

SYMPOSIUM F

Defect- and Impurity-Engineered Semiconductors and Devices III

April 1 – 5, 2002

Chairs

S. Ashok

Electronic Matls & Processing Research Lab
Pennsylvania State Univ
212 EES Building
University Park, PA 16802
814-863-4588

Jacques P. Chevallier

Lab de Phys des Solides
et de Cristallogenese
CNRS
Meudon, 92195 FRANCE
33-1-4507-5340

Noble M. Johnson

Electronic Materials Lab
PARC
Palo Alto, CA 94304
415-812-4160

Bhushan L. Sopori

National Center for Photovoltaics
Natl Renewable Energy Lab
MS 3215
Golden, CO 80401
303-384-6683

Hideyo Okushi

Dept of Matls Fundamentals
Electrotechnical Lab
Ibaraki, 305-8568 JAPAN
81-288-615226

Symposium Support

Biemtron Company, Japan
Eastman Kodak Company
†Jobin Yvon Inc.
MEMC Electronic Materials Inc.
Mitsubishi Silicon America
National Renewable Energy Laboratory
Photowatt
R-DEC Company, Japan
SAIREM
Seik Technotron Corporation
SOITEC SA
SULA Technologies
Thales Research & Technology France
Unisoku Company, Japan
†2002 Spring Exhibitor

Proceedings to be published in both book form and online
(see *ONLINE PUBLICATIONS* at www.mrs.org)
as Volume 719
of the Materials Research Society
Symposium Proceedings Series

* Invited paper

TUTORIAL

ST F: SEMICONDUCTOR DEFECT CHARACTERIZATION BY DEEP LEVEL TRANSIENT SPECTROSCOPY TECHNIQUES

Monday, April 1, 2002
9:00 a.m. - 4:00 p.m.
Salon 1/2 (Marriott)

This tutorial review will focus on deep level transient spectroscopy (DLTS), an extremely sensitive method of characterizing defects in semiconductors. While the DLTS technique has been around for nearly three decades, it has not found widespread usage in industry due to the rather sophisticated equipment and analysis required for proper interpretation of results. The aim of the tutorial is to introduce this elegant and versatile characterization method to materials and device specialists with little or marginal familiarity with the technique. As a result, the attendees will be able to make use of existing commercial DLTS equipment as well as modify them to fit specific tasks of interest. The full-day tutorial will review the basic principles and techniques, present experimental and instrumentation details, address measurement pitfalls and interpretational difficulties, and illustrate with examples from different materials systems.

The tutorial will be useful to all those who are involved in growth and characterization of semiconductor materials, and are currently using or planning to use these techniques in future. The attempt in the first half would be to impart basic principles and skills. The second half would be of a more advanced nature.

An Overview Introduction to DLTS by N.M. Johnson:

- Basic Principles
- Phenomenology of Gap States
- Parameters of Common Interest
- Voltage Controlled Space Charge Layers–Basic Device Physics & Processing
- Origin of Transients & Relaxation Spectroscopy
- Standard Measurements & Analysis–Principles and Practice
- Preparing for Transient Measurements–Importance of C-V, I-V
- How to Obtain Parameters of Interest
- Illustration with Case Studies
- Standard Variants of DLTS–Current, DDLTS, Constant Capacitance Mode & Charge DLTS
- Review of Standard Assumptions & Their Breakdown
- Basic Instrumentation & Their Principles
- Instrumentation & Analysis–Changing Emphasis
- Box Car and Lock-In-Based Instrumentation
- DLTS as Integral Transform
- Relaxation Spectroscopy as Family of Difference Spectroscopy & Higher-Order Spectroscopy
- Isothermal Transient Spectroscopy & Its Advantages
- Fourier DLTS & Laplace DLTS
- Commercial vs. Home-Built Systems, Routine Usage in Industry
- Role of DLTS in Defect Identification & Physics Understanding
- Relation to Other Defect Diagnostic Techniques
- Beyond Standard Analysis
- Important Defect Phenomena–Case Studies (EL2, DX, a-Si:H, MOS Interfaces, Thermal Donors, Radiation-Induced Defects, Etc.)
- Optical Probe-Based Transient Spectroscopy–DLOS, Photocapacitance, etc.

- Applications to Some Current Problems in Semiconductor Materials
- Use & Misuse of DLTS Family of Techniques–Care and Precautions
- Future Prospects

Instructor:

Y.N. Mohapatra, Indian Institute of Technology, Kanpur
(With an introductory overview by **N.M. Johnson, Palo Alto Research Center**)

SESSION F1: DEFECTS AND IMPURITIES IN SEMICONDUCTOR GROWTH

Chairs: Hideyo Okushi and Mario Capizzi
Tuesday Morning, April 2, 2002
Salon 1/2 (Marriott)

8:25 AM WELCOME AND INTRODUCTION

8:30 AM *F1.1

HIGH DOPED P-TYPE GaN GROWN BY ALTERNATIVE CO-DOPING TECHNIQUE. S. Iwai, H. Hirayama, Y. Aoyagi, RIKEN (The Institute of Physical and Chemical Research), Saitama, JAPAN; A. Kinoshita, Waseda Univ, Dept of Chemical Engineering, Tokyo, JAPAN.

Realization of high conductive p-type GaN and AlGaIn is important for optical and electrical devices using nitride compounds. Co-doping is proposed to get high hole concentration in p-type GaN and AlGaIn. In this co-doping method, p-type and n-type impurities are doped simultaneously. The activation energy of acceptor is expected to be reduced by the formation of complexes. In this case, the compensation due to the simultaneous doping should be avoided. If the Mg and Si are supplied at the same time in continuous feeding of TMGa and NH₃, Mg and Si atoms will be distributed randomly in the crystal and compensation is supposed to occur. We have developed alternative co-doping technique. In our technique, GaN is grown by alternative supply of TMGa and NH₃ with a sequence of 1 sec and 3 sec interval for each source gas in a low pressure MOVPE reactor. Mg doping material of Cp₂Mg is supplied during TMGa feeding and Si doping material of TESi is supplied just after the feeding of Mg source within the purging time of TMG before NH₃ feeding time. To keep the stoichiometry of GaN, a small amount of NH₃ is continuously fed into a reactor. Before the NH₃ feeding period, Mg and Si can easily migrate on the Ga surface without NH₃ and make complex to act as a shallow acceptor, predicted by theory^[1]. This migration of on the Ga surface is essential to realize co-doping effect. When Mg and Si are fed simultaneously with TMGa and NH₃, Mg and Si can not so easily and are difficult to make the complex. Hole concentration in Mg doped GaN grown by this alternative feeding technique without Si doping was around 10¹⁸/cm³. With increasing Si feeding rate by this co-doping, hole concentration was increased about 4 times. In the co-doped sample, band to acceptor luminescence shifted to higher energy side than that without Si doping. This result suggests that the acceptor level decreases by this co-doping. Temperature dependencies of hole carrier density were measured from 20 to 250°C. These results indicated that the activation energy of acceptor was reduced and high carrier density was realized.

[1] T. Yamamoto and H. Katayama-Yoshida, Jpn. J. Appl. Phys. 36, L180, (1997).

9:00 AM F1.2

CARBON DOPING IN MBE GROWTH OF WURTZITE AND ZINCBLLENDE GaN. Rob Armitage, Henning Feick, Qing Yang, Eicke R. Weber, Department of Materials Science and Engineering, University of California and Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA.

Understanding the behavior of carbon in GaN is important for several reasons. First of all, significant levels of carbon may be present as a background impurity in both MOCVD and MBE-grown GaN. Secondly, intentional carbon doping has found practical application in the growth of high structural quality semi-insulating wurtzite GaN:C. Although p-type wurtzite GaN:C has not been reported, several groups growing on GaAs substrates obtained carbon-doped zincblende GaN with exceptional p-type conductivity (5e17 holes/cm³ and hole mobility ~100 cm²/V-sec). We study carbon-doped GaN thin films grown by dc-plasma assisted MBE. Several gaseous dopant sources are investigated (carbon tetrachloride, carbon tetrabromide, chloroform, carbon disulfide) in a comparative study of incorporation efficiency, compensating impurities, and parasitic etching of GaN. Co-doping studies of carbon with Mg, O, and As are also included. Several types of substrate (MOCVD GaN templates, sapphire, GaAs, MgO) are

utilized to compare differences in the doping efficiency of wurtzite and zincblende GaN. The carbon-doped samples are characterized by Hall effect, photoluminescence, high-resolution x-ray diffraction, and atomic force microscopy.

9:15 AM F1.3

MICROSTRUCTURE AND OPTICAL PROPERTIES OF GaN FILMS GROWN ON POROUS SiC SUBSTRATE BY MBE. F. Yun, M.A. Reshchikov, L. He, T. King, D. Huang, H. Morkoç, Virginia Commonwealth Univ, Dept. of Electrical Engineering, Richmond, VA; Chae-Deok Lee, R. Feenstra, Carnegie Mellon Univ, Pittsburgh, PA; C.K. Inoki, T.S. Kuan, Univ at Albany, SUNY, Dept of Physics, Albany, NY.

Recent commercially available 6H-SiC substrates have greatly promoted the research interest of GaN growth on this surface. The advantage of SiC over sapphire lies in the fact that the lattice mismatch between SiC and AlN is almost nil, and that between SiC and GaN is much smaller compared to sapphire. The high thermal conductivity of the SiC substrate allows the fabrication of high power/temperature electronics devices. Currently, the high density of threading dislocations in GaN films represents a great obstacle for the improvement of devices. There have been reports of SiC growth on P-SiC substrates, and GaN grown on porous GaN layer on top of SiC substrates. All of them showed improvements in defect reduction and stress alleviation. With the formation of nanometer-scale pores, it is expected that the MBE growth of GaN near the P-SiC surface will be in a growth mode similar to the lateral epitaxial overgrowth as in LEO MOCVD, and the threading dislocations will be annihilated at early stages of growth. P-SiC was prepared by anodization of 6H-SiC (0001) substrates. In this paper, we report growth of GaN films by MBE on P-SiC substrates using ammonia as the N source. The GaN films were grown, under Ga-rich conditions, without insertion of any buffer layer, to a thickness of 0.1-3.5 μm . GaN films were also grown on standard 6H-SiC substrate for comparison. High-resolution X-ray diffraction, atomic force microscopy (AFM), transmission electron microscopy (TEM) techniques were used to study the microstructure and morphology difference of GaN grown on P-SiC and 6H-SiC. A smooth surface of GaN with roughness (rms) of 0.71 nm was obtained with growth on P-SiC substrate. X-ray rocking curve FWHMs of 3.3 arcmin for (002) and 17.7 arcmin for (102) diffractions were recorded for the sub-micron GaN film grown on P-SiC. Optical properties studied by photoluminescence at 15 K demonstrated an exciton peak FWHM of 14 meV, with high quantum efficiency and relatively low yellow luminescence. Growth mechanisms of GaN on top of the nano-porous SiC surface were suggested from TEM and AFM analysis.

9:30 AM F1.4

INFLUENCE OF Be DOPING ON MATERIAL PROPERTIES OF LOW-TEMPERATURE-GROWN GaAs. S. Marcinkevicius, A. Gaarder, J. Siegert, Royal Inst of Technology, Dept of Microelectronics and Information Technology, Kista, SWEDEN; J.-F. Roux, J.-L. Coutaz, Univ Savoie, LAHC, Le Bourget du Lac, FRANCE; A. Wolos, M. Kaminska, Warsaw Univ, Inst of Experimental Physics, Warsaw, POLAND; R. Adomavicius, K. Bertulis, A. Krotkus, Semiconductor Physics Inst, Vilnius, LITHUANIA.

Outstanding properties of low-temperature-grown (LTG) GaAs (sub-picosecond carrier lifetimes, high carrier mobility, enhanced resistivity and breakdown fields) make this material unique for ultrafast optoelectronic and optical applications. Material properties of LTG GaAs, linked to the presence of excess arsenic (As-antisite defect), can further be improved by doping LTG GaAs with Be, which increases the ratio between active and neutral antisite defects. In this contribution we report a multisided experimental investigation performed on Be-doped LTG GaAs layers with different Be concentrations (2.5×10^{17} to $2 \times 10^{19} \text{ cm}^{-3}$) annealed at different temperatures between 500 and 900°C. Enhanced crystalline quality of Be-doped LTG GaAs, as compared to undoped layers, was observed by transmission electron microscopy. Deep donor densities were determined from near infrared absorption spectroscopy. Comprehensive information about electron and hole dynamics was obtained by performing time-resolved photoluminescence, reflectance, transmittance, and photoconduction experiments with femtosecond or picosecond resolution. These time-resolved data sets have been analyzed using a rate equation model, which includes most of the relevant phenomena of carrier dynamics in a semiconductor. Electron trapping times, which determine the response time of a device, were found to vary from a hundred femtoseconds to a few picoseconds. Hole trapping times, establishing the device repetition frequency, have been determined for samples with Be concentrations up to $1.6 \times 10^{18} \text{ cm}^{-3}$ and are about 5 ps. A non-monotonous behavior of the carrier lifetime versus Be-doping level, reported previously, is explained considering the interplay between As antisite defects, Ga vacancies and Be dopants in LTG GaAs. It is found that the optimal properties of Be-doped LTG GaAs are obtained for moderate Be concentrations.

SESSION F2: DOPING ISSUES I
Chairs: Hideyo Okushi and Mario Capizzi
Tuesday Morning, April 2, 2002
Salon 1/2 (Marriott)

10:15 AM *F2.1

TRANSFER DOPING MECHANISM FROM AN AQUEOUS SURFACE LAYER AND THE SURFACE CONDUCTIVITY OF DIAMOND. Lothar Ley, J. Ristein, M. Riedel, F. Maier, M. Stammler, B. Mantel, Institute of Technical Physics, University of Erlangen, Erlangen, GERMANY.

Undoped diamond with a gap of 5.5 eV is a bona fide insulator that nevertheless exhibits a rather substantial p-type surface conductivity (SC). All experimental facts point towards a hole accumulation layer at the diamond surface as the origin for the SC with a Fermi level position that coincides with the VBM. From conductivity measurements performed in ultra high vacuum and atmosphere both on hydrogenated and hydrogen-free surfaces we come to the conclusion that hydrogenation is a necessary but not a sufficient requirement for SC to occur in diamond. Rather, additional species from the atmosphere appear to provide the acceptor that is necessary to form the accumulation layer. We shall give detailed and quantitative evidence that a redox reaction in the mildly acidic aqueous surface layer that always forms on surfaces exposed to air provides the electron sink for the hole accumulation layer. The model accounts for all experimental facts including the fact that only hydrogenated diamond exhibits this kind of SC among all semiconductors.

10:45 AM *F2.2

POSSIBLE SHALLOWING OF NITROGEN DONORS IN DIAMOND. Takehide Miyazaki, AIST, Advanced Semiconductor Research Center, Tsukuba, JAPAN; Tsuyoshi Uda, Joint Research Center for Atom Technology, Tsukuba, JAPAN.

Diamond is a wide band gap semiconductor which has in principle the best electrical properties[1]. For example, an application of its large band gap (5.5 eV) to light sources should be of great potential impact to opto-electronics. A recent status in this direction is that it has been possible to fabricate a prototype of a light-emitting diode based on a p-n junction between p-type [boron (B) doped] and n-type [phosphorus (P) doped] diamond layers[2]. A serious problem in doping of diamond has been left unresolved. It is difficult to dope diamond n-type. P is not the best donor in diamond, because of the low electron mobility of P-doped diamonds (200 $\text{cm}^2/\text{V}\cdot\text{sec}$) relative to the hole mobility (2000 $\text{cm}^2/\text{V}\cdot\text{sec}$) in B-doped counterparts. A cause of this low mobility in the former is understood to be due to formation of P-V (V: vacancy) complexes, which compensate any donors[3]. Nitrogen (N) is an impurity omnipresent in diamond. Although N is a penta-valent element similarly to P, it has been believed that N is a deep donor in diamond[4]. In this study, we challenge this traditional understanding from a theoretical point of view. We show that a complex of a nearest-neighbor pair of two N atoms with a hydrogen (H) atom, the N-H-N defect, might exhibit much shallower donor character than that of isolated N-defect in diamond. We also calculate formation energy of this defect to discuss the conditions in which one might expect preferential generation of N-H-N defects in diamond. [1] L.M. Porter and R.F. Davis, *Mater. Sci. and Eng.* B34, 83 (1995), Table 2. [2] S. Koizumi *et al.*, *Science* 292, 1899 (2001). [3] R. Jones *et al.*, *Appl. Phys. Lett.* 69, 2489 (1996). [4] B.B. Li *et al.*, *Appl. Phys. Lett.* 73, 812 (1998).

11:15 AM F2.3

HYDROGEN-INDUCED P-TYPE CONDUCTIVITY IN DIAMOND: HALL EFFECT AND DEVICE STUDIES. Richard B. Jackman, Oliver A. Williams, Electronic Engineering, University College London, UNITED KINGDOM; Christoph Nebel, Walter Schottky Institut, Technische Universität München, München, Garching, GERMANY.

The realization that surface/near-surface hydrogen within CVD grown diamond films, leads to p-type conduction with little apparent thermal activation, has been one of the most exciting recent developments in the field of diamond electronics. High performance logic circuits that operate at MHz frequencies have been fabricated using this approach. Despite this, the origin of this effect has remained controversial, with differing adsorbates being implicated in surface hole accumulation layers as well as shallow acceptor states being cited. In this paper, ultra-low temperature Hall effect measurements (as low as 0.3K) will be shown, along with a wide range of I-V and C-V measurements, to enable a complete model of the p-type conductivity process to be offered. Device characteristics will be presented which support the model, and the novel use of passivation layers, to isolate adsorbate produced effects, discussed. It will be demonstrated that passivation layers can be used to produce devices which display stability within a range of different atmospheric and thermal conditions, where carrier mobility values of

>400cm²/vs with sheet carrier densities of around 10(13)cm² can be achieved. Interestingly, polycrystalline CVD diamond can be used to achieve remarkably similar results to single crystal material.

11:30 AM F2.4

MULTIPLE DONORS IN ZnO SUBSTRATES. K. Thonke, N. Kerwien, Abt. Halbleiterphysik, Universität Ulm, Ulm, GERMANY; A. Wysmolek, M. Potemski, Grenoble High Magnetic Field Laboratory, Grenoble, FRANCE; A. Waag, R. Sauer, Abt. Halbleiterphysik, Universität Ulm, Ulm, GERMANY.

We investigate by photoluminescence (PL) nominally undoped, commercially available ZnO substrates (from Eagle Picher) grown by seeded chemical vapor transport technique in order to identify residual donors and acceptors. In low temperature PL spectra the dominant emission comes from the decay of bound exciton lines at around 3.36 eV. Zeeman measurements allow the identification of the two strongest lines and some weaker lines in-between as donor-related. From the associated two-electron satellite lines binding energies of the major donors of 40 meV and 60 meV, respectively, can be deduced, consistent with results from Hall effect measurements. Compensating acceptors lead to a donor-acceptor pair transition at 3.22 eV, which turns into a band-acceptor transition for temperatures above 40 K. The acceptor, which likely is nitrogen-related, has a hole binding energy of $E_A = (200 \pm 10)$ meV.

11:45 AM F2.5

NANO-SIZED TE-RICH ISLANDS AS THE BASIS FOR ADVANCE IN P-DOPING OF ZnSe FILMS. J.W. Lau, V.V. Volkov, Y. Zhu, Brookhaven National Laboratory, Upton, NY; I.L. Kuskovsky, Y. Gu, G.F. Neumark, Dept of Applied Physics and Applied Mathematics, Columbia University, New York, NY; W. Lin, O. Maksimov, M.C. Tamargo, Chemistry Department of City College and Graduate Center of CUNY, New York, NY.

