Ohtomo, David A. Muller, Don R. Hamann, John L. Grazul, Bell Labs, Lucent Technologies, NJ.

2:45 PM Z2.4

STRUCTURE SENSITIVITY OF PHOTOCHEMICAL OXIDATION AND REDUCTION REACTIONS ON STTIO₃ SURFACES Jennifer L. Giocondi, Gregory S. Rohrer, Carnegie Mellon University, Dept of Materials Science and Engineering, Pittsburgh, PA.

3:00 PM BREAK

3:30 PM *Z2.5

OXIDE SEMICONDUCTOR JUNCTIONS. Harry L. Tuller, MIT, Dept of Materials Science and Engineering, Cambridge, MA.

4:00 PM <u>Z2.6</u>

AB INITIO CALCULATIONS OF ZrO₂ GRAIN BOUNDARIES AND HETEROGENEOUS INTERFACES. Zugang Mao, Jun He, Susan B. Sinnott, University of Florida, Dept of Materials Science and Engineering, Gainesville, FL; Elizabeth C. Dickey, The Pennsylvania State University, Dept of Materials Science and Engineering, University Park, PA.

4:15 PM Z2.7

CHROMIUM AND LANTHANUM ON TRANSITION ALUMINA SURFACES: THE ROLE OF BULK POINT-DEFECT DISTRIBUTIONS ON CATALYTIC ACTIVITY. S.N. Rashkeev, Vanderbilt University, Dept of Physics and Astronomy, Nashville, TN; K. Sohlberg, Drexel University, Dept of Chemistry, Philadelphia, PA; M.V. Glazov, Alcoa Technical Center, Alcoa Center, PA; J. Novak, Alcoa World Alumina, Port Allen, LA; S.J. Pennycook, Oak Ridge National Laboratory, Solid State Division, Oak Ridge, TN; S.T Pantelides, Vanderbilt University, Dept of Physics and Astronomy, Nashville, TN, and Oak Ridge National Laboratory, Solid State Division, Oak Ridge, TN.

4:30 PM <u>Z2.8</u>

ATOMIC FORCE AND SCANNING TUNNELING MICROSCOPY OF NETWORK-DISRUPTED AMORPHOUS OXIDE INTERFACES: FRACTURE AND SPUTTER MORPHOLOGIES. Christopher C. Umbach and John M. Blakely, Cornell Univ, Dept of Materials Science and Engineering, Ithaca, NY.

4:45 PM Z2.9

OXYGEN ADSORPTION AND OXIDE FORMATION AT Ag(111): ROLE OF THE O-AG INTERACTION IN THE FUNCTION OF SILVER AS AN OXIDATION CATALYST. Weixue Li, Catherine Stampfl, and Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, GERMANY.

> SESSION Z3: POSTER SESSION Chairs: Xiaoqing Q. Pan, Kathleen B. Alexander, C. Barry Carter, Robin W. Grimes and Thomas Wood Monday Evening, December 2, 2002 8:00 PM Exhibition Hall D (Hynes)

Z3.1

SURFACE HYDROXIDE FORMATION ON MeO₂ OXIDES.

<u>Robin W. Grimes</u>, Averyl Tan, C.R. Stanek, Dept. of Materials, Imperial College, London, UNITED KINGDOM; and S. Owens, BNFL, Research and Technology, Rutherford House, Risley, UNITED KINGDOM.

$\mathbf{Z3.2}$

TRANSPORT PROPERTIES OF LOW-ANGLE GRAIN BOUNDARIES IN Fe-DOPED SrTiO₃. <u>R.A. De Souza</u>, J. Fleig and J. Maier, Max Planck Institute for Solid State Research, Stuttgart, GERMANY.

Z3.:

HIGH RESOLUTION ELECTRON MICROSCOPY STUDY ON THE DEFECT STRUCTURE AND STRAIN RELAXATION OF EPITAXIAL Ba_{0.3}Sr_{0.7}TiO₃ THIN FILMS GROWN ON (001) LaAlO₃. Chaojing Lu, <u>Leonid Bendersky</u>, Materials Science and Engineering Laboratory, National Institute of Standards and Technology, Gaithersburg, MD; Kaoshuo Chang, Ichiro Takeuchi, Department of Materials Science and Engineering, University of Maryland, College Park, MD.