ZnSe (E_g of 2.71 eV at room temperature) showed much promise for fabrication of light emitting devices in the blue-green spectral region. However, traditional p-doping with nitrogen has left much to be desired in terms of adequate carrier concentration. As a result, good light emitting devices have been a challenge to achieve with ZnSe. Using the novel d-doping method with small amounts of Te in addition to N, the carrier concentration was observed to improve by about an order of magnitude. Sub-monolayer thick Te layers are co-incorporated along with N into the ZnSe matrix during molecular beam epitaxial growth. Typical Te average concentrations are below 1%. We hypothesize that nitrogen incorporates within localized Te-rich regions. Circumstantial evidences, such as photoluminescence, support our hypothesis of such segregation. X-ray rocking curve data suggests the formation of a second phase within the matrix material. In addition, further evidence is provided with advanced transmission electron microscopy. Dark field images taken with chemically sensitive reflection {200} reveals contrasts that are indicative of Te segregation. Cluster sizes average 5 nm in diameter. Average cluster densities are approximately 8×10^{11} cm² for a Te doped sample, compared with 1×10^{11} cm² for an undoped sample. Te introduced almost an order of magnitude more defects.

SESSION F3: DOPING ISSUES II

Chairs: Mario Capizzi and Bhushan L. Sopori
Tuesday Afternoon, April 2, 2002
Salon 1/2 (Marriott)

1:30 PM F3.1

FABRICATION OF p-TYPE ZnS WITH BLUE-Ag EMISSION BY TRIPLE-CODOPING METHOD. Seiichi Kishimoto, Kochi National College of Technology, Kochi, JAPAN; Seishi Iida, Nagaoka University of Technology, Niigata, JAPAN; Tetsuya Yamamoto, Kochi University of Technology, Kochi, JAPAN; Shigemi Kohiki, Kyusyu Institute of Technology, Fukuoka, JAPAN.

We have succeeded the fabrication of low-resistivity p-type ZnS with blue-Ag emission by triple-codoping using Ag, a Zn-substituting species, In, a Zn-substituting species, and N, a S-substituting species. For the realization of blue-Ag emission, we use In species as co-activators with Ag activators. For the control of conduction type to obtain p-type ZnS thin films, we introduce N species as acceptors into ZnS codoped with Ag and In (ZnS:(Ag, In)). Vapor-phase epitaxial ZnS:(N, Ag, and In) layers were grown on semi-insulating GaAs(100) substrates under hydrogen carrier gas flow using a luminescence-grade unactivated ZnS powder source. Hall-effect measurements at room temperature revealed free hole concentration and mobility values to be $(0.6-1.4) \times 10^{19}$ /cm³ and 10-25 cm² /Vs for ZnS:(N, Ag, and In). For the above films, we find that an emission at 436 nm was dominant from photoluminescence spectra [1]. Based on ab-initio electronic-band-structure calculations, we proposed a model for ZnS:(Ag, In,

and N), in which some of the In species act as coactivators with Ag activators and other In species act as reactive codopants with N acceptors: The main role of In is to delocalize the N-impurity state by improving the incorporation of N species into ZnS. In addition, for ZnS:(In, N), we established that the densities of states calculated by the theoretical calculations are in good agreement with the experimental data obtained by X-ray photo-electron spectroscopy. [1] S. Kishimoto, T. Hasegawa, H. Kinto, O. Matsumoto and S. Iida; The 9th International Conference on II-VI Compounds, November 1-5, Kyoto, Japan, 1999.

1:45 PM F3.2

DOPING OF CuInSe₂ AND CuGaSe₂ BY HYDROGEN. Çetin Kılıç and Alex Zunger, National Renewable Energy Laboratory, Golden, CO.

Chalcopyrite semiconductors CuInSe₂ (band gap = 1.0 eV) and CuGaSe₂ (band gap = 1.7 eV) and their alloys are used as absorber layers in high efficiency polycrystalline thin films solar cells. Whereas CuInSe₂ and its <30% alloy with CuGaSe₂ can be easily doped, once more than 30% CuGaSe₂ is added to CuInSe₂ the doping becomes problematic, and the solar cell efficiency deteriorates. We find that H can convert these materials to n-type due to two possible mechanisms: (a) Our first-principles calculations show that interstitial hydrogen in both CuInSe₂ and CuGaSe₂ acts as a donor, yielding an explanation also for conductivity type conversion. (b) Another explanation for n-type behavior is the passivation of copper vacancies by hydrogen. We will show formation energies and lattice structures for H⁺, H⁰, and H⁻ in CuInSe₂ and CuGaSe₂. We find that H⁺ goes into the Cu-Se bond while H⁰ and H⁻ remain interstitial. Doping chalcopyrites by hydrogen could be a new way to overcome bottleneck.

2:00 PM *F3.3

THEORETICAL INVESTIGATION OF NITROGEN-DOPING EFFECT ON NATIVE DEFECT AGGREGATION PROCESSES IN SILICON. Hiroyuki Kageshima, Akihito Taguchi, NTT Basic Research Labs, NTT Corporation, Atsugi, Kanagawa, JAPAN; Kazumi Wada, Massachusetts Institute of Technology, Cambridge, MA.

Nitrogen-doping in Si have received keen attention because it significantly reduces the concentrations of both void defects and dislocation loops. These experimental observations clearly show that nitrogen effectively suppresses aggregation of both vacancies and Si interstitials during the Si bulk crystal growth. In order to shed light on the nitrogen-doping effect, we investigated interactions between nitrogen atoms and these Si native defects by using first-principles calculations with an ultrasoft potential of N. Comparing total energies of various complexes of nitrogen atoms and Si vacancies, we found a very stable complex composed of two nitrogen atoms and two vacancies (N₂V₂). This complex is very stable because all bonds of the N₂V₂ complex are strong N-Si bonds and there are no dangling bonds. The formation of this complex reduces the concentration of isolated vacancies, resulting in the vacancy aggregation. Additional vacancy association with N₂V₂ needs the reconfiguration of the bonds among the complex, which increases the energy barrier against aggregating in a subsequent chain reaction. These delays evolution of voids. Stable complexes of Si interstitial with nitrogen should be formed, assuming that the dislocation loop suppression by nitrogen would occur in a way similar to the void suppression. The complex should be free of dangling bonds. We will report the energetics of stable configurations of the N-I complexes, based on first-principle calculations.

SESSION F4: GETTERING

Chairs: Bhushan L. Sopori and Fritz G. Kirscht
Tuesday Afternoon, April 2, 2002
Salon 1/2 (Marriott)

3:00 PM *F4.1

RECENT PROGRESSES OF GETTERING IN SILICON. T.Y. Tan, Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC.

For IC fabrications using CZ Si, intrinsic gettering utilizing oxygen precipitates has been extensively studied in the past, with the main efforts concentrated on the engineering and scientific aspects of the creation of gettering sites. The present review, however, will focus on recent progresses on processes and mechanisms of the gettering of metallic impurities from the device active regions to the created gettering regions. The electrical activity and gettering of the metallic impurities in precipitated form will be emphasized.

3:30 PM F4.2

GETTERING BY OVERPRESSURIZED BUBBLES INDUCED BY HIGH-ENERGY-He-IMPLANTATION IN SILICON. Gabrielle Regula, Rachid El Bouayadi, Bernard Pichaud, TECSEN, Marseille,

FRANCE; Sylvie Godey, Romain Delamare, Esidor Ntsoenzok, CERI-CNRS, Orleans, FRANCE; Anton Van Veen, IRI, Delft, THE NETHERLANDS.

Silicon samples were implanted with helium ions at 1.6 MeV with different fluxes (0.4 to 2.0 $\mu\text{A}/\text{cm}^2$) and at the dose of $2 \times 10^{16} \text{ cm}^{-2}$, giving birth to a diluted system of bubbles. During implantation, the temperature could raise up to 373 K for the highest flux used. After implantation, a 1073K annealing for half an hour was performed under neutral atmosphere. For all fluxes used, an unexpected dislocation network surrounding cavities was observed by cross section transmission electron microscopy. Neutron depth profiling measurements showed that there is still a large amount of helium inside these cavities, creating an overpressurized system of bubbles. In order to test the gettering efficiency of these bubbles, gold was sputtered and diffused at high temperatures (1188-1323 K) for few hours (2-4h) before helium implantation. Secondary ion mass spectroscopy measurements showed that helium pressure inside the bubbles does not prevent the cavities to trap gold atoms at their walls. Since gold gettering is limited inside the cavity band, dislocations emitted far from this band are supposed to be hardly involved in the gettering process of gold atoms.

3:45 PM F4.3

DEFECTS INDUCED BY HELIUM IMPLANTATION: INTERACTION WITH BORON AND PHOSPHORUS. F. Cayrel, D.

Alquier, L.M.P., Tours Univ, FRANCE; F. Roqueta, STMicroelectronics, FRANCE; L. Ventura, L.M.P., Tours Univ, FRANCE; C. Dubois, L.P.M. - INSA Lyon, FRANCE; D. Mathiot, PHASE, Strasbourg, FRANCE.

High thermal treatments, applied during power device manufacturing, lead to metal contamination that, even at low concentration, limits device reliability. High dose helium implantation, followed by a suitable thermal anneal induces defects (cavities and dislocations) which are known to trap metal impurities [1-2]. Moreover, papers have enlightened the interaction between these defects and the dopant that drastically influence the structure as well as the electrical characteristics of the devices [3-4]. Understanding this interaction between dopants and He induced defects become then a key point for future devices that will request this gettering technique. In this work, P and N type, $\langle 111 \rangle$, silicon wafers, uniformly doped with B and P (1×10^{18} and $3 \times 10^{18} \text{ at.cm}^{-3}$ respectively), were used. Helium implantation at room temperature (40 keV, $5 \times 10^{16} \text{ He}^+/\text{cm}^2$) followed by furnace annealing for various times from 15 min to 8 h and temperatures up to 1000°C was used to form the defects band. Secondary Ion Mass Spectrometry (SIMS) and Spreading Resistance Profilometry (SRP) were performed to follow respectively the chemical and the electrical profiles of the dopants. The evolution of the defect band was followed using Spectroscopic Ellipsometry (SE). First, we evidence a large segregation of both dopants in the vicinity of the buried layer. In each case, the fraction of gettered dopant was evaluated from the SIMS profiles. Our results exhibit similar behavior for both dopants. Using isochronal treatment, we found a large dependence of the dopant gettering phenomenon upon annealing temperature. Moreover, stability of the gettered fraction can be observed for isothermal annealing. This study has been completed by SRP measurements that allow us to follow the dopant reactivation upon the annealing. These results allow us to better understand the dopant gettering phenomenon, which is of great interest for present and future device fabrication. **References** [1] S.M. Myers and D.M. Follstaedt, J. Appl. Phys 79 (1996), p. 1337. [2] V. Raineri, P.G. Fallica, G. Percolla, A. Battaglia, M. Barbagallo and S.U. Campisano, J. Appl. Phys. 78, (1995), p. 3727. [3] F. Roqueta, D. Alquier, L. Ventura, C. Dubois, R. Jerisian, Nucl. Instr. and Meth. B 183 (2001) pp. 318-322. [4] F. Roqueta, D. Alquier, L. Ventura and B. Lopez, Solid State Phenom. Vols. 82-84 (2002) pp. 279-284.

SESSION F5: DEFECTS IN DEVICES

Chairs: S. Ashok and Reinhart Job
Wednesday Morning, April 3, 2002
Salon 1/2 (Marriott)

8:00 AM *F5.1

EFFICIENT SILICON LIGHT EMITTING DIODES MADE BY DISLOCATION ENGINEERING. K.P. Homewood, M.A. Lourenco, Wai Lek Ng, R.M. Gwilliam, School of Electronics, Computing & Mathematics, G. Shao, S. Ledain, School of Engineering, University of Surrey, Guildford, Surrey, UNITED KINGDOM.

The need for at least partial use of optical data processing on chip is seen as an essential requirement for continuing exponentially increasing processor speed (Moore's Law) beyond the next five to ten years. This is needed to overcome the fundamental interconnect

problem resulting from the non scaling of the transport time of electrons in conventional metal interconnects. The optimum approach is the development of an efficient silicon light emitter that can operate at room temperature. Conventional wisdom has suggested that this is impossible given the indirect nature of the band gap in silicon and the strong thermal quenching of the radiative transitions. This paper describes how efficient room temperature silicon light emitting diodes can be realised and by using entirely conventional ULSI technology. The use here of conventional technology is, given the high tool up costs of the silicon microelectronics industry, considered to be paramount for the introduction of commercially viable optical processing on chip.

8:30 AM F5.2

DEFECT ENGINEERING IN CCD IMAGE SENSORS.

William C. McColgin, Lingadahalli G. Shantharama, and James P.

Lavine, Eastman Kodak Company, Image Sensor Solutions, Rochester, NY.

CCD image sensors provide an excellent example of both high sensitivity of a product to defects and the use of defect engineering to manipulate and control defects. Defect engineering for imagers starts with the epi silicon layer chosen for the uniformity of its electrical properties. The underlying substrate can then be tailored to optimize gettering of heavy-metal contaminants present in the incoming, purchased wafers and added during device fabrication. Such contaminants add noise to imagers that limits their performance. Typically, one or more gettering techniques are employed, since, for some contaminants, the noise contribution of even individual atoms can be measured. Another source of noise in imagers is dangling bond defects at the silicon/gate-dielectric interface. This can be reduced 10x by hydrogen passivation; however, the residual dark current added to an imager pixel from its surface is still orders of magnitude larger than the dark current contribution from ungettered contaminants in the epi layer - unless surface generation is turned off electrically. We will describe the use and effect of these defect engineering techniques for the specific case of a full-frame CCD imager built in p-epi silicon on a p+ substrate.

We have investigated for imager fabrication the effects of different cooling cycles on iron contamination in an attempt to compare gettering from oxygen precipitates with the boron segregation gettering that may also be occurring. In these experiments, we measured iron levels as low as $5\text{E}+7 \text{ cm}^{-3}$ for an estimated gettering efficiency of 99.95%. The final iron concentration was not as low as expected from solubility arguments. We conjecture that at low temperatures, boron segregation gettering and oxygen precipitate gettering no longer work additively and that other sites within the imager portion of the wafer compete with the intended gettering.

8:45 AM F5.3

TRAPPING AND DETRAPPING OF H IN Si: IMPACT ON DIFFUSION PROPERTIES AND SOLAR CELL PROCESSING.

Bhushan Sopor, Yi Zhang, Robert Reedy, Kim Jones, National Renewable Energy Laboratory, Golden, CO; N.M. Ravindra, New Jersey Institute of Technology, Dept of Physics, Newark, NJ; S. Rangan, and S. Ashok, Pennsylvania State University, Department of Engineering Science and Mechanics, University Park, PA.

Hydrogenation is used as a standard process step in fabricating all commercial Si solar cells to passivate impurities and defects. One of the important issues in this process is the need to diffuse H deep into the bulk under reasonable process conditions. Optimum hydrogenation conditions commonly vary for Si produced by different vendors, and the diffusion times and temperatures required are considerably higher than dictated by diffusivity in Si. Generally, these effects are attributed to trapping of H by impurities and defects. We used experimental and theoretical analyses to study the influence of trapping and detrapping of H in Si. We developed a trapping-detrapping model for H diffusion and used it to fit H (or D) profiles in different Si substrates. These results yield best-fit parameters that identify the trapping and detrapping properties. H was introduced in Si substrates of different resistivity, dopant type, impurity concentration, and defect density by low-energy implantation, ECR, and plasma processes. Diffusion profiles were measured by SIMS. In some cases, we annealed samples to study the changes in the diffusion profile and to compare them with our theoretical model. We also studied hydrogenation by PECVD nitridation, which is a very common process in the photovoltaic industry. In this paper, we show that a model invoking bulk and process-induced traps can predict the experimental diffusion profiles. Furthermore, the model can predict the optimum process conditions for passivation of Si solar cells fabricated on different substrates and for different hydrogenation techniques.

9:00 AM F5.4

RADIATION HARDNESS OF AlGaIn/GaN BASED HEMTs.

S.A. Vitusevich, N. Klein, S.V. Danylyuk, Forschungszentrum Jülich,

ISG, Jülich, GERMANY; A.E. Belyaev, R.V. Konakova, A.M. Kurakin, A.E. Rengevich, A.Yu. Avksentiev, Institute of Semiconductor Physics, NASU, Kiev, UKRAINE; B.A. Danilchenko, Institute of Physics, NASU, Kiev, UKRAINE; V. Tilak, J. Smart, A. Vertiatchikh and L.F. Eastman, School of Electrical Engineering, Cornell University, Ithaca, NY.

Wide band-gap heterojunctions based on AlGaIn/GaN structures appear to be very promising for high power and radiation resistant microwave devices including High Electron Mobility Transistors (HEMTs). To realise an excellent potential of Group III-Nitride compound semiconductors for high temperature, high frequency, and high power microwave applications there is a need for physical models describing the device performance and reliability. One of the main issues to be considered is the influence of defects arising under various treatments (in particular, irradiation) on current transport. In this work we present and discuss measurements of steady-state characteristics of AlGaIn/GaN based HEMTs exposed to gamma ray radiation. High performance AlGaIn/GaN HEMT devices have been fabricated using material grown by OMVPE on sapphire substrates. The Hall effect 2DEG sheet charge density and mobility were $1.05 \times 10^{13} \text{ cm}^{-2}$ and $1250 \text{ cm}^2/\text{Vs}$, respectively. The devices with a variety gate length (150-350 nm) and width (100-400 μm) were irradiated by ^{60}Co gamma rays with doses in the range of 10^4 - 10^9 Rad and flux of 10^2 Rad/s at room temperature. Dose dependencies of the basic transistor's operating parameters such as saturation current, I_{sat} , transconductance, g_m , channel conductance, g_c , and threshold voltage, V_T , are analysed. Our study show that visible changes of above mentioned parameters are observed under relatively small doses (10^6 Rad) and strongly depend on the HEMT's topology. The transconductance decreases and threshold voltage increases for all devices while deviation of these parameters from its initial values does not exceed 20% at highest irradiation dose. At the same time variation of the channel conductance as well as saturation current depends to a high extent on the gate voltage, V_g . At $V_g < V_{cr}$, both I_{sat} and g_c show a reversal proportion to the cumulative dosage of radiation. However, at $V_g > V_{cr}$, drain saturation current and channel conductance increase with the cumulative dosage of radiation. The effect is more pronounced in short-length-gate devices. A model describing the role of radiation-induced defects in current transport is presented. This work is supported by the Office of Naval Research under Grant No. N00014-01-1-0828 (Project Monitor Dr. Colin Wood). A.E.B. acknowledges Deutsche Forschungsgemeinschaft for research grant.

9:15 AM F5.5

LOW-TEMPERATURE OPERATION OF DIAMOND SURFACE-CHANNEL FIELD-EFFECT TRANSISTORS. Minoru Tachiki, Hiroaki Ishizaka, Tokishige Banno, Toshikatsu Sakai, Kwang-Soup Song, Hitoshi Umezawa, Hiroshi Kawarada, School of Science & Engineering, Waseda University, Tokyo, JAPAN, CREST, Japan Science and Technology Corporation (JST), JAPAN.

Hydrogen termination of diamond can stabilize the surface structure and also can reduce surface state density. This pinning-free surface is quite favorable when the diamond surface is used for the metal-semiconductor (MES) or metal-insulator-semiconductor (MIS) applications. Furthermore, hydrogen-terminated diamond is attractive for electrical applications because it induces p-type surface conduction even if the diamond is not intentionally doped. Up to now, the fabrication and the operation of field-effect transistors (FETs), single electron transistors (SETs) and ion sensitive FETs (ISFETs) have been demonstrated using a surface conductive layer. To investigate the carrier behavior of the surface conductive layer at low temperature, and to elucidate the formation mechanism of the surface conductive layer, we demonstrated the low-temperature ($\sim 4.5\text{K}$) operation of the diamond FETs for the first time. In this study, we exploit CaF₂ and other insulator materials films to for the MIS structure. In the MISFET characteristics with CaF₂ as a gate insulator, field-effect channel conduction is enhanced at low temperature. Experimental results indicate the surface hole never freeze even at 4.5K, and is well controlled by the field effect. By using the surface conductive layer at low temperature, it is possible to realize the diamond cryoelectronics including superconducting devices, single electron devices, ambipolar devices and so on.

SESSION F6: DEFECT CHARACTERIZATION

Chairs: Takashi Sekiguchi and Gabrielle Regula
Wednesday Morning, April 3, 2002
Salon 1/2 (Marriott)

10:00 AM *F6.1

PHOTOLUMINESCENCE MICROSCOPY OF TEM IRRADIATED DIAMOND SiC AND CUBIC BN. J.W. Steeds, G.A. Evans, E. Shishonok, Department of Physics, University of Bristol, Bristol, UNITED KINGDOM.

Use of a TEM to irradiate wide band-gap semiconductors prior to investigation by low temperature photoluminescence spectroscopy has a number of important advantages. One of these is accurate control of the accelerating voltage so that behaviour near the displacement threshold can be studied as well. This is particularly important for a material such as SiC where, because the atoms have very different masses, Si displacements can be clearly distinguished from C displacements. Another advantage is the ability to carry out local irradiations in well defined areas. Not only does this permit the study of area to area variations but species migrating out of the irradiated area during irradiation may also be identified. Such species are generally interstitial atoms so that a distinction can be made between these and vacancy-related centres that are only observed within the irradiated region itself. Use of isotope-enhanced samples gives rise to splitting of local modes of interstitial-related centres. This technique has been used to study centres in both SiC and diamond and it has recently been used to identify the optical signature of isolated C-C split interstitial dumb-bells in SiC.

10:30 AM F6.2

STM NANOSPECTROSCOPIC STUDY OF DEFECTS IN SEMICONDUCTORS. Koji Maeda, Akira Hida and Yutaka Mera, Dept of Applied Physics, School of Eng., Univ of Tokyo, Bunkyo-ku, Tokyo, JAPAN.

Coupling of scanning tunneling microscopy (STM) with various schemes of optical spectroscopy was found to provide powerful tools for investigation of crystalline defects in bulk semiconducting solids. The simplest instrumentation [1,2] in which the sample is illuminated with a light of variable wavelength allows one to measure the photoabsorption spectrum of even a single defect embedded in the crystal with a spatial resolution as high as nano-meter in scale. The method was applied to a subsurface defect in a bulk GaAs crystal in which the signal was acquired by detecting the change in the tunneling current reflecting a local surface swelling that occurs when the wavelength of the chopped light used for spectroscopic measurements coincides with a photoabsorption spectral peak of the defect. Another scheme using a continuous light of variable wavelength was applied to midgap centers, supposed to be arsenic antisite defects, densely populated in low-temperature-grown GaAs epilayers. Experiments at 90K [3] revealed that light illumination causes reversible transformation of the individual defects to a metastable state with an excitation spectrum very close to one observed for the photo-quenching effect of EL2 centers in bulk GaAs. The local strain field around individual centers could also be imaged with a nano-meter resolution [4] by STM coupled with electric field modulation spectroscopy [5] that enables us to measure accurate spectra of interband optical transitions in the local spot beneath the tip.

[1] A. Hida, Y. Mera, and K. Maeda; Appl. Phys. Lett., 78(21) (2001) 3190-3192.

[2] A. Hida, Y. Mera, and K. Maeda; Solid State Phenomena 78-79 (2001) 419-424.

[3] A. Hida, Y. Mera and K. Maeda; Physica B, in press.

[4] A. Hida, Y. Mera and K. Maeda; Physica B in press.

[5] A. Hida, Y. Mera, and K. Maeda; Appl. Phys. Lett., 78(20) (2001) 3029-3031.

10:45 AM F6.3

NITROGEN-STABILIZED H₂⁺ DEFECTS IN DILUTE GaP:N. A. Janotti, S.B. Zhang, and Su-Huai Wei, National Renewable Energy Laboratory, Golden, CO.

III-V dilute alloy have attracted a lot of attentions recently. The large optical band gap bowing opens up enormous potential for long-wavelength lasing and photovoltaic applications. Because the growth of these materials, by metalorganic chemical vapor deposition (MOCVD) or molecular beam epitaxy (MBE), usually involves H-related precursors, it is essential to understand the formation of H-related defects. In this work we show the important role of nitrogen in stabilizing the H₂⁺ defect complexes in GaP. The H₂⁺ is known to exist in Si with very important applications, but so far, it has never been observed in any conventional III-V semiconductors. The calculated the local vibration modes for H₂⁺ are in very good agreement with the experimentally observed infrared spectrum.

11:00 AM F6.4

CHARACTERIZATION OF DEEP LEVELS IN 3C-SiC BY OPTICAL CAPACITANCE-TRANSIENT SPECTROSCOPY. Yohei Nakamura, Masashi Kato, Masaya Ichimura, Eisuke Arai, Nagoya Inst of Technology, Dept of Electrical and Computer Engineering, Nagoya, JAPAN; Yutaka Tokuda, Aichi Inst of Technology, Dept of Electronics, Aichi, JAPAN.

Since 3C-SiC is grown heteroepitaxially on Si substrates, large area wafers can be produced at low cost. However, at the 3C-SiC/Si

interface, defects are generated due to difference in thermal expansion coefficient and lattice constant. The defects would be extended to epitaxial films, and thus the investigation for the defects in epitaxial films is important. We employed optical capacitance-transient spectroscopy (O-CTS) method to characterize the defects in 3C-SiC on Si. The O-CTS measurement enables us to estimate photo ionization energy and optical cross sections for defects. The sample used in this study was an n-type 3C-SiC film grown on a p-type Si (100) substrate. Schottky barrier diodes were fabricated by evaporating Al and Au as ohmic and Schottky contacts, respectively. In the O-CTS measurement, we observed capacitance transient caused by changing reverse bias under a monochromatic light with a constant photon flux. The energy range of the incident monochromatic light was of 0.5-2.0 eV. The measurement temperature was set at 85 K. In the O-CTS spectrum with 0.5 eV light, a peak is observed at time constant of 1 ms. Considering its peak height, this peak is thought to be due to the ND1 center, which was also observed by deep level transient spectroscopy (DLTS) and found to have a thermal activation energy of 0.3 eV. The optical cross section for the center increases with increasing photon energy up to 0.6 eV and then decreases with increasing photon energy. The apparent photo ionization threshold energy is about 0.45 eV, which is about 0.15 eV larger than the thermal activation energy. This difference is supposed to be the Frank-Condon shift.

11:15 AM F6.5

APPLICATION OF ROOM-TEMPERATURE PHOTO-LUMINESCENCE FOR CHARACTERIZING AS-GROWN AND THERMALLY PROCESSED CZ SILICON. F. Kirscht, B. Orschel, S. Kim, S. Rouvimov, B. Snegirev, M. Fletcher, Mitsubishi Silicon America, Salem, OR; M. Shabani, Mitsubishi Materials Silicon Corporation, Noda-shi, Chiba-Ken, JAPAN; A. Buczkowski, Mitsubishi Silicon America, Salem, OR.

A room-temperature photoluminescence (PL) mapping technique recently developed by BioRad has been exploited for characterizing a variety of features in CZ silicon. Here we present PL studies of oxygen precipitation related defects (OPD), stress relaxation related dislocations (SRD), and doping striations in various heavily doped silicon materials. The sample spectrum includes a variety of dopant species, and the dopant concentration range covers several 10^{14} cm^{-3} to several 10^{19} cm^{-3} . PL intensity in this doping concentration range is controlled by three basic recombination mechanisms: radiative recombination competing with multi phonon Shockley-Read-Hall (SRH) and Auger recombination. In addition, certain enhancement of radiative recombination due to localized lattice disorder is speculated. In the case of lightly boron-doped, precipitation-annealed silicon, intentionally metal-contaminated samples with different OPD levels revealed a metal-specific PL variation with OPD density. For the relatively slow diffuser iron, the PL intensity increased with OPD density. In this case, PL is primarily controlled by highly SRH recombination-active Fe dissolved in the silicon lattice, not by the OPDs themselves. Higher OPD density led to progressive gettering of Fe and higher PL. For fast diffusers copper and nickel, which also are less active recombination centers in B-doped silicon, the PL yield is going down with increasing OPD density. In this case, PL intensity is not controlled by dissolved metal impurities but by metal-decorated OPDs. The information gained is complementary to data obtained from carrier recombination based techniques, such as PCD or SPV. However, an additional advantage of PL is its spatial resolution and applicability to detecting grown-in features, such as doping striations, and thermally induced defects, such as OPDs and SRDs, in the case of heavily doped silicon. This information is principally not possible using techniques such as PCD or SPV. Besides applicability to bare polished and epitaxial wafers, we found a high potential of PL applications to device-processed Si wafers. Examples include SRD analysis and assessment of relative cleanliness of epitaxial silicon close to device regions. The detected dislocations originated either from misfit stress at epi interfaces or local stress at device structures. Locally reduced PL yield, due to increased SRH recombination at a defect site, allows SRD detection at a spatial resolution close to 1 micrometer. The impact of added deep-level centers (due to heavy metal gettering) on the defect contrast is yet to be understood. At present, the actual threshold contamination levels of specific metals where a contaminated defect (such as SRDs or OPDs) becomes detectable by PL remain unknown. Nevertheless, a reasonable relationship between relative cleanliness of silicon beneath certain device structures and actual device yield could be established. In other examples, the impact of epi misfit-related and diffusion-induced SRD density on device yield is illustrated.

11:30 AM F6.6

APPLICATION OF X-RAY SYNCHROTRON TECHNIQUES TO THE CHARACTERIZATION OF THE CHEMICAL NATURE AND RECOMBINATION ACTIVITY OF LIFETIME LIMITING DEFECTS IN SOLAR CELLS. T. Buonassisi, O.F. Vyvenko, A.A. Istratov, E.R. Weber, University of California, Berkeley, CA; R.

Schindler, Fraunhofer Institute for Solar Energy Systems, Freiburg, GERMANY.

The improvement of low-cost photovoltaic cells based on multi-crystalline silicon requires the identification of efficiency-limiting grown-in and process-induced microdefects in the solar cell material. This identification is ideally based on a combination of spatially resolved electrical characterization with chemical analysis. For this purpose a novel, synchrotron-radiation based analytical technique has been developed, X-ray Beam Induced Current (XBIC), that can be directly correlated with X-ray microprobe Fluorescence (XRF) mapping for the analysis of shunts and lifetime limiting defects in solar cells. XBIC is a lifetime-sensitive technique, which uses an X-ray beam focused to a spot size of several square microns to generate electron-hole pairs, which are then collected by the p-n junction of the solar cell. The XBIC signal is measured simultaneously with the XRF signal, which characterizes the chemical nature of the sample excited by the beam, including e.g. impurity precipitates. This combination enables us to study the chemical nature of the defects and impurities and their recombination activity in-situ and to map metal clusters with a micron-scale resolution. In our first experiments with this novel approach, the impurities located at the shunt regions determined using thermography were mapped using XRF and XBIC. In all shunt locations analyzed so far, metal clusters consisting of nickel, copper, iron, titanium, chromium, and zinc were found. The possible correlations and impact of these impurities on the formation of shunts are discussed. Additionally, we have established correlations between metal distributions and lifetime maps in as-grown and hydrogen passivated mc-Si. While metal clusters were often found in the lower-lifetime regions of the solar cell, some extended defects which also showed strong contrast in XBIC maps did not have any detectable metal contamination. The role of metals in the enhancement of recombination activity of lattice defects in Si solar cells will be discussed in detail.

11:45 AM F6.7

MULTI-MODEL PARAMETERIZATION OF POINT DEFECT PROPERTIES IN SILICON. Thomas Frewen and Talid Sinno, Dept. of Chemical Engineering, University of Pennsylvania, Philadelphia, PA; Erich Dornberger, Christian Hoess, and Robert Hoelzl, Wacker Siltronic AG, Burghausen, GERMANY; Harmut Bracht, Institut für Metallforschung, University of Münster, Münster, GERMANY.

The thermophysical properties of native point defects in crystalline silicon, namely self-interstitials and vacancies, are critical for defect and dopant dynamics modeling and simulation. Models for the evolution of defects and dopants during silicon crystal growth and device processing continue to be only semi-quantitatively predictive and not robust. An outstanding challenge is the generation of a single set of point defect parameters that can be used to model defect and dopant distributions in both crystal growth (high temperature) and wafer processing (low temperature). An integrated approach to thermophysical property prediction in silicon has been developed that exploits simultaneously data from crystal growth, point defect self-diffusion measurements, and metal atom (zinc) diffusion profiles in wafers. Czochralski (CZ) crystal growth experiments are performed with continuously varying pull rates, leading to complex transient behavior for point defect diffusion and reaction that cannot be captured with steady-state analyses. These experiments provide a rich database for parameterization. The data from these experiments is combined with data from Zn wafer in-diffusion experiments at several temperatures. Simultaneous parameter fitting to both these transient experimental systems is performed using Simulated Annealing (SA), a stochastic global optimization method suited for complex objective functions with multiple local minima. Several approaches for considering multiple objective functions are investigated and compared with regard to convergence properties and computational expense. It is shown that the simultaneous consideration of multiple experimental datasets greatly decreases the number of plausible parameter sets, and should therefore increase resultant model accuracy and robustness. The large number of objective function evaluations associated with SA optimization (typically tens to hundreds of thousands) is a limiting factor in the present calculations, especially for two-dimensional transient finite element models of CZ crystal growth. A highly efficient implementation based on adaptive mesh generation and time integration is employed to reduce the calculation time.

SESSION F7: SEMICONDUCTOR NANOCAVITIES AND NANOSTRUCTURES

Chairs: E. V. K. Rao and Tony E. Haynes
Wednesday Afternoon, April 3, 2002
Salon 1/2 (Marriott)

1:30 PM *F7.1

FUNCTIONAL VOIDS BY GAS ION IMPLANTATION FOR

Voids in semiconductor crystals can be induced by gas ion implantation and annealing. Depending on the implanted dose, environment, and/or thermal budget, gas bubbles can be formed already in the as-implanted samples or after annealing. During thermal treatments gas atoms can dissolve in the matrix, agglomerate and/or evaporate from the surface. To be used in semiconductor processing the method for void formation should not introduce contamination and its integrability with standard semiconductor processing should be demonstrated. To date, void formation based on He ion implantation is the most widely and deeply investigated and its integrability will be demonstrated. Voids and bubbles can also be formed by ion implantation of several different species. The relative void or bubble formation will be also briefly discussed. Applications of voids in semiconductors processing for device fabrication are for enhanced materials, improved device performances or even as in situ nano sensors. Examples are SMART-CUT, self-gettering semiconductors, polycrystalline layers with high thermal stability, lifetime engineering, improved reliability of devices and sensors for interstitials. The specific application requires the right combination of implanted ion, implantation parameters setting, accurate thermal treatments and the proper integration in the device fabrication or material processing. The main topics for the different applications will be critically discussed

2:00 PM F7.2
ROLE OF IMPLANTED-HELIUM IN THE GROWTH OF CAVITIES IN SILICON. Esidor Ntsoenzok, Romain Delamare, CERI-CNRS, Orleans, FRANCE; Gabrielle Regula, Bernard Pichaud, TECSN, Marseille, FRANCE; Jeremie Grisolia, Alain Claverie, CEMES, Toulouse, FRANCE; Anton Van Veen, IRI, Delft, THE NETHERLANDS.

Cavities induced by helium implantation can have many applications including the gettering of metallic impurities. The thermal growth of these cavities are however unclear yet. Particularly the role of the helium must be clearly addressed. Helium can lead to the formation of overpressured cavities with a different growth behavior. Implantation near the silicon surface result to a fast thermal exodiffusion of helium while that process is slower for deeper implantation. Then the first cavities can be considered as helium free and the second ones growth in helium-rich environment. Silicon was implanted with both 50 keV and 1.55 MeV helium ions. The growth of cavities was studied by TEM measurements performed on samples after annealing at different temperatures. The first results showed that there is a difference in the organization of cavities. The cavities obtained by 50 keV implantation energy present an increase of their size with the sample depth i.e. the smallest cavities are near the surface and the biggest are in the bulk. In the case of the high implantation energy, cavities are more homogeneous. In addition, cavities induced by 50 keV are more faceted and bigger than they are when 1.55 MeV is used. These differences are probably connected to the desorption rate of helium. This study also allows the way to study the interactions between the surface and the cavities since the growth process of cavities is greatly influenced by the surface when using the lower implantation energy and hardly influenced for the higher energy. The role of both helium and surface in the growth of cavities will be widely discussed in this paper.

2:15 PM F7.3
INTERACTION BETWEEN SI-INTERSTITIALS AND HELIUM-IMPLANTATION RELATED DEFECTS FOR CAVITY STABILISATION. Anita Peeva, Jorge Kaschny, Reinhard Kogler, Wolfgang Skorupa, Forschungszentrum Rossendorf, Dresden, GERMANY.

The effect of interstitial type defects, on the evolution of He-implantation induced cavities in Si has been studied by Transmission Electron Microscopy (TEM). It has been demonstrated that the He cavities are stabilised by the interstitial type defects in silicon during annealing. Interstitial type defects were formed by Si ion implantation into Si and subsequent annealing. Si ions were implanted into n-type (100) oriented CZ-Si wafers at 1.7 MeV to the fluences between 5×10^{13} at/cm² and 2×10^{14} at/cm². The Si ion energy and fluences were chosen in such a way to prevent the proximity of the surface and to create interstitial type defects with different size, from small interstitial clusters to extended defects, in the projected ion range (R_P) region after annealing at 850°C for 30 min. The He ions were implanted at 470 kV to the fluence of 1×10^{16} at/cm² into the region where the previously formed Si interstitial type defects were located. The corresponding He peak concentration is lower than the critical one reported in the literature as a threshold for formation of He cavities. The samples were annealed at 700°C for 30 or 60 minutes in order to study the defect evolution. No visible cavities are formed in the as-implanted state after the He implantation. After an anneal at 700°C for 30 min the TEM

micrographs of both the reference sample only with He implant and the sample with He implant and the previously formed dislocations show existence of a cavity layer located in the R_P region. After longer annealing at 700°C for 60 min the reference sample shows no cavities while in the sample with the dislocations cavities are seen. The cavities are found to be located in the place where the pre-existing dislocations are observed. The cavities in silicon are known as a sink for interstitials released by the interstitial type defects. In the reference sample the flow of interstitials released by the interstitial type defects around the cavities in the same temperature regime can be captured by the cavity internal surface. If a great amount of interstitials is trapped at the cavity surface an epitaxial growth can occur, and the empty volume shrinks. The pre-existing dislocations are another sink and probably the preferred one for the interstitials. The pre-existing dislocations can get the interstitials which in the reference sample are trapped in the internal surface of the cavities, and prevent the cavity disappearance.

2:30 PM F7.4
COMPARATIVE RAMAN AND TEM ANALYSIS OF THE EVOLUTION OF PLATELET DEFECTS IN PLASMA HYDROGENATED AND ANNEALED CZOCHRALSKI SILICON. Reinhart Job, Alexander G. Ulyashin, Wolfgang R. Fahrner, Univ of Hagen (LGBE), Hagen, GERMANY; Marie-France Beaufort, Jean-Francois Barbot, Univ of Poitiers, Futuroscope Chasseneuil, FRANCE.

By Raman spectroscopy the formation of H₂ molecules in platelets and their evolution upon annealing were studied. Transmission electron microscopy (TEM) was applied for comparison. Standard p- and n-type (100)-oriented Cz Si wafers were hydrogenated by a plasma treatment at 250°C and subsequently annealed up to 600°C/air. H₂ molecules did appear only as nearly free species in platelets/voids (Raman shift ~ 4150 cm⁻¹). The Raman intensities of the H₂ vibration modes exhibited significant intensity modulations in dependence on the annealing temperature for both p- and n-type substrates. These intensity modulations can be explained by the evolution of (111)- and (100)-oriented platelets. The latter ones are oriented parallel to the wafer surface. At lower temperatures (350°C) (111)-oriented platelets and at higher temperatures (550°C) (100)-oriented platelets are predominant in the subsurface regions of the treated samples. This conclusion from Raman spectroscopy was proofed by TEM investigations. In case of p-type substrates the Raman intensities were significant higher than for n-type material. The higher H₂ Raman intensities in p-type Cz Si can be explained by the amphoteric character of hydrogen. In p-type material hydrogen mainly exists as positively charged H⁺ species, i.e. an electric field gradient occurs between the positively charged plasma and these H⁺ species. Therefore hydrogen is forced to move into deep wafer regions, where platelets are created and filled with H₂. In n-type material hydrogen is in the negative H⁻ or neutral H⁰ state and the driving force for the hydrogen migration is lower. So in p-type material the region over-saturated by hydrogen is wider, resulting in higher total amount of platelet formation and therefore larger H₂ concentrations located inside these platelets. The TEM investigations underline the Raman results and show that by non-destructive Raman spectroscopy the evolution of platelets can be monitored.