$\mathbf{Z3.4}$

SYNTHESIS AND PHOTOCATALYTIC PROPERTIES OF NEW VISIBLE LIGHT DRIVEN INDIUM OXIDE PHOTOCATALYSTS. Jiang Yin, Jinhua Ye, National Institute for Materials Science (NIMS), Ecomaterials Center, Tsukuba, JAPAN; Zhigang Zou, National Institute of Advanced Industrial Science and Technology (AIST), Photoreaction Control Center (PCRC), Tsukuba, JAPAN.

$\mathbf{Z3.5}$

CHARACTERIZATION OF INTERFACIAL CHEMISTRY AND THE EFFECTS ON SINGLE CRYSTAL GROWTH OF PMN-PT. <u>Edward P. Gorzkowski</u>, Helen M. Chan, Martin P. Harmer, Lehigh University, Materials Research Center, Bethlehem, PA.

<u>Z3.6</u>

ATOMIC STRUCTURE-ELECTRICAL PROPERTY RELATIONSHIPS IN KrF LASER IRRADIATED SURFACE OF POROUS SILICA FILMS. <u>Hyun-Dam Jeong</u>^a, Jung-Bae Kim^a, Sun-Young Lee^b, Jin-Heong Yim^a, Yi-Yeol Lyu^a, and Jae-Geun Park^a; ^aPolymer Lab., Samsung Advanced Institute of Technology, Suwon-city, Kyungki-do, KOREA; ^bManufacturing Technology Center, Samsung Electronics Co., Ltd., Yongin-city, Kyungki-do, KOREA.

Z3.7

THE EFFECT OF SURFACE LAYER ON THE DIELECTRIC BEHAVIOR OF COMPLEX OXIDE THIN FILMS. <u>Dingquan Xiao</u>, Linli Meng, Dept of Materials Science, Sichuan University, Chengdu, P.R. CHINA.

Z3.8

TEM INVESTIGATION OF THE CORE/CLAD INTERFACE OF La₂O₃-Al₂O₃-SiO₂ GLASSES FOR HIGH POWER FIBER LASERS. Shang-Cong Cheng, Matthew J. Dejneka, Corning Inc, Science and Technology, Corning, NY.

$\mathbf{Z3.9}$

EFFECT OF EPITAXIAL STRAIN ON THE METAL-INSULATOR TRANSITION CHARACTERISTICS OF NdNiO₃. <u>Ashutosh Tiwari</u>, J. Narayan, Department of Materials Science and Engineering, North Carolina State University, Raleigh, NC.

Z3.10

CHARACTERIZATION OF POROUS PT/ALUMINA FILMS PRODUCED BY HYBRID GAS-TO-PARTICLE CONVERSION AND CHEMICAL VAPOR DEPOSITION. Q.T. Nguyen, S.H. Ehrman, Dept of Chemical Engineering, College Park, MD.

Z3.11

THE EFFECT OF OXIDE COATING OF COPPER NANOPARTICLES ON POLARIZED LIGHT SCATTERING. Jung Hyeun Kim, Sheryl H. Ehrman, Univ MD, College Park, MD; George W. Muholland, Thomas A. Germer, NIST, Gaithersburg, MD.

Z3.12

IR SPECTRA OF PHOTOCHEMICALLY GROWN SUBOXIDES AT THE Si/SiO₂ INTERFACE. <u>Peter Hess</u>, Jochen Lambers, Univ of Heidelberg, Inst of Physical Chemistry, Heidelberg, GERMANY.

Z3.13

Abstract Withdrawn

<u>Z3.14</u> Abstract Withdrawn

Z3.15

SYNTHESIS OF ZEOLITE-CONFINED RuO₂ NANOCLUSTERS FOR AEROBIC OXIDATION CATALYSIS. Bi-Zeng Zhan, Mary Anne White, Dalhousie University, Dept. of Chemistry and Institute for Research in Materials, Halifax, Nova Scotia, CANADA.

Z3.16

CHARACTERIZATION OF NONSTOICHIOMETRIC ZINC OXIDE NANOPARTICLE PREPARED BY DECOMPOSITION OF ZINC PEROXIDE NANOPARTICLE. <u>Naofumi Uekawa</u>, Naomi Mochizuki, Kazuyuki Kakegawa, Chiba Univ, Dept of Materials Technology, Chiba, JAPAN; Jyunichi Kajiwara, FM Giken Co. Ltd., Chiba, JAPAN.

Z3.17

POLYCRYSTALLINE COPPER CHROMITE (CuCr₂O₄) CATALYST THIN FILMS PREPARED BY METAL ORGANIC CHEMICAL VAPOR DEPOSITION. <u>Yuneng Chang</u>, Chianghung Lin, Beeyu Lee Department of Chemical Engineering, Lunghwa University of Science and Technology Gueishan, Taoyuan, TAIWAN, R.O.C.

$\mathbf{Z3.18}$

SPINEL ZINC CHROMITE (ZnCr2O4) THIN FILMS PREPAREDBY METAL ORGANIC CHEMICAL VAPOR DEPOSITION.Yuneng Chang, Chichih Chung, Huankuang Pen, Department ofChemical Engineering, Lunghwa University of Science and TechnologyGueishan, Taoyuan, TAIWAN, R.O.C.

Z3.19

LOW-TEMPERATURE GROWTH OF SILICON DIOXIDE THIN FILMS BY VUV PHOTO-OXIDATION. Atsuyuki Fukano and Hiroyuki Oyanag, National Institute of Advanced Industrial Science and Technology, Ibaraki, JAPAN.

<u>Z3.20</u>

CORRELATION BETWEEN MAGNETORESISTANCE, DC RESISTIVITY AND MICROSTRUCTURE OF SrRuO₃ THIN FILMS. <u>Khaled Khamchane</u>, Robert Gunnarsson, Zdravko Ivanov, Chalmers University of Technology, Dept of Microelectronics and Nanoscience; Andrei Vorobyev, Per Rundqvist, Spartak Gevorgian, Chalmers University of Technology, Dept of Microelectronics.

Z3.21

Abstract Withdrawn

Z3.22

THE EFFECT OF OXIDE INTERFACE ON MINERALIZATION. Jingjing Liu, Shuzheng Zhang, Lisheng Qin, and Kecheng Gong, Polymer Structure & Modification Res. Lab., South China Uni. of Tech., Guangzhou, P.R. CHINA.

Z3.23

THEORETICAL STUDIES OF POINT DEFECT SEGREGATION TO THE $\Sigma = 5$ TWIST BOUNDARY IN SrTiO₃. <u>R. Astala</u>, P.D. Bristowe, Univ Cambridge, Cambridge, UNITED KINGDOM.

Z3.24

THE EFFECT OF Y ON THE STRENGTH OF FeCrAl ALLOY/SAPPHIRE INTERFACES. <u>S.N. Basu</u>, Department of Manufacturing Engineering, Boston University, Boston, MA; V. Gupta, Department of Mechanical and Aerospace Engineering, UCLA, Los Angeles, CA.

Z3.25

EFFECT OF THIN Y₂O₃ FILMS ON IN-SITU FORMED CAO COATINGS ON V-4%Cr-4%Ti IN LIQUID 2.8 AT % Ca-Li. J.-H. Park, A. Sawada, K. Natesan, and R.F. Mattas^a, Energy Technology Division and ^a Technology Development Division, Argonne National Laboratory, Argonne, IL.

Z3.26

Abstract Withdrawn

Z3.27

EFFECT OF LANTHANUM MANGANITE MODIFICATION BY CALCIUM AND/OR FLUORINE ON THE BONDING STRENGTH, MOBILITY AND REACTIVITY OF THE LATTICE AND SURFACE OXYGEN. Vladislav A. Sadykov, Tatyana G. Kuznetsova, Andrei V. Simakov, V.A. Rogov, V.I. Zaikovskii, E.A. Paukshtis, E.M. Moroz, D.I. Kochubei, B.N. Novgorodov, V.P. Ivanov, S.N. Trukhan, G.S. Litvak, N.N. Bulgakov, Boreskov Inst. Catalysis, Novosibirsk, RUSSIA; V.V. Lunin, Lomonosov Moscow State Univ., Chem. Dep., Moscow, RUSSIA; E. Kemnitz, Ints. for Chemistry, Humboldt Univ., Berlin, GERMANY.