2:45 PM F7.5
ONSET OF BLISTERING AND THIN LAYERS EXFOLIATION OF ION IMPLANTED AND HYDROGEN PLASMA TREATED SILICON. Alexander Ulyashin, Reinhart Job, Wolfgang R. Fahrner, University of Hagen, Dept. of Electrical Engineering, Hagen, GERMANY; Anatolii Frantskevich, Belarussian State Polytechnical Academy, Dept. of Electronic Devices, Minsk, BELARUS; Alexander Usenko, Silicon Wafer Technologies Inc., Newark, NJ.

The onset time for surface blistering and exfoliation of thin layers at different temperatures were studied for n and p-type Cz Si implanted by H or He ions (100 keV, doses 1E15 - 1E16 cm⁻²) and then hydrogenated from a plasma. The surface blistering process as a function of annealing temperature and annealing time was studied by optical and scanning electron microscopy (SEM). Raman spectroscopy was used for the investigation of the evolution of Si-H bonds after the post hydrogenation annealing. It was found that the release of the hydrogen from the sub-surface layer and accumulation in buried defect region during the annealing is responsible for the onset of blistering for low-dose H/He implanted and then hydrogen plasma treated samples. The complete layer transfer for silicon samples, joined to a supporting wafer was realized for low-dose implanted ($\sim 1E16$ cm⁻²) samples. It was found that the process of the blistering and exfoliation is controlled by the hydrogenation and annealing parameters as well as by the heat pre-treatment of the ion-implanted samples. The mechanism of the hydrogen-induced exfoliation of silicon induced by hydrogen and nano-cavities preliminary formed by ion implantation is discussed.

3:30 PM F7.6**CAVITY FORMATION IN SI-COVERED Ge ISLANDS.**

M. Kammiller^a, F.M. Ross, R.M. Tromp and R. Hull^a, ^aUniversity of Virginia, Department of MSE, Charlottesville, VA; IBM T.J. Watson Research Center, Yorktown Heights, NY.

In our ultra high vacuum transmission electron microscope (UHV-TEM) we have been studying the behavior of defects in Ge and SiGe layers grown on electron-transparent Si substrates. The UHV-TEM gives us the unique opportunity to observe, in real time, the formation of thin films and self-assembled islands and the motion of defects such as dislocations during chemical vapor deposition carried out in the microscope polepiece. We are now applying this technique to the study of other important defects, including cavities. We have observed that electron beam irradiation of Ge islands which are overgrown with Si triggers the formation of spherical cavities similar to the bubbles generated by He implantation. The cavities form because of the separation of vacancies and interstitials by the strain field of the buried Ge island. The ability to control the position and size of these cavities by adjusting the dose and the strain field may be useful in defect engineering for devices, while also allowing us to investigate the physical mechanisms which control cavity formation. We will present video-rate observations of the formation and motion of these cavities in the spatially varying strain fields generated by the islands, and compare the results with cavities generated by He implantation. The influence of strain fields on the dynamics of the cavities as well as their nucleation and disappearance as a function of irradiation and temperature will be discussed.

3:45 PM F7.7

INTERFACIAL STATES AND STARK SHIFTS IN RED EMITTING InAlAs QUANTUM DOTS: DISCRIMINATION OF DEFECT LEVELS AND QD ENERGY LEVELS. R. Leon, J. Ibanez, Jet Propulsion Laboratory, Pasadena, CA; J. Siegert, S. Marcinkevicius, Department of Microelectronics and Information Technology, Royal Institute of Technology, SWEDEN; T. Paskova, B. Monemar, Department of Physics and Measurement Technology, Linköping University, Linköping, SWEDEN; S. Chaparro, C. Navarro, S. Johnson, and Y.H. Zhang, Center for Solid State Electronics Research & Dept. of Electrical Engineering, Arizona State University, Tempe, AZ.

Optical and transport measurements in diodes containing multilayers of InAlAs quantum dots (QDs) embedded in n- and p-type AlGaAs were performed as Capacitance-Voltage (C-V), deep level transient spectroscopy (DLTS), continuous wave and time resolved photoluminescence (PL) spectroscopy, and cathodoluminescence (CL) spectroscopy and imaging. These measurements show that while red emission from QD states is obtained at ~1.8 eV, interfacial states dominate the optical properties and affect carrier transport in these QDs. Interfacial defects provide non-radiative recombination path(s) which reduces the QD carrier lifetime to tens of picoseconds (down from ~1 ns for purely radiative decay) and produce DLTS peaks in both p and n type structures. Reduction of the filling pulses to ~1 microsecond allows isolation or deconvolution of the electron and hole levels from the QDs, which have apparent capture cross sections orders of magnitude larger than the dot/barrier interfacial defects. Changes in DLTS peak structure and shifts in electron and hole QD energy levels with applied electric field are also presented.

4:00 PM F7.8

DYNAMICS OF PHOTOEXCITED CARRIERS IN InAs QUANTUM DOTS SPATIALLY ALIGNED BY MISFIT DISLOCATIONS. J. Siegert, A. Gaarder, S. Marcinkevicius, Royal Inst of Technology, Dept of Microelectronics and Information Technology, Kista, SWEDEN; R. Leon, Jet Propulsion Laboratory, California Inst of Technology, Pasadena, CA; S. Chaparro, S.R. Johnson, and Y.H. Zhang, Arizona State Univ, Center for Solid State Electronics Research and Dept of Electrical Engineering, Tempe, AZ.

One of the ways to form ordered patterns of quantum dots (QDs) is to produce them on misfit dislocations deliberately introduced into the structure. During such growth, a square pattern of misfit dislocations is transferred into well-separated rows of sharply aligned QDs. In the studied samples, the dislocation patterns were formed with the help of a metastable structure, which relaxes during post growth annealing through a self-organized process leading to the formation of gradual surface undulations, acting as preferential sites for the nucleation of the QDs. However, dislocations may also have a negative effect behaving as nonradiative recombination centres and reducing carrier lifetimes. In the present work we address this aspect of ordered InAs quantum dot structures by studying photoexcited carrier dynamics with the help of time-resolved photoluminescence (PL) in a wide temperature and excitation intensity range. The main differences between the PL of the ordered QD and randomly oriented reference QD samples are the following: The spectra of the ordered QD samples show a much narrower width, suggesting much smaller QD size

variations. The PL decay time in the ordered QDs (100 - 200 ps) is too short to be determined by the radiative recombination, besides, it increases with increased photoexcitation intensity. The excitation power dependence of the PL intensity for the ordered QDs is superlinear. These experimental observations are explained by the influence of saturable carrier traps, present in the ordered QD samples. The origin of these traps will be discussed.

SESSION F8: POSTER SESSION

Chairs: Jacques P. Chevallier and S. Ashok

Wednesday Evening, April 3, 2002

8:00 PM

Salon 1-7 (Marriott)

F8.1

IMPURITY EFFECTS ON THE DISLOCATION ACTIVITIES IN Si. Ichiro Yonenaga, Institute for Materials Research, Tohoku University, Sendai, JAPAN.

Establishment of the knowledge on dislocation-impurity interaction is important from both the fundamental and practical viewpoints for development of semiconductor technology as well known in oxygen-dislocation interaction in Si. In current advanced technology, large diameter Si crystals heavily doped with electrically active impurities are exclusively used as the substrate material for the epitaxial growth of clean wafers without grown-in defects. However, easy slip generation of slip/dislocations within large diameter Si wafers becomes serious problems during device fabrication process because of the own self-weight. Recently, dislocation-free Si crystals without the Dash necking process, which was a standard for over 40 years, has been successfully grown by the Czochralski technique with heavy doping of certain impurities. However, far less is known on the dynamic activities of dislocations in Si heavily doped with electrically active impurities.

This paper reports on the dynamic activity of dislocations in Si crystals doped with acceptor (B) and donor (P, As and Sb) to various concentrations up to $2.5 \times 10^{20} \text{ cm}^{-3}$ in comparison with those in undoped and O-doped Si crystals. Suppression of the generation of dislocations from a surface scratch is found for Si doped with B, P and As to a concentration higher than $1 \times 10^{19} \text{ cm}^{-3}$ and the critical stress for dislocation generation increases with the impurity concentration, which is interpreted in terms of dislocation locking due to impurity segregation. The velocity of dislocations in B, P and As doped crystals increases with increasing the concentration.

F8.2

INTRINSIC POINT DEFECTS AND OXYGEN INTERACTION IN HEAVILY DOPED SILICON. Pierre Laveant, Peter Werner, Norbert Engler, Gerhard Gerth and Ulrich Goesele, Max Planck Institute of Microstructure Physics, Halle(Saale), GERMANY.

Carbon diffusion in Si is dominated by the so-called kick-out mechanism characterized by an interaction between C atoms and self-interstitials (I). As a result, a diffusion process at high C concentration causes a local undersaturation of I. This behavior can result in a reduction of the enhanced diffusion of dopants (TED of, e.g., boron) and is technologically applied in the heavily C-doped SiGe-base of hetero-bipolar transistors. Nevertheless, little is known about the influence of carbon on other point defects, such as vacancies, and impurities, such as oxygen. Samples of Si hetero-structures have been grown by molecular beam epitaxy (MBE) to investigate the corresponding influence of a high C content and of different dopants and impurities. Two topics will be brought into focus: i) the influence of vacancies V (Frank-Turnbull-mechanism) and the formation of SiC clusters as a source of V. ii) The oxygen out-diffusion from the substrate into the doped layers and a related gettering/complex formation. Such a mutual behavior (formation of complexes and precipitation) is discussed also on the base of the simulations of diffusion.

F8.3

ELECTRICALLY ACTIVE BORON-HYDROGEN COMPLEXES IN IRRADIATED SILICON. Nikolai Yarykin, Olga Feklisova, Inst. Microelectronics Technology RAS, Chernogolovka, RUSSIA; Joerg Weber, Dresden University of Technology, Dresden, GERMANY.

Two new electrically active radiation defects are observed using the DLTS and MCTS techniques in boron-doped silicon, which was hydrogenated before the room-temperature high-energy electron irradiation. Hydrogenation was performed by chemical etching in acid solutions and by treatment in hydrogen/deuterium plasma at temperatures below 500 K. Concentrations of the new centers can exceed those of other prominent radiation defects and always follow the depth distribution of the pre-formed boron-hydrogen pairs. The new radiation defects are not detected in non-hydrogenated samples and in hydrogenated boron-free (aluminum- and phosphorus-doped)

crystals. These findings indicate the boron-hydrogen-related nature of the centers. Comparison with other radiation defects indicates the interstitial nature of the observed centers. One of the new centers reveals a charge-driven configuration metastability. The energy levels associated with each configuration are determined and transformation kinetics are studied including the effect of deuterium substitution for hydrogen. The metastable center anneals out at 360 K. The other center is more stable and can be alternatively formed by subsequent hydrogenation of irradiated boron-doped silicon. Although the (non-hydrogenated) precursor of the center is not yet determined, formation and annealing kinetics of the precursor are studied in silicon crystals with different contents of oxygen and carbon impurities. The possible reactions of irradiation-induced interstitial boron in silicon are discussed.

F8.4
HYDROGEN PENETRATION AND REDISTRIBUTION DURING AND AFTER CHEMICAL ETCHING OF SILICON. Nikolai Yarykin, Olga Feklisova, Eugene Yakimov, Inst of Microelectronics Technology RAS, Chernogolovka, RUSSIA; Joerg Weber, Dresden University of Technology, Dresden, GERMANY.

Hydrogen penetration into silicon during wet chemical etching and its redistribution and formation of complexes with other defects during subsequent electrical/thermal treatments is investigated both experimentally and by computer simulation. Experimentally, the CV-profiling of net dopant concentrations was performed on Schottky diodes prepared on hydrogenated samples, and depth distributions of electrically active hydrogen-related centers were measured by the DLTS technique. The simulation program took into account the drift/diffusion of hydrogen in different charge states and its interaction with other defects. It is established that the unknown conditions at the etching surface prevent the unambiguous determination of the hydrogen diffusivity from the fitting of the simulated depth profiles to the final hydrogen complex profiles, which are usually measured experimentally. However, the detection of relaxation of the atomic hydrogen distribution after termination of the chemical etching process, allows us to estimate the concentration of mobile hydrogen near the surface and to determine the hydrogen diffusivity, which is close to the value extrapolated from the high-temperature experiments. From the fitting procedure a capture radius for the boron-hydrogen pair formation is calculated, which is close to the previously reported values and implies that electrostatic interaction governs the reaction. In contrast, the effective distance for hydrogen interaction with donors (including phosphorus as well as oxygen- and nitrogen-related thermal donors) in n-type silicon is much shorter than expected from the currently accepted structure of the energy levels of isolated hydrogen in silicon.

F8.5
EVOLUTION OF NUCLEATION SITES AND BUBBLE PRECURSORS IN SILICON AS A FUNCTION OF HELIUM IMPLANTED DOSE. Changlong Liu, R. Delamare, E. Ntsoenzok, CERI-CNRS, Orleans, FRANCE; D. Alquier, Laboratoire LMP, Tours, FRANCE; G. Regula, B. Pichaud, Laboratoire TECSEN, UMR 6122, Universite d'Aix-Marseille III, FRANCE; A. Van Veen, IRI, Delft University of Technology, Delft, THE NETHERLANDS.

(111) Oriented silicon samples were implanted at room temperature with 1.55 MeV ^3He ions in the dose range of 5×10^{15} to 5×10^{16} ions/cm². Cross-section transmission electron microscopy (XTEM) was used to study the evolution of bubbles and extended defects during subsequent thermal annealing. Meanwhile, techniques, such as thermal desorption spectroscopy (TDS) and nuclear reaction analysis (NRA), were adopted to check the He desorption from bubbles and bubble precursors. TEM results show that a large band of defects consisting of bubbles and/or dislocation loops are produced in the samples implanted to the doses higher than 1×10^{16} ions/cm² and during subsequent high temperature annealing. The dislocation loops were mainly found to extend away from the buried layer. The clusters of He bubbles in the buried layer act as the sources of the dislocation loops. No bubbles were observed in the low dose implanted samples even after thermal annealing treatment. TDS and NRA measurements show that the He desorption behaviour is quite different for the different dose implanted samples. This is mainly due to the desorption from the different sources, i.e. smaller vacancy-like clusters in the lower doses and bubbles or cavities in the higher doses. The formation of vacancy-like clusters in the low dose He implanted samples are further confirmed by the measurements of positron annihilation spectroscopy (PAS). These vacancy-like clusters act as the precursors of bubbles formed in the high doses. The results are qualitatively discussed. Key words: silicon, He implant, XTEM, bubbles, dislocation loops, vacancy-like defects.

F8.6
PARTIAL ANNEALING OF DEFECTS IN BORON-IMPLANTED P-TYPE SILICON BY HYDROGEN IMPLANTATION.

Yutaka Tokuda, Aichi Institute of Technology, Dept of Electronics, Toyota, JAPAN; Hiroyuki Iwata, Aichi Institute of Technology, Research Institute for Industrial Technology, Toyota, JAPAN.

We have already shown the partial annealing of electron traps in phosphorus-implanted n-type silicon by subsequent hydrogen implantation [1]. In this work, the effects of hydrogen implantation on hole traps produced in p-type silicon by boron implantation have been studied by deep-level transient spectroscopy (DLTS). Schottky contacts were fabricated by evaporation of Ti on implanted surfaces for DLTS measurements. The 300-keV boron implantation to a dose of 1×10^{19} cm⁻² induces four hole traps with thermal emission activation energies of 0.21, 0.35, 0.46 and 0.55 eV. Subsequent hydrogen implantation were performed to a dose of 2×10^{10} cm⁻² with energies of 60, 90, 120 and 150 keV. A substantial decrease in concentration is observed for the trap(0.46) with thermal emission activation energy of 0.46 eV after hydrogen implantation with energies of 120 and 150 keV whose projected ranges are deeper than that for the 300-keV boron implantation. The peak concentration of 2.0×10^{13} cm⁻³ in depth for the trap(0.46) after boron implantation decreases to the concentration of 7.6×10^{12} cm⁻³ after subsequent hydrogen implantation with the energy of 120 keV. This partial annealing is ascribed to the reaction of preexisting defects with point defects produced by hydrogen implantation. The effects of hydrogen implantation on other hole traps produced by boron implantation will be reported. [1] A. Ito and Y. Tokuda, J. Appl. Phys. 82, 1053 (1997).

F8.7
INVESTIGATION OF SUBSTRATE DAMAGE UNDER DIFFERENT MODES OF HYDROGEN PLASMA IMMERSION ION IMPLANTATION. Ricky K.Y. Fu, Paul K. Chu, Dept of Physics and Materials Science, City University of Hong Kong, Kowloon, HONG KONG; W.Y. Cheung, S.P. Wong, Dept of Electronic Engineering, Chinese University of Hong Kong, Shatin, HONG KONG.

Silicon-on-insulator (SOI) synthesized by the wafer bonding / ion-cut process is now commercially available. Hydrogen is typically introduced into the donor wafer using beam-line ion implantation. The implanted hydrogen ions are mass and energy filtered resulting in a well-defined hydrogen in-depth distribution. Plasma immersion ion implantation (PIII) is a viable alternative to beam-line ion implantation in this application and if conducted properly, better efficiency and lower production costs can be achieved. However, in the absence of ion / mass analysis, multiple ion species such as H1+, H2+ and H3+ are formed in the plasma and co-implanted into the wafer, thereby causing not only broadened hydrogen in-depth distribution but also different degree of surface damage compared to beam-line implantation. To compare the damage and defects created by hydrogen PIII, we conducted experiments using three modes: (1) 30 ms short pulse PIII, (2) 500 ms long pulse PIII, and (3) direct current PIII. Dynamic secondary ion mass spectrometry (SIMS) is employed to determine the hydrogen depth profiles and surface doses. The crystal disorder of the as-implanted samples is examined by channeling Rutherford Backscattering spectrometry (RBS). Our results show that the DC mode yields the least crystal damage, followed by long pulse PIII. The short pulse mode suffers mainly from the non-zero rise and fall time of the pulse and gives rise to a broader hydrogen distribution. The surface damage is primarily caused by low-energy ion bombardment and atom displacement due to nuclear stopping near the substrate surface. Our data suggest that the DC PIII mode is more preferred provided that there is sufficient sample cooling.

F8.8
PHOTO-INDUCED DISSOCIATION AND OPTICAL CROSS SECTION OF Si-H AND S-H COMPLEXES IN GaAs AND AlGaAs. M. Barbe, F. Bailly, J. Chevallier, Laboratoire de Physique des Solides et de Cristallogénèse, CNRS, Meudon, FRANCE; S. Silvestre, D. Lorient-Bernard, L. Kurowski, E. Constant, Institut d'Electronique et de MicroElectronique du Nord, CNRS, Villeneuve d'Ascq, FRANCE; M. Constant, Laboratoire de Spectrochimie Infrarouge et Raman, CNRS, Universite des Sciences et Technologies de Lille, Villeneuve d'Ascq, FRANCE.