Z3.28

COMPOSITIONAL IMAGING OF THE "CORE-SHELL" STRUCTURE IN BaTiO₃ BASED CERAMICS. <u>Dae-Chul Park</u>, Isao Sakaguchi, Naoki Ohashi, Shunichi Hishida, and Hajime Haneda, Advanced Materials Laboratory, National Institute for Materials Science, Ibaraki, JAPAN; Jun-ich Itoh, Mitsui Mining & Smelting Co., Ltd, Saitama, JAPAN.

$\mathbf{Z3.29}$

COMPARISON OF Al₂O₃ FILMS GROWN BY ATOMIC LAYER DEPOSITION AND REACTIVE SPUTTERING. Giovanna Scarel, Evangelis K. Evangelou, Sandro Ferrari, Sabina Spiga, Grazia Tallarida, Claudia Wiemer, and <u>Marco Fanciulli</u>, Laboratorio MDM-INFM, Agrate Brianza (MI) ITALY; Elizabeth E. Hoppe and Carolyn R. Aita, ACE Laboratory and Department of Materials Engineering, Milwaukee, WI; Andrei Zenkevich and Yuri Lebedinskii, Moscow Engineering Physics Institute, Moskow, RUSSIA.

Z3.30

CROSS SECTION ANALYSIS OF ANODIZED NIOBIUM OXIDE FILMS. Hiroshi Moriyama, Ryusuke Osada, Yuko Iizuka, Toho Univ, Dept of Chemistry, Funabashi, JAPAN; Takashi Mochizuki, Sanshin Ltd, Shiojiri, Nagano, JAPAN.

Z3.31

STUDY OF PORE ARCHITECTURE IN SILICON OXIDE THIN FILMS BY VARIABLE ENERGY POSITRON ANNIHILATION SPECTROSCOPY. Kenji Ito, Yoshinori Kobayashi, Runsheng Yu, Kouichi Hirata, Hisashi Togashi, National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki, JAPAN.

Z3.32

USING STRAIN TO DYNAMICALLY TUNE THE PROPERTIES $\begin{array}{l} {\rm OF\ La}_{0.5}{\rm Sr}_{0.5}{\rm MnO}_3 \ {\rm ON\ BaTiO}_3. \ \underline{\rm Darren\ Dale}, \ {\rm Cornell\ Univ,\ Dept} \\ {\rm Materials\ Science\ and\ Engineering,\ Ithaca,\ NY;\ Aaron\ Fleet,\ Cornell \end{array}$ Univ, School of Applied and Engineering Physics, Ithaca, NY; J.D. Brock, Cornell Univ, School of Applied and Engineering Physics, Ithaca, NY; Yuri Suzuki, Cornell Univ, Dept Materials Science and Engineering, Ithaca, NY.

Z3.33

STABILIZATION OF INDIUM TIN OXIDE FILMS AT VERY HIGH TEMPERATURES. Otto J. Gregory, Everett E. Crisman, <u>Tao You</u> and Michael Platek, University of Rhode Island, Sensors and Surface Technology Partnership, Department of Chemical Engineering, Kingston, RI.

Z3.34

SELECTIVE CATALYTIC REDUCTION OF NOX BY HYDRO-CARBONS OVER ALUMINA-BASED NANOCOMPOSITES <u>Pemakorn Pitukmanorom</u> and Jackie Y. Ying, Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA.

Z3.35 EPITAXIAL OXIDE HETEROSTRUCTURES FOR CHEMICAL SENSING APPLICATIONS. <u>Wonwoo Kim</u>, Juan Dominguez and Xiaoqing Pan, University of Michigan, Dept. of Materials Science, Ann Arbor, MI.

<u>Z3.36</u>

THE STRONG METAL SUPPORT INTERACTION IN THE Pd/TIN OXIDE MODEL SYSTEM FOR CHEMICAL SENSORS. Juan Dominguez, Xiaoqing Pan, University of Michigan, Dept of Materials Science, Ann Arbor, MI; George Graham, Ford Research Lab, Dearborn, MI.

<u>Z3.</u>37

STRUCTURES OF OXIDES FORMED ON METALS DUE TO ATOMIC OXYGEN EXPOSURE. Long Li, Judith C. Yang, Materials Science and Engineering Dept, University of Pittsburgh, Pittsburgh, PA.