The passivation effect of dopants in crystalline semiconductors by formation of hydrogen-dopant complexes is a well established phenomenon. A critical point for the fabrication of devices affected by such a passivation effect is to find out efficient dopant reactivation processes. Besides conventional thermal dissociation, hydrogen-dopant complexes can be dissociated under hot electron excitation, minority carrier injection or photoexcitation. For a given photon density, UV illumination has been found to be very efficient to dissociate Si-H complexes in GaAs at 300 K and at 100 K as well while near above band gap illumination induces a much smaller dissociation effect. In this work, we first present a determination of the optical cross section of Si-H complexes in GaAs for different wavelengths by modeling of the photon density dependence of the extra sheet carrier concentration induced by illumination in the range 1×10^{16} cm⁻² - 1×10^{22} cm⁻² of

photon densities. The sheet carrier concentrations have been measured either by Hall effect and conductivity experiments or by Raman scattering experiments through the analysis of the phonon-plasmon interaction. This cross section exhibits a threshold energy at 3.5 eV which is interpreted as the excitation energy from the bonding state to the antibonding state of Si-H bonds in GaAs. We also show that a UV induced dissociation of Si-H and S-H complexes occurs in AlGaAs and in 2D AlGaAs-GaAs heterostructures at 300 K. The evolution of the extra sheet carrier concentration at low photon densities presents a loss of free carriers which might be attributed to the filling of surface states as the dopants are progressively reactivated. In AlGaAs and in 2D AlGaAs-GaAs heterostructures, the replacement of hydrogen by deuterium in the complexes shows that the Si-D and S-D complexes are significantly more stable than the Si-H and S-H complexes as previously found in GaAs:Si,H.

F8.9
INFLUENCE OF HIGHLY DEFECTED δ -LAYERS ON P-N STRUCTURE PROPERTIES. B.S. Sokolovskii, V.K. Pysarevskii, R.M. Kovtun, Ivan Franko National Univ, Dept of Physics, Lviv, UKRAINE.

It has been developed an analytical model describing the influence of highly defected δ -layers located in the base region of p-n structure on reverse branches of current-voltage characteristics. The highly defected δ -layers, which are usually formed by ion implantation and widely used in fabrication of semiconductor devices, is assumed to can be characterized by the velocity of interfacial recombination of nonequilibrium carriers. By considering the carrier transport in the base region of p-n structure it has been obtain analytical expressions for spatial dependencies of the minority carrier concentration and the current through the reverse biased p-n junction. It has been shown that the reverse current caused by the carrier generation in the defected layer depends on the layer location, with the layer manifesting itself when it is at the distance from the space charge region of order or less than the diffusion length of minority carriers. At these conditions the reverse current monotonously increases at rising the velocity of interfacial recombination and does not depend on the applied voltage. In the case when the distance of the defect layer is of order of the Debye screening length the reverse current ceases to be a saturation current, i.e. it increases at rising the reverse bias. When the space charge region reaches the defected layer the substantial increase of the excess current takes place. In this case the situation is analogous to punch-through effect in p-n structure with thin base region.

F8.10
Abstract Withdrawn.

F8.11
DEEP LEVEL STUDY IN EPITAXIAL 4H-SiC GROWN ON SUBSTRATES INCLINED TOWARD $\langle 1\bar{1}00 \rangle$. Masashi Kato, Masaya Ichimura, Eisuke Arai, Nagoya Institute of Technology, Dept of Electrical and Computer Engineering, Nagoya, JAPAN; Shigehiro Nishino, Kyoto Institute of Technology, Dept of Electronics and Information Science, Kyoto, JAPAN.

4H-SiC epitaxial layers are generally grown on (0001) face substrates inclined toward $\langle 11\bar{2}0 \rangle$ direction. Recently, it has been reported that good epitaxial layers can be grown even on substrates inclined toward $\langle 1\bar{1}00 \rangle$ direction. In this study, we fabricated 4H-SiC epitaxial layer grown on substrates inclined toward these two kinds of directions and characterized them by deep level transient spectroscopy (DLTS). 4H-SiC epilayers were grown on (0001) Si face of 4H-SiC substrates inclined 8 degree toward $\langle 11\bar{2}0 \rangle$ and $\langle 1\bar{1}00 \rangle$ directions by the cold wall chemical vapor deposition method. Source gases were Si₂Cl₆ and C₃H₈ with H₂ carrier gas and growth temperature was 1550°C. We grew 6 and 20 μm thick 4H-SiC sample pairs. The each pair was simultaneously grown in a furnace. After the growth, Ni was evaporated on the C face of the samples and was annealed in order to form the ohmic contacts. The Au was evaporated on the epitaxial layer as the Schottky contacts. From the capacitance voltage (C-V) measurements, all the samples have net donor concentrations of $2.4 \times 10^{15} \text{ cm}^{-3}$. The 6 μm thick samples grown on different substrates show DLTS spectra very similar to each other for temperature range up to 550 K. The peak height in the spectra corresponds to concentration of 10^{12} - 10^{13} cm^{-3} and, the sum of the deep level concentrations is of the order of 10^{13} - 10^{14} cm^{-3} for both the samples. The same peaks are observed for the 20 μm thick samples. The sum of the deep level concentrations for the 20 μm thick samples is 10^{12} - 10^{13} cm^{-3} , which is one order of smaller than that for the 6 μm thick samples. The DLTS results indicate that the deep level concentration does not depend on the inclined direction of substrates but depends on the epilayer thickness.

F8.12
INFLUENCE OF SUBSTRATE SURFACE MORPHOLOGY ON

DEFECT GENERATION DURING SILICON CARBIDE SINGLE CRYSTAL GROWTH. Myung Yoon Um, Jae Kyeong Jeong, Bum Seok Kim, Hoon Ju Na, In Bok Song, and Hyeong Joon Kim, School of Materials Science and Engineering, Seoul National University, Seoul, KOREA.

Although it is well known that one of the major factors limiting the extent of the successful application of silicon carbide is the influence of the grown-in screw dislocations on device performance, their formation mechanism is still not fully understood. We had focused our efforts on getting a better understanding of substrate surface morphology's influence on defect generation. Silicon carbide single crystals were grown on various substrates by physical vapor transport method. Substrates used in this experiment were treated in different mechanical polishing using paste and chemical gas treatment. To investigate the defect evolution with respect to the substrate treatment before the growth, the grown crystals were examined by optical micrograph, scanning electron microscopy, atomic force microscopy and molten KOH etching technique. The dislocation density of the grown SiC crystals were determined by AFM, after they were etched by molten KOH at 550°C for 10 minutes. Substrate polished by 0.25 μm diamond paste showed uniformly distributed small scratches with RMS roughness of 10.8 Å while substrate polished by 6 μm diamond paste had nonuniformly large scratches with RMS roughness of 66.7 Å. The RMS roughness of the seed polished by 0.25 μm diamond paste was reduced to 6 Å by chemical hydrogen etching for 10 minutes at 1500°C. SiC single crystal was grown simultaneously on a substrate polished by 0.25 μm diamond paste and by 6 μm diamond paste, mounted side by side. The SiC grown on a substrate polished by 0.25 μm diamond paste had a edge/screw dislocation density of $6.1 \times 10^3/\text{cm}^2$ without micropipes. Hydrogen etched sample had a edge/screw dislocation density of $7.3 \times 10^2/\text{cm}^2$ without micropipes. On the other hand, the SiC grown on a substrate polished by 6 μm diamond paste had a edge/screw dislocation density of $5.1 \times 10^4/\text{cm}^2$, two orders of magnitude of higher than the hydrogen etched sample and four micropipes in this sample.

F8.13
Ni-Si ION BEAM MIXING INTO SiC FOR STABLE LOW TEMPERATURE OHMIC CONTACT. A.M. Elsamadicy, D. Ila, R. Zimmerman, M. Vora, J.J. Weimer, J.K. Hirvonen, J.D. Demaree.

We have used Ion Beam Mixing in introducing a Nickel-Silicon system to form a Nickel Silicide (Ni₂Si) in Silicon Carbide surface. Formation of Nickel Silicide (Ni₂Si) is investigated as possible ohmic contact to heavily nitrogen doped n-type 4H-SiC and 6HSiC. Nickel and Silicon have been electron evaporated to the SiC substrate surface while a beam of Argon Ion was used simultaneously, to assist the Ni-Si Ion mixing into the Substrate surface. Ni and Si were evaporated with various densities to study the optimum doses of Ni and Si for the formation of (Ni₂Si). We enhanced the ohmic property by electron gun evaporation of (Ni₂Si) on the Substrates surface. SIRIM code was used to predict the depth of the Ion Mixing zone. The (Ni₂Si) contacts were formed at room temperature as well as at substrates elevated temperatures. Contact resistivities and I-V characteristics were measured at temperatures between 100°C to 700°C. To investigate the electric properties, I-V characteristics were studied for the samples at each annealing temperature. Both Rutherford Backscattering Spectroscopy (RBS) and Auger Electron Spectroscopy (AES) were used for depth profiling of the (Ni₂Si), Si, and C. X-Ray Photoemission Spectroscopy (XPS) was used to study the chemical structure of the (Ni₂Si)/SiC interface. Acknowledgment Research sponsored in part by the NASA-Alabama Space Grant Consortium and the Ctr. for Irradiation of Materials of Alabama A&M University.

F8.14
Transferred to F9.7

F8.15
RAMAN AND FTIR STUDIES OF SILICON CARBIDE STRUCTURE DAMAGED BY HEAVY ION IMPLANTATION. Claudiu I. Muntele, Iulia C. Muntele, Daryush Ila, Center for Irradiation of Materials, Alabama A&M University, Normal, AL; David B. Poker, Dale K. Hensley, Solid State Division, Oak Ridge National Laboratory, Oak Ridge, TN.

The work reported here deals with studying the defects induced by heavy ion implantation as well as the degree of crystalline lattice recovery after annealing in a high purity argon environment between 600 and 1600°C. We implanted silicon carbide with Pd and Au ions at levels between 1014 and 1016 ions/cm², and used micro-Raman and FTIR techniques for investigating the lattice properties at various stages during the fabrication process. Research centers around the world have been involved for the past few years in developing gas sensors based on silicon carbide for applications in high temperature (800°C) environments, which practically eliminates other semiconductor materials. When hydrogen detection is desired, the

most suitable combination appears to be palladium, either implanted into silicon carbide or deposited on its surface. The sensors obtained by implantation are more stable in time at high temperatures, but the signal is less uniform than in the case of deposited sensors, because the p-n junction created by ion implantation has a poor quality due to the defects induced. Detailed discussions on Raman and FTIR spectra taken on 4H and 6H silicon carbide samples, as well as quantitative results of the damage level evolution with the annealing temperature, will be presented during this meeting. Research sponsored by the NASA Grant No. NG3-2302, and partially by the Center for Irradiation of Materials of Alabama A&M University and U.S. Department of Energy under contract DE-AC05-00OR22725 with the Oak Ridge National Laboratory, managed by UT-Battelle, LLC.

F8.16

CHARACTERIZATION OF SILICON CARBIDE IMPLANTED WITH EITHER B OR Al USING THERMAL ADMITTANCE SPECTROSCOPY. S.R. Smith, M.A. Capano, A.O. Ewvaraye, Air Force Research Laboratory, Materials Directorate.

We have measured the thermal activation energies for shallow acceptors in ion-implanted silicon carbide using Thermal Admittance Spectroscopy. The substrates were n/n⁺ epilayers. The implantation plus annealing produced p-type layers that were acceptable for characterization. The specimens were annealed in Ar at 1600°C, after which Ni Schottky diodes were fabricated on the specimens. Annealing times were 5, 15, 30, and 60 minutes. A shallow level that did not correspond to known levels was found in some of the specimens after annealing. Energy shifts were noted as the annealing progressed. In some of the specimens, band bending allowed the detection of both the p-type impurities and the residual n-type impurities in the substrate. Measurements of the electrically active p-type dopants were compared to a control specimen implanted with Ar. From this study, we conclude that at least one shallow donor level is introduced into the bandgap by implantation damage. Further more, the defects associated with these shallow levels may affect the device performance by destabilizing the lattice occupation of the implanted species, and limit the lifetime of the carriers.

F8.17

OPTICAL METHODS FOR DEFECT CHARACTERIZATION IN LIGHT ION IMPLANTED SILICON CARBIDE. Julia C. Muntele, Claudiu I. Muntele, Daryush Ila, Center for Irradiation of Materials, Alabama A&M University, Normal, AL; James Thompson, Department of Chemistry, Alabama A&M University, Normal, AL; David B. Poker, Dale K. Hensley, Solid State Division, Oak Ridge National Laboratory, Oak Ridge, TN.

The work reported in this paper deals with studying the defects induced by light ion (Al, N, He) implantation in the most commonly used species of silicon carbide, 4H and 6H, both p-type (Al doped) and n-type (N-doped). Confocal Micro-Raman (MR) and Fourier Transform Infra-Red (FTIR) techniques have been used for monitoring the spectral regions of amorphous silicon (480 to 540 cm⁻¹) and carbon (1300 to 1600 cm⁻¹). Broad peaks form in these regions because of silicon and carbon atoms relocated as interstitials, translating into a locally stressed crystalline lattice. The locally relaxed lattice at these atoms locations of origin also gives a broadening of the characteristic Raman peaks of each type of material (976, 798, 789, and 767 cm⁻¹ for 6H, and 965, 798, and 776 cm⁻¹ for 4H), besides the presence of the peaks of amorphous silicon and carbon. Furthermore, if any of the two phenomena exceeds the other, then a shift of the peak towards higher or lower wavenumbers is observable. UV/Vis Optical Absorption (OA) Spectroscopy has also been employed as a good tool for dopant and carrier trapping levels embedded in the band gap of the silicon carbide material. Detailed quantitative results on all the types of samples mentioned earlier will be presented during the meeting. Data were collected from virgin samples, as implanted, and after annealing at various temperatures between 600 and 1600°C. MR and FTIR results correlated with SRIM simulated vacancies, primary and secondary ion distributions and OA results will be shown. Acknowledgements This work is supported by the Center for Irradiation of Materials at Alabama A&M University and NASA-GRC Contract No. NAG3-2123. The work at ORNL was sponsored by the U.S. Department of Energy under contract DE-AC05-00OR22725 with the Oak Ridge National Laboratory, managed by UT-Battelle, LLC.

F8.18

ELECTRICAL CHARACTERIZATION OF LASER-IRRADIATED 4H-SiC WAFER. I. Salama, School of Optics/CREOL, Department of Mechanical, Materials, and Aerospace Engineering, University of Central Florida, Orlando, FL; N. Quick, Applicote Associates, Lake Mary, FL; A. Kar, School of Optics/CREOL, Department of Mechanical, Materials and Aerospace Engineering, University of Central Florida, Orlando, FL; Gilyong Chung, Sterling Semiconductor Inc., Tampa, FL.

Highly conductive tracks are generated in low-doped epilayers on 4H-SiC wafers using a laser-direct write technique. The current-voltage characteristics are measured to study the effect of the applied voltage on the electric resistance and the surface contact of the irradiated tracks. Transmission Line Method (TLM) will be used to determine the contact resistance, sheet resistance and charge carrier concentration. The effect of multiple irradiations on the electronic properties of the fabricated tracks was investigated and compared with the effect of the conventional annealing process. A laser doping process was used to achieve n-type as well as p-type impurity doping in the substrate. The electronic properties of the doped tracks are measured and compared with those of the untreated wafers. Microstructural observation and surface analysis of the irradiated tracks are discussed.

F8.19

THERMODYNAMICS OF SITE OCCUPATION OF SOLUTES IN COMPOUNDS. Gary S. Collins, Matthew O. Zacate, Dept of Physics, Washington State University, Pullman, WA.

The partition of a dilute concentration of solute atoms among substitutional and interstitial lattice sites is governed by reactions that transfer the solute from one site to another. For highly-ordered compounds, it has been shown using the law of mass action that, in the absence of interactions among defects and solutes, site-fractions of solutes are governed not only by energies of the solute in the various sites but also by concentrations of intrinsic elementary point defects (vacancies, antisite atoms or host-interstitials) and corresponding partial energies of formation of the defects [1]. This is because equilibrium defects in compounds must preserve the homogeneity of the phase and therefore can only exist in combinations such as an antisite pair formed by atom exchange or Schottky defect formed by removal of a formula unit of the compound, leaving behind vacancies. As a consequence, simulation of solute site fractions requires knowledge of solute site-energies and energies of all elementary point defects. These considerations apply for both 'line' compounds and compounds having a wide phase-field width made possible by structural point defects. In this paper, the thermodynamic model for solute site preferences described in ref. [1] is extended in two ways to correspond better with real material systems. First, in addition to substitutional and interstitial sites, solute sites are considered in lattice 'sinks' such as dislocations or grain boundaries. Second, effects of interactions among defects and solutes are explored using simple near-neighbor interaction models. - This work was supported in part by the NSF under grant DMR 00-91681. [1] Gary S. Collins and Matthew O. Zacate (submitted.)

F8.20

PASSIVATION OF THE NATIVE POINT DEFECTS IN LOW-TEMPERATURE-GROWN GaAs. V.V. Chaldyshev, A.E. Kunitsyn, D.A. Vasyukov, Ioffe Institute, St. Petersburg, RUSSIA; V.A. Kagadei, Research Institute of Semiconductor Devices, Tomsk, RUSSIA; D.I. Proskurovsky, Institute of High Current Electronics, Tomsk, RUSSIA; V.V. Preobrazhenskii, M.A. Putyato, and B.R. Semiyagin, Institute of Semiconductor Physics, Novosibirsk, RUSSIA.

A huge amount of native point defects is the main feature of the GaAs films grown by molecular-beam epitaxy at low temperature (LT). The most important of them are arsenic antisites, which create midgap donor levels with concentration up to $1 \times 10^{20} \text{ cm}^{-3}$. These deep donors are in part compensated by deep acceptors related to gallium vacancies. Such metastable system of native point defects transforms in nanoscale clusters upon post-growth anneals. In this paper we report about influence of hydrogenation on the native point defect system in LT GaAs. The LT GaAs films were grown at 200°C and were either undoped or unintentionally doped with Si or Be. The treatment in atomic hydrogen was performed at various temperatures and with different durations. Two main phenomena have been revealed, which are associated with the hydrogenation. The one of them is a retardation of the precipitation of the excess arsenic upon anneals. The other is a reduction in the electrical compensation of the arsenic-antisite-defect-related deep donors. Both phenomena are discussed in terms of formation of stable complexes between gallium vacancies and hydrogen atoms.

F8.21

COMPARATIVE ANALYSIS OF MBE-GROWN GaN FILMS ON SiC, ZnO AND LiGaO₂ SUBSTRATES. F. Yun, M.A. Reshchikov, L. He, T. King, D. Huang, H. Morkoç, Virginia Commonwealth Univ, Richmond, VA; Jeff Nause, Cermet, Inc., Atlanta, GA; Gene Cantwell, Eagle Picher Technologies, LLC, Miami, OK; H. Paul Maruska, CPI Crystal Photonics, Inc., Sanford, FL; C.W. Litton, Air Force Research Laboratory (AFRL/MLPS), Wright Patterson AFB, OH.

Since GaN substrates are not yet commercially available, other substrates with better lattice match and/or stacking match to GaN

are of interest. Sapphire, though with a large lattice and thermal mismatch, is still the standard substrate on which GaN films have been grown successfully with the aid of buffer layers and lateral overgrowth. ZnO, with very close lattice match and the same stacking order to GaN, is expected to greatly reduce the extended defect density of GaN films while providing single polarity films. SiC substrate is a promising candidate for high power electronic devices due to its superb thermal conductivity. LiGaO₂ is beginning to emerge as a useful substrate since the (111) surface matches well with GaN lattice (0001), though with the drawback of poor thermal conductivity. In this paper, we investigate different heteroepitaxial systems, namely, GaN/SiC, GaN/ZnO, and GaN/LiGaO₂, all grown in the same MBE system in Ga-rich conditions, in a similar fashion. GaN films were grown to a thickness of 1-2 μm in the temperature range of 610-650°C, on SiC, ZnO (O-face), and LiGaO₂. No buffer layers were used. The latter two substrates were subject to a chemical etch, prior to loading into the MBE chamber. Smooth AFM images were obtained for GaN films, and chemical etching of substrates was demonstrated to be beneficial for growth on both ZnO and LiGaO₂. X-ray rocking curve measurements showed the best FWHM for (002) GaN diffraction to be 2.0 arcmin, and that for (102) to be 13.9 arcmin, for a GaN film grown on SiC. Preliminary photoluminescence measurements at 15K showed the FWHMs of excitonic peaks to be 13, 16, and 23 meV, for GaN/ZnO, GaN/SiC, and GaN/LiGaO₂, respectively. A comparison of strain conditions on different substrates is discussed.