Z3.38

NEW RESULTS OF IRON OXIDE MICROSTRUCTURE IN HIGH-TEMPERARURE OXIDATION. Bae-Kyun Kim and Jerzy A. Szpunar, McGill Univ, Dept. of Mining, Metals and Materials Engineering, Montreal, CANADA.

Z3.39

INTERFACIAL PHASE FORMATION IN Cu-Mg THIN FILMS GROWN ON OXIDIZED Si. <u>M.J. Frederick</u>, R. Goswami, G. Ramanath, Rensselaer Polytechnic Institute, Dept of Materials Science and Engineering, Troy, NY.

Z3.40

SURFACE CHEMISTRY OF MESOPOROUS MATERIALS:

EFFECT OF NANOSCALE PORE SPACE CONFINEMENT. Yifeng Wang, Charles Bryan, Sandia National Laboratories, Carlsbad, NM; Huifang Xu, Department of Earth and Planetary Sciences, University of New Mexico, Albuquerque, NM; Phil Pohl, C. Jeffrey Brinker, Sandia National Laboratories, Albuquerque, NM.

Z3.41

THE RELATIONSHIP BETWEEN MICROSTRUCTURE PROCESSING AND ELECTRONIC PROPERTIES OF BULK COMPOSITE FERROELECTRICS. Jennifer Synowczynski, Samuel Hirsch and Bonnie Gersten, Weapons and Materials Research Directorate, Army Research Laboratory, Aberdeen Proving Grounds, MD.

Z3.42

COMPUTATIONAL STUDIES OF CATECHOL AND WATER INTERACTIONS WITH TITANIUM OXIDE NANOPARTICLES. P. $Zapol^a$, P.C. $Redfern^b$, M.C. Thurnauer^b, T. $Rajh^b$, and L.A. Curtiss^{a, b}, ^aMaterials Science and ^bChemistry Divisions, Argonne National Laboratory, Argonne, IL.

OXIDATION OF SI-SINGLE CRYSTAL BY ATOMIC OXYGEN SPECIES. Judith C. Yang, Maja Randjelovic, University of Pittsburgh, Materials Science and Engineering Department, Pittsburgh, PA.

Z3.44

TREATMENT OF (100) KTaO₃ FOR ATOMICALLY-FLAT SURFACES. Hyung-jin Bae, Jennifer Sigman, D.P. Norton, Univ. of Florida, Dept of Materials Science and Engr, Gainesville, FL; Lynn Boatner, Solid State Div, Oak Ridge National Laboratory, Oak Ridge, TN.

Z3.45

METALORGANIC CHEMICAL VAPOR DEPOSITION OF ALUMINUM OXIDE ON SILICON NITRIDE: FORMATION OF INTERFACIAL SiO $_x$ N $_y$. Anindya Dasgupta, Abhijit Roy Chowdhuri, and Christos G. Takoudis, University of Illinois at Chicago, Dept of Chemical Engineering, Chicago, IL.

Z3.46

INFLUENCE OF STRUCTURE AND CHEMISTRY ON PIEZOELECTRIC PROPERTIES OF PZT IN A MEMS POWER GENERATION APPLICATION. L.M.R. Eakins, D.E. Eakins, C.D. Richards, M.G. Norton, R.F. Richards, and D.F. Bahr, Mechanical and Materials Engineering, Washington State University, Pullman, WA.

Z3.47

OBSERVATIONS OF TiO₂ SURFACE USING TOTALLY REFLECTED X-RAY IN-PLANE DIFFRACTION UNDER UV IRRADIATION. T. Horiuchi, H. Ochi, K. Kaisei, K. Ishida and K. Matsushige, Kyoto Univ., Dept. of Electronic Science and Engineering, Kyoto, JAPAN.

Z3.48

INTERACTION OF ULTRATHIN Cu₂O LAYERS ON WO₃ CHEMIRESISTIVE SENSING FILMS. A. El Madi, G. Bernhardt, R.S. Pilling, R.J. Lad, B.G. Frederick, Laboratory for Surface Science & Technology, University of Maine, Orono, ME.