F8.22

CORRELATION OF SURFACE MORPHOLOGIES WITH Mn COMPOSITIONS Ga_{1-x}Mn_xAs EPILAYERS GROWN BY LIQUID PHASE EPITAXY. Hwa Mok Kim, Jae Hyeon Leem, Seung Yoo Choi, Deuk Young Kim and Tae Won Kang, Dongguk Univ, Seoul, KOREA.

We investigated the correlation between as-grown surface morphologies and Mn compositions of Ga_{1-x}Mn_xAs epilayers – a III-V diluted magnetic semiconductor – grown by liquid phase epitaxy (LPE). Ga_{1-x}Mn_xAs epilayers were grown at 595°C from 50%Ga 50%Bi mixed solvent. The grown layers were characterized by energy dispersive x-ray analysis (EDS) and atomic force microscopy (AFM). The Mn composition measured by EDS after growth process was varied from 1 to 7%. As increasing Mn composition surface morphologies of as-grown Ga_{1-x}Mn_xAs epilayers were varied. At higher Mn compositions, the morphology of the surface layers degrades strongly, preventing removal of the solution-melt from it.

F8.23

PROBING THE ALLOY DISTRIBUTION IN Al_xGa_{1-x}N WIDE-BANDGAP SEMICONDUCTORS VIA UV-PHOTOLUMINESCENCE. Leah Bergman, Sandra Wright, Xiangbai Chen, Tim Householder, David McIlroy, Wei Jiang Yeh, Department of Physics, University of Idaho; Stephen Terrell, Department of Mechanical Engineering, University of Idaho; Robert Davis, Department of Materials Science and Engineering, North Carolina State University.

A key issue for an alloy-based optical device is the nature of the distribution of its atomic constituents; the distribution impacts the width of the emission spectral-line. In general terms an alloy can be classified according to its atomic arrangements as either ordered, random distributed, or phase separated. The latter consists of aggregate-type-defects, and its emission line is expected to be broader relative to that of an ordered or random distributed alloy. Our study focuses on the photoluminescence (PL) properties of wide-bandgap Al_xGa_{1-x}N of composition 0 ≤ x ≤ 0.7. Ten films were grown via MOCVD on SiC substrates, with thickness ~3 nm. The optical system consists of a SHG UV laser of 244 nm (5.01 eV) excitation line and of a confocal microscope high-resolution Raman system, with probing spot diameter ~500 nm. Our results concerning the functional dependence of the PL linewidth with composition concur with the model calculation of excitonic emission of a random distributed alloy. This implies that the PL broadening in our samples is mainly due to random spatial fluctuation at the nano-scale regime of the Al and Ga atoms, and that no aggregation is taking place. In order to gain further insight into the effect of the random distribution on the PL characteristics, the effective probing volume has to be considered. The effective probing volume, which is due to the absorption length at a given alloy composition, can be estimated via knowledge of the probing spot size and absorption coefficient, and moreover can be varied via the confocal hole. The dependence of the PL lineshape on the effective volume was studied for two samples of 0.12 and 0.4 composition. The maximum probing volumes were calculated to be ~300x10⁴ nm³ and ~400x10⁴ nm³ respectively. Upon reducing these volumes by about 20% to 60%, the 0.12 sample exhibited no significant variation in its lineshape. In contrast, the 0.4 sample exhibited fluctuation in both line width and peak position on the order of a few meV. These results will be discussed in terms of the composition-dependent volume of the exciton in the AlGaIn alloys.

Acknowledgments: The author greatly acknowledges the NASA Idaho Space Grant Consortium for supporting this research.

F8.24

EFFECT OF ALUMINIUM COMPOSITION ON EXTENDED DEFECTS IN (Al_xGa_{1-x})_{0.51}In_{0.49}P EPITAXIAL LAYERS MEASURED BY ISOTHERMAL DLTS. H.F. Lim^a, S.J. Chua^{a,b}, D.Z. Chi^b, J.R. Dong^b and C.B. Soh^a; ^aCentre for Optoelectronics, Department of Electrical and Computer Engineering, National University of Singapore, SINGAPORE; ^bInstitute of Materials Research & Engineering, SINGAPORE.

Isothermal deep level transient spectroscopy (DLTS) technique was used to investigate deep level defects in (Al_xGa_{1-x})_{0.51}In_{0.49}P epitaxial layers grown by metal organic chemical vapour deposition (MOCVD) on GaAs substrate. The samples were grown with V/III ratio of 50, at a temperature of 675°C and pressure of 100 mbar. The aluminium composition, x, was varied, keeping all other growth parameters constant. In this study, it was found that there is severe temperature dependence of the DLTS signals for all the samples and this is explained in terms of the presence of noticeable capture barriers for electrons as well as the presence of a repulsive Coulombic barrier, which impedes the charge carriers to reach thermal equilibrium during the filling process. With high aluminium content, DX-like centers affect the capture process. The capture time constant, capture cross-section and trap concentration were observed to vary linearly with temperature change. It was also found that there is a logarithmic relation between the emission time constant and activation energy with filling pulse width and there is a linear relationship between capture cross-section with filling pulse width. The DLTS spectrum of all the traps have been found to be broader than that expected for a point-type defect, implying that they may be associated with a complex or extended defect. The observation of logarithmic capture mechanism further supports this speculation. The effect of composition, x, on the extended defects in the (Al_xGa_{1-x})_{0.51}In_{0.49}P epitaxial layers will be discussed in this paper.

F8.25

THE EFFECT OF DISLOCATIONS AND DEFECTS ON THERMAL CONDUCTION IN GaN FILMS. Jie Zou, Dmitri Kotchetkov, Alexander A. Balandin, Univ of California at Riverside, Dept of Electrical Engineering, Riverside, CA; Doru I. Florescu, Fred H. Pollak, Brooklyn College of the City Univ of New York, Physics Department, Brooklyn, NY.

GaN as well as other group III nitrides are viewed as highly promising for semiconductor optoelectronic and electronic applications. The wide band gap of GaN makes it suitable for high power density and high-temperature operation. Proposed applications of GaN-based devices such as microwave power sources, laser diodes and ultra-high power switches rely heavily on the possibility of removing high density of excess heat from the device active area. The latter, in turn, depends on the thermal conductivity values in GaN and related compounds. Despite the significant practical importance of the knowledge of heat conduction in GaN layers and a number of recent experimental reports [1] on the thermal conductivity values, theoretical investigation of the subject lagged behind. To date, the available theoretical models of thermal conductivity in GaN are limited to calculations of the intrinsic theoretical limit that do not consider defects and impurities. Thus, a realistic theoretical model which would allow us to investigate the effects of dislocations, point defects and impurities on the thermal conductivity of GaN grown on SiC and sapphire substrates is needed. In this talk, we will present such a model together with results of the calculation of thermal conductivity in wurzite GaN films characterized by realistic material parameters specific for a given growth technique. The effect of threading dislocations, vacancies, and impurities is analyzed. The predicted variations of the thermal conductivity with respect to dislocation density and doping concentration are in good agreement with recent experimental data [2]. The developed model can be used for thermal budget calculation in high-power density GaN devices. [1]. D.I. Florescu, V.M. Asnin, F.H. Pollak, et. al., Appl. Phys. Lett., 77, 1464 (2000). [2]. D. Kotchetkov, J. Zou, A.A. Balandin, D.I. Florescu, and F.H. Pollak, Appl. Phys. Lett., (to appear in December, 2001).

F8.26

COMPARATIVE INVESTIGATION OF PHOTOLUMINESCENCE OF Si- AND In-DOPED GaN/AlGaIn MULTIQUANTUM WELLS. W.H. Sun, L.S. Wang, and S.J. Chua, Institute of Material Research and Engineering, SINGAPORE.

Major developments in wide-gap III-V nitride semiconductors have been recently led to the commercial production of high-brightness UV/blue/green/amber light-emitting diodes(LEDs) and to the demonstration of room-temperature(RT)violet laser light emission under pulsed and continuous-wave operation. Impurity doping in active layers is one of many interesting topics when one grows

structural materials for fabricating those devices above. Employing low pressure metalorganic chemical deposition, Si- and In-doped GaN/AlGaIn multiquantum wells (MQWs) with serial Si- and In-doping levels, respectively, have been grown. Photoluminescence (PL) measurements have been performed on Si- and In-doped GaN/AlGaIn MQWs in the temperature range of 77-330K. In those two kinds of doping, there newly appear several different features in their PL spectra, which redshift with the sample temperature. Comparing the behavior of those features in PL spectra, we have investigated their mechanisms.

F8.27

INCORPORATION OF HIGHLY CONCENTRATED IRON IMPURITIES IN InP BY HIGH TEMPERATURE ION IMPLANTATION. T. Cesca, A. Gasparotto, N. El Habra, A. Coati, INFN and Physics Dept, Padova, ITALY; F. Boscherini, B. Fraboni, F. Priolo, E.C. Moreira, INFN and Physics Dept, Bologna, ITALY; G. Ciatto, F. D'Acapito, CNR and INFN, ESRF, Grenoble, FRANCE.

Among other impurities in InP Fe plays a special and important role. Thanks to its midgap deep acceptor character, Fe doping is employed to produce bulk and epitaxial semi-insulating InP and is widely used in the optoelectronic device technology. Furthermore, intracenter d-shell transitions between Fe^{2+} states could be exploited to produce a light emitter in the mid-IR region. In order to display these properties, due to their chemical nature, Fe atoms have to be substitutionally located in a regular lattice. Major drawbacks are due to the limited Fe solubility ($\leq 1 \times 10^{17} \text{ cm}^{-3}$) and its strong reactivity with the crystal defects. We employed ion implantation as a non-equilibrium technique to overcome the solubility limitations and introduce a high concentration of active Fe atoms in the InP lattice; in order to reduce the damage production and avoid Fe-defect reactions we heated the substrate at a temperature $T \geq 200^\circ\text{C}$ during the implantation. With this method local electrical compensation and semi-insulating layer formation in substrates with n-doping up to $1 \times 10^{19} \text{ cm}^{-3}$ has been obtained. A detailed investigation of the implant induced crystal modifications, with special attention paid to the local structure around the Fe implanted atoms, is presented here. RBS- and PIXE-channeling together with XAFS measurements were used as main characterization tools; XRD and TEM were also employed. The results show a very interesting situation: beside to a crystal damage strongly reduced by dynamical annealing effects, the as-implanted samples show a high concentration of substitutional Fe atoms; following annealing treatments in the 300 - 600°C range cause a reduction of the substitutional Fe fraction, probably related to the formation of Fe-P clusters. Correlation with the electrical properties and application perspectives of these high Fe-density implanted InP will also be discussed.

F8.28

RAMAN SCATTERING SPECTRA IN Be-IMPLANTED GaN EPILAYERS. W.H. Sun, L.S. Wang and S.J. Chua, Institute of Material Research and Engineering, Singapore, SINGAPORE.

Ion-implantation has been an interesting topic on impurity-doping in GaN. Raman measurement is a strong tool for the characterization of semiconductors. We have investigated the Raman scattering spectra in Be-implanted GaN epilayers. (a) In as-implanted GaN, new Raman bands at ~ 310 , ~ 350 , ~ 370 , 669 cm^{-1} appeared. From phonon-dispersion curves for hexagonal GaN, the $\sim 310 \text{ cm}^{-1}$ and 669 cm^{-1} bands were assigned to the highest acoustic-phonon branch and the optical-phonon branch at the Brillouin zone boundaries, respectively. Comparing to Raman spectra from GaN samples implanted with other species of ions, such as Mg and C ions, we discuss the origins of the ~ 350 and $\sim 370 \text{ cm}^{-1}$ peaks (b) Two sharp bands at 168 and 199 cm^{-1} were observed in the Raman spectra of Be-implanted GaN after post-implantation annealing treatments. We attentively assign these two bands to Be-related local vibrational modes.

F8.29

DIFFRACTION CONTRAST IMAGE ANALYSIS ON THE DEFECTS OF THE GaAs CRYSTALS CAUSED BY ECR CLEANING PROCESS. Shang-Cong Cheng, Mike X. Ouyang, Corning Inc, Science and Technology, Corning, NY.

Cross-sectional and plan-view TEM techniques were used to study the defects on (110) facets of GaAs crystals caused by ECR hydrogen and argon plasma cleaning process used to remove the native oxides. It is found that the densities of the defects are dependent on the ECR gas type, anode voltage and the etching time. By TEM diffraction contrast image analysis, the crystal defects are determined as Frank dislocation loops at the {111} planes of the GaAs crystal. The details of the TEM analysis procedures are described in the paper. In order to obtain a damage free and oxygen free (110) surface of the GaAs crystal, the control of the ECR process parameters is critical.

F8.30

THE DIFFUSION OF INDIUM IN LEAD TELLURIDE. M.P. Darieł, Z. Dashevsky and S. Shusterman, Ben-Gurion University of the Negev, Dept. of Materials Engineering, Beer-Sheva, ISRAEL.

The addition of indium transforms a p-type PbTe into n-type PbTe when the concentration of the negative charge carriers, contributed by In atoms occupying Pb lattice sites and that act as donors, outweighs the initial positive charge concentration. Indium was diffused from a gaseous source at a series of temperatures into two kinds of p-type PbTe single crystals, grown in the Czochralski technique: (a) PbTe doped with 1 at. % Na; (b) off-stoichiometric PbTe with excess Te. In the former, Na atoms substitute for Pb atoms and act as acceptors, in the second case, excess Te generates structural Pb lattice vacancies that act as acceptors. In both instances the initial constant concentration of the positive charge carriers was determined by Hall effect measurements at low temperature. The location of the n - p junction (generated by the influx of In in the course of the diffusion anneal) was determined using a hot-probe technique, whereby the location of the change of sign of the Seebeck coefficient is determined within a resolution of $10 \mu\text{m}$. At that location, the concentration of electrons contributed by the incoming In equals the initial concentration of holes. The surface In-concentration, at different temperatures in the 500 to 750°C range, was determined by electron microprobe measurements. On the basis of these data points, the effective diffusivities of In in PbTe were calculated using the solution of the uni-dimensional diffusion equation for a constant surface source. The results for the diffusion of In in PbTe with excess Te can be expressed as $D = D_0 \exp(-E_a/kT)$ with $(-E_a = 1.4 \pm 0.1 \text{ eV})$, $D_0 = (9 \pm 2) \cdot 10^{-2} \text{ cm}^2/\text{sec}$. The effective diffusivities of In in PbTe(Na) are lower by a factor of 20 but with a similar activation energy. These results are consistent with an interstitial diffusion mechanism of In in both kinds of p-type PbTe and with the much larger number of available free Pb-lattice sites in off-stoichiometric PbTe with excess Te.

F8.31

NATIVE DEFECT FORMATION AND IONIZATION ENERGIES IN CADMIUM TELLURIDE. John E. Jaffe, Mary Bliss, Pacific Northwest National Laboratory, Richland, WA.

Deep intrinsic levels near the middle of the band gap in CdTe, 0.60 to 0.75 eV above the valence band maximum, have been reported in several experiments. Based on earlier electronic structure calculations, these features have been attributed to the second ionization level of the Cd vacancy, while the Te antisite, possibly complexed with a Cd vacancy, has also been suggested to account for some midgap levels. Using high-accuracy LDA calculations with full lattice relaxation out to third neighbors, we show that (i) both acceptor states of the Cd vacancy are shallow, (ii) the donor states of an isolated antisite are both more than 1 eV above the valence band maximum, (iii) the antisite-vacancy complex is very stable and (iv) this complex does indeed have acceptor states near midgap in CdTe and may account for the intrinsic defect states in that energy range. The lower energy of the complex relative to separated antisite and vacancy is shown to result partly from enhanced lattice relaxation: the bridging Te between the antisite and vacancy can move away from the former and towards the latter with little steric hindrance.

F8.32

BEHAVIOR OF COPPER IN CdGeAs₂ CRYSTALS. Valeriy G. Voevodin, Olga V. Voevodina, Svetlana A. Bereznyaya, Zoya V. Korotchenko, Siberian Physico-Technical Institute, Tomsk, RUSSIA; Melvin C. Ohmer, Jonathan T. Goldstein, Nils C. Fernelius, Air Force Research Lab, Materials Directorate, MLPSO, Wright-Patterson Air Force Base, OH.

We present an investigation of diffusion and melt doping of Cu in CdGeAs₂. Cu was found to be an acceptor, its introduction in the melt allowed the controlled introduction of holes from $\sim 8 \times 10^{16} \text{ cm}^{-3}$ to $\sim 1 \times 10^{18} \text{ cm}^{-3}$. Introduction of Cu from the melt was also found to improve the homogeneity of the crystal. The saturation solubility of Cu introduced via diffusion doping was found to have an exponential dependence on the diffusion temperature, from 450°C to 600°C , obeying the equation $N = N_0 \exp(-\Delta H/kT)$ with the parameters $N_0 = 6 \times 10^{19} \text{ cm}^{-3}$, $\Delta H = 0.3 \text{ eV}$, and k is the Boltzmann constant. From 600°C to 650°C , the saturation solubility was found to *shape decrease* exponentially with temperature.

F8.33

CONTROL OF VALENCE STATES FOR ZnO AND ZnS WITH A WIDE-BAND GAP BY A CO-DOPING METHOD. Tetsuya Yamamoto, Kochi Univ. of Technology, Dept of Electronic and Photonic Systems Engineering, Kochi, JAPAN.

We discuss what causes the differences in properties of p-type doping using a nitrogen species among ZnO, ZnS and ZnTe as a reference

based on the electronic structures and the Madelung energy calculated by ab-initio electronic-band-structure calculations, and the thermodynamic parameter which is the formation enthalpy of the solid compounds, Zn_3N_2 . Nitrogen doping gives rise to localized impurity states at the top of the valence band for ZnO and ZnS while it causes a delocalized ones for ZnTe. Holes in the narrow bands for ZnO and ZnS are localized by repulsion effects. The Madelung energies for the three N-doped semiconductors are found to be increased. For ZnTe, based on the calculated results, we find that Zn vacancies, which behave as acceptors, cause a decrease in the Madelung energy. Considering that Zn-deficient ZnTe is more stable, the Zn vacancy compensates the increase of the Madelung energy by the incorporation of the nitrogen into ZnTe. In addition, the differences in the formation enthalpy between the materials and the Zn_3N_2 indicate the high affinity between Zn and N for N-doped ZnTe compared with N-doped ZnO or ZnS. In order to solve the N-doping problem above in ZnO and ZnS, we propose a co-doping method using the N acceptors and donors as a reactive codopants. The deliberate co-doping of the donors is essential for the delocalization of the impurity states at the acceptors and the stabilization of the ionic charge distributions in p-type highly doped semiconductors. The donor is not the p-type killer but a good by-player who activates acceptors, i.e., the reactive codopant. Based on theoretical calculations, Ga or Al species is suitable for the use as reactive codopants for ZnO and Ga or In for ZnS. We will discuss the experimental data of the two semiconductors.

F8.34
PERTURBATION OF COPPER SUBSTITUTIONAL DEFECT CONCENTRATIONS IN CdS/CdTe HETEROJUNCTION DEVICES. D. Albin, R. Dhere, T. Gessert, M.J. Romero, Y. Yan, S. Asher, and S. Johnston, National Renewable Energy Laboratory, Golden, CO.

The efficacy of implementing terrestrial-based photovoltaics is dictated by trade-offs in device performance, cost, and reliability. Presently, the highest efficiency polycrystalline CdS/CdTe superstrate solar cells utilize backcontacts containing copper as an intentional dopant. Accelerated stress data correlates copper diffusion from this contact with performance degradation. The use of nitric-phosphoric acid etching prior to contacting is shown to impede the diffusion of Cu from the backcontact as shown by secondary ion mass spectroscopy. Simultaneous stress test hardening is observed in these acid-etched devices. Transmission electron microscopy and x-ray diffraction of etched surfaces reveal the conversion of surface CdTe to a Te-rich matrix. This converted surface layer is approximately 100-200 nm thick and exists both at the film surface and down grain boundaries. Deep level transient spectroscopy of etched and non-etched devices show that the formation of this Te-rich matrix strongly favors the formation of defect levels at (Ev + 0.28 to 0.34 eV). These levels are believed to be associated with Cu_{Cd} substitutional defects and are localized in the vicinity of the backcontact.