Z3.49

SURFACE ELECTRICAL MEASUREMENTS ON PHOTO-CATALYSIS OF RUTILE TiO₂(110). <u>K. Kaisei</u>, K. Ishida, T. Horiuchi, K. Matsushige, Kyoto University, Dept of Electronic Science and Engineering, Kyoto, JAPAN.

Z3.50

X-RAY MEASUREMENTS OF THE INTRINSIC SURFACE EFFECT ON FERROELECTRICITY IN PbTiO₃ FILMS. D.D. Fong, S.K. Streiffer, J.A. Eastman, O. Auciello, P.H. Fuoss, G.B. Stephenson, Argonne National Laboratory, Materials Science Division, Argonne, IL; Carol Thompson, Northern Illinois Univ, Dept of Physics, DeKalb, IL; Y. Yacoby, M. Sowwan, Hebrew Univ, Racah Inst of Physics, Jerusalem, ISRAEL; R. Pindak, Brookhaven National Laboratory, National Synchrotron Light Source, Upton, NY; R. Clarke, Univ of Michigan, Randall Laboratory of Physics, Ann Arbor, MI; E.A. Stern, Univ of Washington, Dept of Physics, Seattle, WA.

Z3.51

CHEMICAL STRUCTURE OF N ATOMS INCORPORATED INTO 1NM-THICK $\mathrm{SiO}_2/\mathrm{Si}$ AS REVEALED WITH THE DISSOLUTION AND HYDROGENATION IN HYDROFLUORIC ACID. Naomi Mizuta, Satoru Watanabe, Fujitsu Laboratories Ltd, Kanagawa, JAPAN.

Z3.52 GROWTH KINETICS AND INTERFACE CHEMISTRY OF SUBSTITUTIONAL DOPING IN SrTiO₃ FILMS. <u>Akira Ohtomo</u>, Harold Y. Hwang, David A. Muller, Bell Labs, Lucent Technologies, NJ

Z3.53

MICROSTRUCTURAL CHARACTERIZATION BY SPECTRO-SCOPIC ELLIPSOMETRY OF ALUMINIUM OXIDE THIN FILMS GROWN BY LOW PRESSURE MOCVD. M.P. Singh and S.A. Shivashankar, Materials Research Centre, Indian Institute of Science, Banglore, INDIA; G. Raghavan and A.K. Tyagi, Materials Science Division, Indira Gandhi Centre for Atomic Research, Kalpakkam, INDIA

Z3.54

LATTICE STRAIN CONTROL AT OXIDE HETEROINTERFACES. K. Terai, T. Fujii, H. Koinuma, Department of Innovative and JAPAN; M. Lippmaa, Institute for Solid State Physics, University of Tokyo, JAPAN; P. Ahmet, T. Chikyow, National Institute for Materials Science, Tsukuba, JAPAN; M. Kawasaki, Institute for Materials Research, Tohoku Univ., Sendai, JAPAN.

Z3.55

WATER MOLECULE ADSORPTION PROPERTIES ON THE SURFACE OF THE PROMISING NEW PHOTO-CATALYST InVO₄ FOR WATER DECOMPOSITION IN THE VISIBLE WAVE-LENGTH REGION. <u>Mitsutake Oshikiri</u>, Jinhua Ye, NIMS, Tsukuba, JAPAN; Mauro Boero, AIST, Tsukuba, JAPAN.

> SESSION Z4: Chairs: Thomas Wood and Kathleen B. Alexander Tuesday Morning, December 3, 2002 Independence West (Sheraton)

NOTE EARLY START

 $8:00~\text{AM}~\underline{*Z4.1}_{\text{AND}}$ characterisation of Ni thin films on PEROVSKITE-BASED SUBSTRATES. J. Yu, <u>M. Yeadon</u>, IMRE, Singapore and Dept of Materials Science, National University of Singapore, SINGAPORE; J.H. Haeni and D.G. Schlom, MSE Dept, Penn State University, State College, PA; W. Tian and X.Q. Pan, MSE Dept, Univ of Michigan, Ann Arbor, MI; R. Clarke, Physics Dept, Univ of Michigan, Ann Arbor, MI.