F8.35
LASER ENGINEERING OF BARRIER STRUCTURES BASED ON SOLID SOLUTION $ZnCdHgTe$. Galina Khlyap, State Pedagogical University, Drogobych, UKRAINE.

The narrow-gap semiconductor $ZnCdHgTe$ is proposed as a material alternative to the world-wide known compound $HgCdTe$ due to improved electric properties. The abstract for the first time deals with the problem of the artificial defects generation by using CO₂-laser radiation on the surface of $ZnCdHgTe$ epitaxial layers grown by the modified liquid-phase epitaxy on CdTe substrates. Electrical investigations carried out at the room temperature had shown the current-voltage and capacitance-voltage dependencies typical for the metal-semiconductor barrier structure. The epilayer surface studies had demonstrated that the cell-like relief has replaced the initial tessellated structure observed on the as-grown samples. The detailed numerical analysis of the experimental measurements and morphological investigations of the film surface showed that the boundaries of the cells formed under the laser irradiation are appeared as the regions of accumulation of derived charged defects of different type of conductivity supplying free charge carriers under the applied electric field.

F8.36
AN EXPERIMENTAL ANALYSIS OF THE INFLUENCE OF DEFECTS ON THE BUCKLING OF COMPRESSED THIN FILMS. M.-W. Moon, K.H. Oh, School of Material Science and Engineering, Seoul Nat'l Univ, Seoul, KOREA; J.-W. Chung, K.-R. Lee, Future Technology Research Division, KIST, Seoul, KOREA; R. Wang, Department of Metals and Materials Engineering, University of British Columbia, Vancouver, CANADA; A.G. Evans, Princeton Materials Institute, Princeton Univ, Princeton, NJ.

The role of imperfections on the initiation and propagation of buckle driven delaminations in compressed thin films has been demonstrated

using experiments performed with diamond-like carbon (DLC) films deposited onto glass substrates. The surface topologies and interface separations have been characterized by using the Atomic Force Microscope (AFM) and the Focused Ion Beam (FIB) imaging system. The wavelengths and amplitudes of numerous imperfections have been measured by AFM and the interface separations characterized on cross sections made with the FIB. Chemical analysis of several sites, performed using Auger Electron Spectroscopy (AES), has revealed the origin of the imperfections. The incidence of buckles has been correlated with the imperfection wavelength. The findings have been rationalized in terms of theoretical results for the effect of imperfections on the energy release rate.

F8.37
FIRST-PRINCIPLES SIMULATION OF HYDROGEN INTERACTION IN AMORPHOUS SILICON NITRIDE. Peter Kroll, Institute of Inorganic Chemistry, RWTH Aachen, GERMANY.

We investigated structure and properties of amorphous hydrogenated silicon nitride ($a-SiN_x:H$) using density functional methods. We concentrated on the calculation of vibrational spectra, which can be compared with Raman spectra accessible through the experiment, and their relation to specific properties of the structure. Models of $a-SiN_x:H$ were generated from random networks we prepared earlier for $a-SiN_x$. In addition we investigated the N-H terminated surfaces of $\beta-Si_3N_4$ and the crystal phase Si_2N_2NH . A comparison between N-H bond vibrations at surfaces and in the bulk shows that within the bulk the frequency of N-H bond stretching ($\approx 3000\text{ cm}^{-1}$) is considerably lower than at the surface ($\approx 3300\text{ cm}^{-1}$). We attribute this decrease of the force constant for this vibration to secondary interaction through space of hydrogen with nearby atoms. This influence is also responsible for the asymmetric peak shape. Car-Parrinello molecular dynamic simulations at elevated temperatures show hopping of bulk hydrogen between typically two bonding sites. Moreover, the preferred migration of hydrogen atoms occurs through interaction with adjacent N atoms.

F8.38
GROWTH DIRECTIONAL FEATURES OF SILICON NANOWIRES OBTAINED USING SILICON-MONOXIDE SOURCE MATERIALS. T.-Y. Tan, Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC; S.T. Lee, Center of Super-Diamond and Advanced Films (COSDAF) & Department of Physics and Materials Science, City University of Hong Kong, Hong Kong SAR, CHINA; U. Goesele, Max-Planck-Institute of Microstructure Physics, Halle, GERMANY.

Experimental results showed that most silicon nanowires (SiNW) grown using Si monoxide source materials are oriented in the $\langle 112 \rangle$ direction, some in the $\langle 110 \rangle$ direction, but hardly any in the $\langle 100 \rangle$ or $\langle 111 \rangle$ directions. These SiNW growth directional features may be understood by considering 4 mechanism-based criteria that concerns with the stability of a Si atom occupying a surface site, the Si {111} surface stability in the presence of oxygen, the stepped Si {111} surface layer lateral growth process, and the effect of dislocations in providing {111} surface steps. Analyses of SiNW growth in accordance with these criteria showed that $\langle 112 \rangle$ and $\langle 110 \rangle$ are the preferred SiNW growth directions, but $\langle 111 \rangle$ and $\langle 100 \rangle$ are not.

F8.39
STRAIN RELAXATION AND DISLOCATION DENSITY OF SiGe FILMS IN MICRON SIZE WINDOW WITH DIFFERENT MASK MATERIALS GROWN BY MBE. Xiang-jiu Zhang, Hui Xiong, Jihuang Hu, Zuiming Jiang, Yongliang Fan, Dongzhi Hu, Jun Lin, Yuerui Chen, Surface Physics Laboratory, Fudan University, Shanghai, P.R. CHINA.

Many authors reported that for heteroepitaxial growth the misfit dislocation density in the epitaxial layers would be varied if they were grown in small finite area of different sizes. In this paper we will report that the mask material was another factor, which would make obvious influence to the strain relaxation and the dislocation density of the SiGe films in micron size windows grown by MBE. In the experiments Si(001) wafers were used as the substrates and three kinds of materials were used as the masks, which were SiO_2 , Si_3N_4 , and the combined mask made by SiO_2 and Si_3N_4 films. $Si_{0.8}Ge_{0.2}$ films of 220nm were grown both in the micron size windows and at the large area of the same Si substrate by MBE. Experiment results showed that both the strain relaxation and the dislocation density were effected by the window size and the mask material. For the samples with the same mask material but different window sizes, as the window size reduced the dislocation density in the SiGe films in the windows would decrease correspondingly, but the strain relaxation in these films would not vary monotonically. The strain in the SiGe film grown in the windows of $20 \times 20\ \mu m^2$ was higher than that in the large area, but it was interesting to see that the strain

reduced along with the reducing of window size as the window size was smaller than $20 \times 20 \mu\text{m}^2$. For the samples with different mask materials but same size windows, the strain relaxation and the dislocation density in the SiGe films were also different. In the three kinds of samples, the dislocation density in SiGe films grown in the windows of Si_3N_4 mask was highest, and that in the windows of combined material mask was the lowest.

Annealing effect for these samples was also studied. Samples were annealed successfully at 620°C , 670°C , 770°C and 870°C for 30 minutes. The strain relaxation and the dislocation density in the SiGe film grown in large area increased greatly after annealing, but that in the SiGe films in the windows of $3 \times 3 \mu\text{m}^2$ was less changed. Especially for the sample with the combined mask material of SiO_2 and Si_3N_4 films the strain relaxation and the dislocation density only changed a little even it was annealed at 870°C . A qualitative explanation for these experimental results based on the edge induced strain relaxation effect was suggested.

F8.40

THE ROLE OF INTERFACES IN THIN FILM SOLAR CELLS.

Manuel J. Romero, M.M. Al-Jassim, R.G. Dhere, M.A. Contreras, F.S. Hasoon, T.A. Gessert, and H.R. Moutinho, National Renewable Energy Laboratory, Golden, CO.

Thin film II-VI and I-III-VI solar cells are the most promising for cost-effective, large-scale power generation for future terrestrial photovoltaics. A world-record efficiency of 18.8% has been demonstrated for $\text{Cu}(\text{In,Ga})\text{Se}_2$ solar cells fabricated by the three-stage process. Although these developments are very promising, further increase in efficiency will critically depend on a better understanding of the absorbers and how processing influences efficiency, reproducibility of fabrication, and long-term stability. Issues which are critical and on which progress has to be made are on interfaces associated with the absorbers. Both II-VI and I-III-VI thin films exhibit grain boundaries, which might be understood as homointerfaces. Heterointerfaces such as CdTe/CdS or CIGS/CdS are responsible for the mechanisms of carrier collection. The access to these micro- and nanosystems requires techniques of high spatial resolution. Beam injection methods, such as electron beam induced current (EBIC) and cathodoluminescence (CL) have been used to determine electrical and optical properties at the interfaces. In this contribution, we investigate the role of both internal and external interfaces in the functionality of thin film solar cells. For CdTe/CdS , a detailed study of the effects of grain boundaries and the Te/CdTe or $\text{ZnTe}/\text{Cu}/\text{CdTe}$ interfaces for back contacting has been conducted. On the other hand, for $\text{Cu}(\text{In,Ga})\text{Se}_2$ is commonly accepted that grain boundaries are passivated and carrier recombination at grain boundaries might be neglected in describing the cell operation. However, we show that grain boundary recombination is strongly dependent on the electric field distribution across the absorber. Additionally, we have studied several CIGS solar cells processed with different buffer layers showing that the absorber/buffer layer interface is indeed critical in the definition of the mechanisms for carrier collection.

F8.41

THE ELIMINATION OF ION IMPLANTATION DAMAGE AT THE SOURCE/DRAIN JUNCTION OF POLY-Si TFTS. Sang-Hoon Jung, Min-Cheol Lee, Kee-Chan Park and Min-Koo Han.

Polycrystalline silicon thin film transistors (poly-Si TFTs) crystallized by excimer laser annealing (ELA) of amorphous silicon (a-Si) are promising devices for active matrix displays (AMDs). However, ion implantation, which is usually used for doping process, creates considerable structural damage to the poly-Si layer and it was reported that defects at source/drain junction are not completely eliminated by ELA activation process due to laser beam attenuation near the gate edge. These defects are responsible for the large leakage current of poly-Si TFTs. The purpose of our work is to propose a simple poly-Si TFT with large lateral grains at the drain junction where the ion implantation damage is successfully eliminated. We located large grains at the drain junction by performing source/drain ion implantation prior to excimer laser annealing of active silicon film. The crystallization of a-Si and the dopant activation were simultaneously accomplished by single ELA process step. We have observed by TEM that large poly-Si grains were successfully grown from the source/drain region to the channel region by TEM due to different melting conditions between the implanted source/drain region and non-implanted channel region. The leakage current of the proposed TFT with large grains at the drain junction, decreased by one order compared with a conventional TFT that has many grain boundaries and residual implantation damage at the drain junction. The proposed poly-Si TFT, of which mobility is over $170 \text{cm}^2/\text{Vs}$, exhibits a large on/off current ratio exceeding 4×10^7 without LDD or offset structure. The improvement of electrical characteristics of the proposed poly-Si TFT is due to large grains at the drain junction.

F8.42

STUDY OF Er-RELATED DEFECTS IN a-Si:H:Er FILMS USED IN LIGHT EMITTING HETEROSTRUCTURES. A. Nazarov, Ja. Vovk, V. Lysenko, Institute of Semiconductor Physics, NASU, Kyiv, UKRAINE; O. Kon'kov, E. Terukov, Ioffe Physical and Technical Institute, RAS, Saint Petersburg, RUSSIA; S. Ashok, Dept of Engr Science, Pennsylvania State University, University Park, PA.

This work addresses defect issues relating to Er-doping of hydrogenated amorphous silicon films in amorphous/crystalline(a-Si:H:Er / n-Si) heterostructures used as light emitters. The a-Si:H:Er films were deposited on Si by chemical vapor deposition (CVD) or magnetron assistance deposition (MASD). The defects were evaluated by thermally activated current spectroscopy (TACS) and high-frequency (1 MHz) capacitance-voltage (C-V) characteristics measured at 77 K. For charging of the traps, visible light illumination was used at low temperatures and thermal-bias stress at high temperatures. Observed TAC spectra display no dependence on the film deposited technique, and the signal amplitude increases monotonically with the Er concentration in the a-Si:H film. Traps that have activation energies in the range 0.10 - 0.35 eV and 0.5 - 0.6 eV are charged under both light and thermal-bias stress, and may be associated with the deep levels in the bandgap of a-Si:H. The high-temperature current peaks with activation energies of 0.8-0.9 eV emerge only under thermal-bias stress and are strongly dependent on the charging temperature. It is suggested the these high-temperature thermally activated processes are related to polarization of the Er-O bonds in the amorphous matrix of a-Si:H. C-V measurements show that charging of the structure by negative substrate bias leads to net electron trapping in the a-Si:H(Er) film, whereas charging by positive bias results in net hole trapping. Thus, forward biasing the structure results in occupation of the deep levels located in the upper half of the a-Si:H band gap, while reverse bias causes charging of the deep levels located in the bottom half of the band gap. The plausible origin of the observed deep levels and polarization effects is discussed.

F8.43

LOW-TEMPERATURE PROPERTIES OF COMPENSATED Ge FILMS USED FOR CRYOGENIC THERMOMETERS. V.F. Mitin, V.V. Kholevchuk, Inst of Semiconductor Physics, NASU, Kiev, UKRAINE; V.K. Dugaev, M. Vieira, Dept of Electronics and Communications, ISEL, Lisbon, PORTUGAL.

Ge films are obtained by thermal evaporation of Ge in vacuum on semi-insulating GaAs substrates, and the temperature microsensors for cryogenic applications are designed. The electrical properties of Ge film depend on technology of their preparation. They are determined by the diffusion of Ga and As atoms from the GaAs substrate and by the structural perfection of the film. As a result, the Ge films are heavily doped and compensated. We present the results of experimental and theoretical study of temperature and magnetic field dependences of resistance at low temperatures. The behavior of resistance on the temperature and magnetic field depends on the doping level and compensation degree. The resistance demonstrates a strong dependence on both temperature and magnetic field at ultralow temperatures. At $T > 0.5 \text{ K}$ the magnetoresistance is small and positive over the whole range of applied fields. At lower temperatures the magnetoresistance is negative. At $T < 0.3 \text{ K}$, a gigantic negative magnetoresistance up to 100% is observed. This magnetoresistance saturates for fields above 1 T. These effects can be explained by the Anderson localization in a vicinity of mobility edge. We apply the scaling theory of localization, matching it to the weak localization theory for the electron energies above the mobility edge, and to the variable-range hopping conductivity for the localized states below the edge. The computer simulations of the temperature dependences show a good agreement with experimental data. The calculated effect of magnetic field is in a qualitative agreement with the experiment but lower in magnitude.

F8.44

X-RAY PHOTOELECTRON AND RAMAN SPECTROSCOPY STUDIES OF SULFUR IMPURITY INCORPORATED NANOCRYSTALLINE CARBON THIN FILMS DEPOSITED BY HFCVD FOR ELECTRONIC DISPLAYS. S. Gupta, Department of Physics, University of Puerto Rico; B.R. Weiner, Department of Chemistry, University of Puerto Rico; G. Morell, Department of Physical Sciences, University of Puerto Rico, San Juan, PR.

Results are reported on structural properties of sulfur incorporated nanocrystalline carbon (n-C: S) thin films grown on molybdenum substrates by hot-filament chemical vapor deposition (HFCVD) technique from methane-hydrogen (CH_4/H_2) and hydrogen sulfide-hydrogen ($\text{H}_2\text{S}/\text{H}_2$) gas feedstocks. All of the films were grown for 20-30 minutes and the thicknesses were around 0.5 micron. The structural bondings in thin films are studied as a function of substrate temperature (500-900°C) and sulfur concentration (100-500 ppm of H_2S) using Raman scattering (RS) and X-ray photoelectron

spectroscopy (XPS) techniques. While RS was used to identify the various carbon bonding configurations, XPS was utilized to study the electronic structure of these nanocrystalline carbon thin films with a view to control and optimize the growth parameters and consequently engineer electronic properties for vacuum microelectronics such as field emission displays. The Raman analyses were performed in terms of the variation in positions of D and G Raman bands, full-width at half maxima of G band and the ratio of their intensities $I(D)/I(G)$. These results clearly indicate the gradual clustering/ordering of sp^2 C sites leads into a network. The in-plane correlation length (L_a) which is related to $I(D)/I(G)$ ratio is also determined as a function of both substrate temperature and sulfur concentration and found to decrease with increasing both the process variables. The XPS C1s core level and valence band (VB) spectra of these films are compared with those of graphite and the composite (sp^3 and sp^2 bonded carbon) nature of the films is apparent. These results are also compared with those grown without sulfur (i.e. intrinsic material) at a particular substrate temperature and sulfur concentration. The SEM and AFM results support the conclusions drawn on the basis of RS and XPS investigations. This is a new and important development in engineering the carbon-based material through defects and impurity incorporation as viable cold-cathodes.

SESSION F9: HYDROGEN-DEFECT INTERACTION WITH SEMICONDUCTORS

Chairs: Noble M. Johnson and Jacques P. Chevallier
Thursday Morning, April 4, 2002
Salon 1/2 (Marriott)

8:00 AM *F9.1

HYDROGEN PASSIVATION AS A TOOL TO ENGINEER PROPAGATION LOSSES IN PHOTONIC CIRCUITS ON InP. E.V.K. Rao^a, B. Theys^b and B. Thedrez^c, ^aCNRS/LPN, Bagneux, FRANCE; ^bCNRS/LPSC, Meudon, FRANCE; ^cOPTO+/ALCATEL, Marcoussis, FRANCE.

The photonic circuits (PICs) operating in the 1.56 μm wavelength window contain side-by-side on the same chip the active (lasers, amplifiers, modulators, etc.) and passive components (straight or curved guides, interconnects, Y-junctions, etc.) monolithically integrated on a single InP substrate. Depending on the functionality of the circuit, high propagation losses in the passive sections can be a severe limitation to achieve optimal circuit performances. Such situations are often encountered in the presently developed photonic integration technologies since the free carriers in p- and n-InP cladding layers prevailing on either side of the passive waveguides could significantly contribute to propagation losses (through absorption and/or scattering). This talk precisely addresses the latter issue where we show that a spatially localized hydrogenation permits to engineer the losses in passive sections – **reduce them significantly** –, by neutralizing the active dopants through H-dopant interactions.

After a rapid overview on presently developed photonic integration technologies on InP, the different physical mechanisms controlling propagation losses are surveyed in the first part to highlight the prominent contribution of free holes in p-InP cladding layer through intervalence band absorption (IVBA). In the second part, the optical and electrical properties of deliberately hydrogenated p-InP and InGaAsP/InP double hetero-structures (DHS) are detailed to underline the high efficiency of atomic hydrogen to neutralize the commonly employed Zn and Be acceptor dopants in InP. Finally, after demonstrating the high thermal stability of H-acceptor complexes, few examples of photonic circuits successfully fabricated on InP for WDM (wavelength division multi-plexing) applications using spatially localized hydrogenation to reduce propagation losses will also be presented.

8:30 AM *F9.2

EFFECTS OF HYDROGEN ON THE DEEP LEVELS IN Si, ZnO AND DIAMOND STUDIED BY CATHODOLUMINESCENCE. Takashi Sekiguchi, Nanomaterials Lab, National Institute for Materials Science, Tsukuba, JAPAN.

It is widely recognized that hydrogen shows very complex behavior in various semiconductors. We are interested in the effect of hydrogen on the deep levels and have studied the change of luminescence properties of deep levels due to hydrogen incorporation by means of cathodoluminescence. In this presentation, the effects of hydrogen on the deep level luminescence in Si, ZnO and Diamond are reviewed. It is well known that hydrogen passivates deep levels in Si. However, the D-line luminescence that is related to dislocation is not passivated by hydrogen. Moreover, this emission is often enhanced by hydrogen treatment. This mechanism is interpreted as follows. Plastic deformation usually introduces not only dislocations but also point

defects in the crystals. Hydrogen effectively passivates point defects acting as nonradiative centers but not dislocations. On the other hand, point defects due to the off-stoichiometry or impurities endow visible luminescence in ZnO. We have found that hydrogen plasma treatment completely passivates such visible luminescence and, in turn, markedly enhances band-edge emission in ultraviolet region. In diamond, hydrogen related centers produce a broad emission around 540 nm in wavelength. Since homoepitaxial diamond films are usually grown in hydrogen plasma enhanced chemical vapor deposition, hydrogen is incorporated in the subsurface region of the films. Such hydrogen not only acts as the luminescence center but also creates the surface conductive layer. Detailed experiments revealed that hydrogen in diamond has metastable states and electron beam irradiation changes their energy states.