8:30 AM <u>*Z4.2</u> ISLAND SHAPE SELECTION AND INSTABILITY IN EPITAXIAL GROWTH. E.G. Wang, M.Z. Li, J. Wu, B.G. Liu, Institute of Physics and International Center for Quantum Structures, Chinese Academy of Sciences, Beijing, CHINA; J. Wendelken, and Z. Zhang, Oak Ridge National Lab, Oak Ridge, TN.

9:00 AM <u>Z4.3</u>

ELECTRON MICROSCOPY CHARACTERIZATION OF THIN-FILM YTTRIUM STABILIZED ZIRCONIA AND CERIA ON MgO. J. Bentley, P.F. Becher, I. Kosacki, and C.M. Rouleau[†], Oak Ridge National Laboratory, Metals and Ceramics Division ([†]Solid State Division), Oak Ridge, TN.

9:15 AM <u>Z4.4</u>

LAYER INTERMIXING DURING METAL/METAL-OXIDE ADSORPTION: Ti/SAPPHIRE(0001). C. Verdozzi, Department of Physics, California State University Nortridge, Nortridge, CA; P.A. Schultz, Sandia National Laboratories, Albuquerque, NM; Ruqian Wu, Department of Physics and Astronomy, University of California, Arb, Department of Hydrox Arr Force Research Laboratory, Kirtland AFB, NM; Nicholas Kioussis, Department of Physics, California State University Nortridge, Nortridge, CA.

9:30 AM Z4.5

DIRECT DETERMINATION OF EPITAXIAL INTERFACE STRUCTURES. Yizhak Yacoby, Hebrew University, Racah Institute of Physics, Jerusalem, ISRAEL; <u>Ron Pindak</u>, NSLS, Brookhaven National Lab, Upton, NY; Ed Stern, Dept of Physics, Univ of Washington, Seattle, WA; Julie Cross, Dale Brewe, PNC-CAT, Advanced Photon Source, Argonne National Lab, Argonne, IL; Eric Dufresne, MHATT-CAT, Advanced Photon Source, Argonne National Lab, Argonne, IL; Roy Clarke, Dept of Physics, Univ of Michigan, Ann Arbor, MI.

9:45 AM BREAK

10:15 AM <u>*Z4.6</u>

GRAIN BOUNDARY SEGREGATION IN TITANIUM DIOXIDE: EVALUATION OF RELATIVE DRIVING FORCES FOR SEGREGATION. Elizabeth C. Dickey, Qinglei Wang, Guoda D. Lian, Pennsylvania State University, Department of Materials Science and Engineering, University Park, PA.

10:45 AM Z4.7

HOW THICK IS THAT OXIDE? David D. Allred, R. Steven Turley, Guillermo Acosta, Shannon Lunt, Kristi Adamson, Elke Jackson, Michael Newey, Raymond Rios, Richard Sandberg, and Nick Webb, Brigham Young University, Department of Physics and Astronomy, Provo, UT.

11:00 AM Z4.8

MOLECULAR DYNAMICS SIMULATIONS OF THE INTERFACE STRUCTURE AND CHEMISTRY OF INTERGRANULAR FILMS. Stephen H. Garofalini, Weiwei Luo, and Shanghong Zhang, Department of Ceramic and Materials Engineering, Rutgers University, Piscataway, NJ.

11:15 AM <u>Z4.9</u>

STABILITY OF INTERGRANULAR GLASSY FILMS IN CERAMICS. Catherine M. Bishop, W. Craig Carter, MIT, Dept. of Materials Science and Engineering, Cambridge, MA.

11:30 AM Z4.10

THE WETTING OF ALUMINA GRAIN BOUNDARIES BY MOLTEN GLASS. John E. Blendell, Amanda K. Slocum, Bernard J. Hockey, Jong-Sook Lee, Sheldon M. Wiederhorn and Mark D. Vaudin, Materials Science and Engineering Laboratory, National Institute of Standards and Technology, Gaithersburg, MD.

11:45 AM <u>Z4.11</u>

EFFECTS OF THE AMORPHOUS OXIDE INTERGRANULAR LAYER STRUCTURE AND BONDING ON FRACTURE TOUGHNESS IN HIGHLY PURE SILICON NITRIDE. Alexander Ziegler, Lawrence Livermore National Laboratory, University of California, Livermore, CA; Christian Kisielowski, Lawrence Berkeley National Laboratory, University of California, Berkeley, CA; Michael J. Hoffmann, IKM, University of Karlsruhe, Karlsruhe, GERMANY; Robert O. Ritchie, Lawrence Berkeley National Laboratory, University of California, Berkeley, CA.

> SESSION Z5: Chairs: Xiaoqing Q. Pan and Thomas Wood Tuesday Afternoon, December 3, 2002 Independence West (Sheraton)

1:30 PM <u>Z5.1</u>

REACTIVE SOLID STATE DEWETTING: CAVITY FORMATION AT THE INTERFACE IN THE SYSTEM Ag-Ni-O. Henri de Monestrol, Lelia Schmirgeld Mignot, Sylvie Poissonnet and Georges Martin, SRMP, CEA Saclay, Gif sur Yvette, FRANCE.

1:45 PM Z5.2

IMAGING BURIED STRUCTURES WITH THE PHOTO-ELECTRON EMISSION MICROSCOPE. K. Siegrist, V.W. Ballarotto, M. Breban, E.D. Williams, Department of Physics, University of Maryland, College Park, MD, and the Laboratory for Physical Sciences, College Park, MD.

2:00 PM <u>*Z5.3</u>

STRUCTURE AND PROPERTY OF OXIDE INTERFACE AND OXIDE NANO-MATERIALS CHARACTERIZED BY COMPLEX HRTEM AND PROPERTY IMAGING TECHNIQUE. J.J. Kai, Fu-Rong Chen, Center of Electron Microscopy, Dept. of Engineering and System Science, National Tsing Hua University, Hsin Chu, TAIWAN.

2:30 PM *Z5.4

BONDING AND MANIPULATION OF COPPER-ALUMINA INTERFACES. Christina Scheu, Max-Planck-Institut fuer Metallforschung, Stuttgart, GERMANY.

3:00 PM BREAK

3:30 PM *Z5.5

ELECTROCHEMICAL BEHAVIOR OF SURFACE-MODIFIED AND DOPED ELECTRODE MATERIALS FOR HIGH-POWER LITHIUM ION BATTERIES. Jun Liu, Khalil Amine, Chemical Technology Division, Argonne National Laboratory, Argonne, IL.

4:00 PM <u>Z5.6</u>

ELECTROCHEMICAL PROPERTIES OF COPPER OXIDE SURFACES, BURIED INTERFACES, AND SUBSURFACE ZONES AND THEIR USE TO CHARACTERIZE THESE ENTITIES. David L. Cocke, Gill Chair of Chemistry and Chemical Engineering, Lamar University, Beaumont, TX; Mohammad A. Hossain, Gill Chair Research Group, Lamar University, Beaumont, TX; Donald E. Mencer, Department of Chemistry, Wilkes University, Wilkes-Barre, PA; Hylton McWhinney, Department of Chemistry, Prairie View A&M University, Prairie View, TX; Jose R. Parga, Institute Technology of Saltillo, Department of Metallurgy and Materials Science, Saltillo Coah., MEXICO; Mohammad Y.A. Mollah, Department of Chemistry, University of Dhaka, Dhaka, BANGLADESH; Donald Naugle, Department of Physics, Texas A&M University, College Station, TX; Mehmet Kesmez, Gill Chair Research Group, Lamar University, Beaumont, TX.

4:15 PM <u>Z5.7</u>

INTERFACE CONDUCTION BETWEEN CONDUCTIVE ReO₃ THIN FILM AND NdBa₂Cu₃O₆ THIN FILM. Manabu Ohkubo, Kumiko Fukai, Matsuo Kohji, Nobuyuki Iwata and <u>Hiroshi</u> <u>Yamamoto</u>, Department of Electronics & Computer Science, College of Science & Technology, Nihon University, Chiba, JAPAN.

4:30 PM <u>Z5.8</u>

METAL-SUPPORT INTERACTIONS IN MODEL AUTOMOTIVE-EXHAUST CATALYSTS: EFFECTS OF GAS ON INTERFACIAL STRUCTURE. George Graham, Ford Research Laboratory, Chemical Engineering Department, Dearborn, MI; Haiping Sun, University of Michigan, Department of Materials Science and Engineering, Ann Arbor, MI.