9:00 AM *F9.3

THEORY OF HYDROGEN IN DIAMOND. J.P. Goss, R. Jones, School of Physics, University of Exeter, Exeter, Devon, UNITED KINGDOM; M.I. Heggie, C.P. Ewels, CPES, University of Sussex, Falmer, Brighton, UNITED KINGDOM; P.R. Briddon, Department of Physics, University of Newcastle upon Tyne, Newcastle upon Tyne, UNITED KINGDOM; S. Öberg, Department of Mathematics, Luleå University of Technology, Luleå, SWEDEN.

Ab initio cluster and super-cell methods are used to investigate the local geometry and optical properties of hydrogen defects in diamond. Special attention is given to the single isolated species, hydrogen dimers and complexes with important donors, acceptors and extended defects. It is shown that H^+ is highly mobile and H_2^+ is the most stable dimer. Hydrogen is readily trapped by B, N and P. We assign the 3107 cm to a N-H pair. The role of surface hydrogen termination with regards to the phenomenon of surface hole conduction in diamond is also discussed.

9:30 AM F9.4

REVERSIBLE NITROGEN PASSIVATION BY HYDROGEN IN III-N-V COMPOUNDS. M. Capizzi, A. Polimeni, G. Baldassarri H.v.H., M. Bissiri, A. Augieri, INFN and Dept. of Physics, Univ. of Rome I, Rome, ITALY; A. Amore Bonapasta, CNR-ICMAT, Monterotondo, ITALY; Fan Jiang, M. Stavola, Dept. of Physics, Lehigh Univ., Bethlehem, PA; M. Fischer, A. Forchel, Universität Würzburg, Technische Physik, Würzburg, GERMANY.

Hydrogen is present in most steps of semiconductor growth and device processing and, because of its high diffusivity and strong chemical activity, it may sizably change the electronic properties of the host material. Therefore, great attention has been paid to the effects of H introduction in elemental Si and binary compounds as InP, GaAs, and GaN. Here, we report on the effects of atomic hydrogen irradiation on the optical properties of $(\text{InGa})\text{As}_{1-y}\text{N}_y/\text{GaAs}$ heterostructures, a system of increasing interest for telecommunications. By investigating samples with concentration, y , of the isoelectronic impurity N varying in a wide range, we have found that: (i) for $y \leq 0.001$, photoluminescence lines due to exciton recombination in N-related complexes are fully quenched upon hydrogenation; (ii) in the alloy limit ($y \geq 0.01$) and for increasing H dose, the $(\text{InGa})(\text{AsN})$ band gap blue-shifts toward the value it has in the N-free material; (iii) in the same alloy limit, H insertion into the lattice fully counterbalances the strong modification induced by N on the dependence of the $(\text{InGa})(\text{AsN})$ band gap on external perturbations (e.g., temperature and magnetic field); (iv) for all N contents, a complete recovery of the optical properties the material had before hydrogenation is obtained by thermally annealing the samples. These results are the first example of passivation by H of an isoelectronic impurity. They highlight the strongly localized character the N wavefunction maintains in $(\text{InGa})\text{As}$ for values of y that usually characterize an alloy. Consistently, infrared absorption measurements show the formation of N-H bonds, also predicted by a theoretical investigation of H equilibrium sites in $(\text{InGa})(\text{AsN})$. This suggests a mechanism for N passivation by H. Finally, preliminary results on the effect H irradiation has on other isoelectronic systems, as GaP:N and Zn(STe), will be presented.

10:15 AM F9.5

DOPING OF OXIDIZED FLOAT ZONE SILICON BY THERMAL DONORS - A LOW THERMAL BUDGET DOPING METHOD FOR DEVICE APPLICATION. Reinhart Job, Alexander G. Ulyashin, Wolfgang R. Fahrner, Univ of Hagen (LGBE), Hagen, GERMANY; Eddy Simoen, Cor Claeys, IMEC, Leuven, BELGIUM; Franz-Josef Niedernostheide, Hans-Joachim Schulze, Infineon AG, Munich, GERMANY; Guido Tonelli, IFN, Pisa, ITALY.

Hydrogen enhanced formation of thermal donors (TDs), i.e. oxygen related 'old' TODs, can be observed in Czochralski (Cz) silicon after applying a plasma hydrogenation at 250°C (60 min) and subsequent annealing at 450°C in air (>15 min) [1]. By such processes deep p-n junctions were created in p-type Cz Si wafers due to counter doping

by TODs [1]. In the present study TD formation was studied also in oxygen enriched high resistive float zone (FZ) silicon. Such substrates are used e.g. for radiation hard detectors or high voltage devices. RF Plasma hydrogenation (110 MHz, 50 W) was carried out at 250°C for 1 h. Subsequent annealing was done at 450°C/air for up to 50 h. The plasma treated and annealed oxidized FZ Si samples were analyzed by spreading resistance probe (SRP), capacitance-voltage (C-V) and DLTS measurements. Also Raman measurements and scanning electron microscopy were applied for the analysis. SRP measurements show that doping by TDs occurs up to deep wafer regions, i.e. >100 μm. Due to DLTS and C-V measurements one can state that the FZ material is not dominated by the formation of TODs (as in similar treated Cz Si [1]), but also a significant shallow thermal donor concentration (STD) occurs. In the FZ material TOD formation is lower than in Cz Si, since despite the oxidation the interstitial oxygen concentration is rather low (10E17 1/cm³). Therefore, in FZ Si STDs are of comparable importance like the TODs. Due to the higher O_i concentration, in Cz Si the STDs play a negligible role in comparison with the TODs. Finally, a low thermal budget doping technology on base of hydrogen supported TD formation and some high voltage test devices (diodes) will be discussed. [1] MRS Symp. Proc. Series, Vol. 513, p. 337 (1998).

10:30 AM F9.6

HYDROGEN PLATELET LAYER IN SILICON FORMED FROM HYDROGEN TRAPPED ONTO MICROBUBBLES OF GASES.

Alexander Usenko, Silicon Wafer Technologies, Inc., Newark, NJ; William Carr, Bo Chen, New Jersey Institute of Technology, Newark, NJ.

Features of a process of delamination of crystalline silicon layer from silicon wafer along hydrogen platelet layer formed by RF plasma hydrogenation are described. The process involves first making a buried trap layer. Ion implantation of inert or low-soluble gases is used to form the trap layer. The traps are microbubbles that appear along R_p plane of implanted ions. Results for argon, helium, and hydrogen implantation are compared. Wafers thus processed with an initial implant to levels below 2x10¹⁶cm⁻² are then hydrogenated with a RF plasma. During hydrogenation, an atomic hydrogen diffuses into the silicon wafer and collects onto internal surfaces of the microbubbles. Then the hydrogen increases the internal surface of the microbubbles by growing a platelet type extensions to the microbubbles. The extensions grow preferably along the buried layer plane (i.e. < 100 > plane). A silicon layer above the layer of grown platelets were delaminated through pre-bonding/cut/post-bonding sequence as in the Smart-cut process. The plasma hydrogenation of the trap layer may be used as a step in a process of fabricating of SOI wafers with a very thin top crystalline silicon layer. Also, implant doses needed to form the microbubble trap layer are much lower than doses of direct implantation of hydrogen in the Smart-cut process. Temperature range of 300°C to 450°C during the hydrogenation process allows effectively grow extended hydrogen platelets from the microbubbles. Mechanisms of nucleation of platelets as extensions of inert gas microbubbles are suggested. Control of hydrogen outdiffusion/platelet growth with thermal trajectory during plasma processing is discussed.

10:45 AM F9.7

THERMAL EVOLUTION OF DEUTERIUM IN 4H-SiC BY NUCLEAR METHODS. Romain Delamare, Esidor Ntsoenzok, Thierry Sauvage, CERI-CNRS, Orleans, FRANCE; Andrei Shiryayev, A. van Veen, IRI-Delft University of Technology, Delft, THE NETHERLANDS.

Hydrogen can have many exciting interests in silicon carbide since it can passivate defects and SiC is known to contain many. In addition it can also passivates dopants. Then it is very useful to understand what is its evolution during thermal treatments. Nuclear reaction analysis {NRA} is a powerful tool for an accurate study of deuterium in SiC. 4H-SiC was implanted with 30 keV D⁺ at room temperature with a fluence of 5E16 D / cm². The profiles of deuterium were measured by both the nuclear reaction {NRA} ²H (³He, ¹H) ⁴He and SIMS. To investigate the thermal evolution of deuterium, we applied thermal annealing with temperature up to 1300°C. Measurements by NRA didn't show any evolution until 1000°C while after a treatment at 1150°C, we found a decrease of about 30% of deuterium by a tail toward the surface. In addition Ruthrford back scattering {RBS} and ion channeling techniques were used in order to study both the evolution of defects in the matrix and the position of deuterium. Implantation of deuterium induces small clusters at R_p but with annealing, cavities can be found in the sample. We will also discuss how these defects affect the deuterium moving.

11:00 AM F9.8

ELECTRON-BEAM-INDUCED REACTIVATION OF Si DOPANTS IN HYDROGENATED AND DEUTERATED 2D AlGaAs HETEROSTRUCTURES. APPLICATION TO THE FABRICATION OF NANOSTRUCTURES. Ludovic Kurowski, Sarah Silvestre,

Dorothee Loridant-Bernard, Eugene Constant, Institut d'Electronique et de Microelectronique du Nord, Villeneuve d'Ascq, FRANCE; Michel Barbe, Jacques Chevallier, Laboratoire de Physique des Solides et de Cristallogene, Meudon, FRANCE; Monique Constant, Laboratoire de Spectrochimie Infrarouge et Raman, Villeneuve d'Ascq, FRANCE.

Hydrogen incorporation in n-type Si-doped GaAs epilayers is now a well-known process. Our interest is the stability of SiH complexes when submitted to an electron beam. Then, we study the role of hot electron injection in the dissociation of the SiH (or SiD) complexes which appears in n-type Si-doped GaAs epilayer and also in 2D-AlGaAs heterostructures exposed to a hydrogen or deuterium plasma. Firstly, we present Hall effect measurements obtained on hydrogenated and deuterated GaAs epilayers with different thicknesses (0.2 and 0.35 μm) and Si planar-doped AlGaAs/GaAs/InGaAs heterostructures exposed to an electron beam with different injection energies (10 to 50 keV). On one hand, we observe that the reactivation of Si dopants is weaker when deuterium is used. On the other hand, the study of this reactivation versus injection energies of electrons suggests an energetic electron excitation effect more than a minority carrier generation effect. Moreover, for the 0.2 μm thick GaAs epilayer and the 2D heterostructures, we observe that the free carrier density does not vary significantly for weak electron densities, and as a consequence, the reactivation of the Si dopants occurs above an electron dose threshold. This phenomenon might be attributed to the filling of surface states as the dopants are progressively reactivated. Finally, because of the electron dose threshold as well as their high electron mobility properties, Si planar-doped AlGaAs/GaAs/InGaAs heterostructures are particularly interesting to reactivate dopants, with a good contrast, using an electron beam irradiation. Also, it could open the fabrication of high mobility 1D or 2D mesoscopic structures for electronic or optoelectronic applications.

SESSION F10: ION IMPLANTATION I

Chairs: Esidor Ntsoenzok and Wolfgang Skorupa
Thursday Morning, April 4, 2002
Salon 1/2 (Marriott)

11:15 AM *F10.1

VACANCY IMPLANTATION— NO LONGER JUST A MYTH.

T.E. Haynes, R. Kalyanaraman, and O.W. Holland, Oak Ridge National Laboratory, Oak Ridge, TN; H.-J. Gossmann, D.C. Jacobson, and C.S. Rafferty, Agere Systems, Murray Hill, NJ.

In spite of the fact that interstitials and vacancies are produced in equal numbers (as Frenkel pairs or FPs) during ion implantation, it is well known in silicon that the interstitial-type defects overwhelmingly dominate the evolution of the system after implantation. The mutual annihilation of vacancies and interstitials arising from the FPs can be nearly perfect but each implanted atom itself adds an extra atom (interstitial) to the system as described by the so-called "plus-one" model. Consequently, such phenomena as enhanced diffusion, electrical activation, and dislocation growth and dissolution, etc., can be described quantitatively by considering only the interstitial interactions. This situation has made the properties of interstitial-type defects relatively easy to detect and measure and provided a useful tool for interstitial-based defect engineering. However, truly effective defect engineering requires a more complete understanding that includes knowledge of the behavior of vacancy-type defects and independent control of the vacancy concentration. There is a real need for a "vacancy implanter" in our defect-engineering toolkit. We have recently shown that MeV implantation can be used in combination with spatial separation between the vacancies and recoils to produce well-controlled vacancy supersaturations. This presentation will review recent experiments based on this concept of a vacancy implanter. These experiments have revealed the properties of vacancy-rich environments in silicon such as the energetics and kinetics of vacancy clustering and cluster dissolution. In addition, new effects resulting from implantation through interfaces and in channeling directions have been discovered. This presentation will discuss significant technological implications of these results for dopant activation and strain engineering.

11:45 AM F10.2

CREATION OF INTERNAL POINT DEFECT SOURCES IN SILICON BY CARBON IMPLANTATION. Maik Häberlen, Jörg K.N. Lindner, Bernd Stritzker, University of Augsburg, Institute of Physics, Augsburg, GERMANY.

It is generally accepted that point defects play a major role in the diffusion of dopants in silicon. Therefore it is interesting to establish techniques to create sources and drains of selfinterstitials and vacancies. In this contribution it is demonstrated by cross-sectional and energy-filtered TEM that amorphous SiC_x nanoprecipitates, which are formed during low-temperature high-dose implantation of

carbon into silicon, constitute such sources or drains. The formation of amorphous SiC_x nanoclusters in silicon is the result of both the negligible room temperature solubility of carbon in crystalline silicon and the stopping of carbon ions in silicon. The implantation conditions at which such nanoclusters are created have been extensively studied. Since the atomic density of silicon in amorphous SiC is significantly reduced compared to the atomic density of crystalline silicon, the nanocluster formation involves emission of Si self-interstitials. Vice versa, crystallization of these nanoclusters into SiC crystalites at 850-900°C requires the incorporation of Si self-interstitials into the recrystallization volume to adjust the Si atomic density of the amorphous phase to the higher value of crystalline SiC. The required interstitial flux to the recrystallizing SiC precipitates leads to the formation of voids in the silicon host lattice unless that interstitials can be provided by edge-type dislocations which are formed as a primary defect at elevated implantation temperatures.

SESSION F11: ION IMPLANTATION II
Chairs: Esidor Ntsoenzok and Wolfgang Skorupa
Thursday Afternoon, April 4, 2002
Salon 1/2 (Marriott)

1:30 PM F11.1

ELECTRICAL SIGNATURE OF ION-IMPLANTATION INDUCED DEFECTS IN N-SILICON IN THE DEFECT CLUSTER REGIME STUDIED USING DLTS AND ISOTHERMAL TRANSIENT SPECTROSCOPIES. Samarendra P. Singh, Vineet Rao, Y.N. Mohapatra, Dept of Physics, Indian Institute of Technology Kanpur, INDIA; Sanjay Rangan, S. Ashok, Dept of Engg Science and Mechanics, Pennsylvania State University, University Park, PA.

There is at present considerable controversy regarding electrical activity and possible signatures of defect clusters in silicon. In this paper we report detailed electrical signature of ion implantation induced defects in n-type epitaxial silicon using DLTS, isothermal time analyzed transient spectroscopy (TATS) and high resolution Laplace-DLTS. The defects are created using 33 keV Ar ions at a dose of 10^{14} cm⁻² and subsequent rapid thermal annealing in the temperature range of 350°C to 600°C. Though conventional DLTS shows several point defect-like mid-gap deep traps, it is shown not to be a reliable guide to the study of the dominant traps in this case. The emission time constants at any particular temperature are observed to depend on filling pulse width i.e. time for capture. Isothermal spectroscopies such as TATS and Laplace-DLTS show that emission time constants become progressively slower with increasing filling time. For a short filling pulse of 1ms, a trap with activation energy of about 0.3eV is observed. This trap however gives up its charge to deeper levels for longer filling times. The activation energy of the dominant trap (appearing at all temperatures between 230K-270K) deepens from 0.43 to 0.65eV increasing linearly with logarithm of filling time varying from 10ms to 1s. A still deeper trap appearing above 270K has activation energy in the range of 0.54-0.62eV. Contrary to the view that few dominant point-defect like traps are observed electrically in presence of ion-implantation induced defect clusters, our results show that the band gap may be replete with bands of trap states; however their occupation and hence observation depends on experimental conditions dictating dynamics of carrier capture and emission at these traps. Probable models, based on multiple charge nature of clusters and volume defects, giving rise to these unusual features will be discussed.

1:45 PM F11.2

DOSE RATE AND TEMPERATURE DEPENDENCE OF ION-BEAM-INDUCED DEFECT EVOLUTION IN Si AND SiC STUDIED BY CHANNELING IMPLANTATION. M. Posselt, L. Bischoff, J. Teichert, Forschungszentrum Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, GERMANY; A. Ster, Research Institute for Technical Physics and Materials Science, Budapest, HUNGARY.

The shape of ion range profiles obtained by channeling implantation depends strongly on the implanted dose. This behavior is caused by enhanced dechanneling of the incident ions due to the buildup of ion-beam-induced damage. In this work, the competing influence of dose rate and temperature on the dose dependence of the profile shape is investigated. 70 keV channeling implantation of Ge into Si and 6H-SiC was performed, using doses between 5×10^{12} and 6×10^{14} cm⁻². The implantation temperature varied between RT and 580°C. The use of a focused ion beam system enabled the application of two very different dose rates (10^{18} and 10^{11} cm⁻²s⁻¹). The depth distributions of Ge were measured by secondary ion mass spectrometry. The dose rate and temperature effects found are explained in terms of intracascade damage relaxation. The time scales for defect reduction and annealing are estimated. The characteristics

of ion-beam-induced damage evolution in Si and SiC are found to be different. Based on the qualitative discussion of the experimental results, a simple phenomenological model is developed in order to describe the dechanneling effect of the defects formed during ion bombardment. The use of this model in atomistic computer simulations yields Ge depth profiles which agree well with the measured data.

2:00 PM F11.3

DEFECT ACCUMULATION AND RECOVERY IN ION-IMPLANTED 6H-SiC. W. Jiang and W.J. Weber, Pacific Northwest National Laboratory, Richland, WA.

Results from a several-years effort on the ion implantation effects in 6H-SiC will be summarized. Single crystal wafers of the <0001>-oriented 6H-SiC polytype were irradiated at different temperatures (150 - 870 K) using a variety of ion species (H⁺ to Au⁺). Ion fluences were chosen to produce implantation damage that ranged from dilute point-defect concentrations to a fully amorphous state. The disorder on both the Si and C sublattices has been simultaneously studied in situ using a combination of Rutherford backscattering spectrometry and nuclear reaction analysis in channeling geometry. Multiple crystallographic axes have been used to determine the disordering behavior along different orientations. Isochronal annealing for 20 min has been performed on the implanted samples over a wide temperature range. After each annealing step, the remaining disorder was determined at lower temperatures to quench the annealing processes. The disorder accumulation for all ion species is consistent with a combined direct-impact and defect-stimulated (DI/DS) model for amorphization. A lower level of disorder on both the Si and C sublattices is observed along the <0001> axis than along the <1102> and <1011> axes to low doses, which suggests that some of the Si and C defects, such as single and split interstitial defects, are well aligned with the <0001> axis. Along the latter two axes, the rate of C disordering is higher than that of Si disordering due to a smaller displacement energy on the C sublattice. The fraction of irradiation-induced defects surviving simultaneous recovery processes decreases with decreasing ion mass and with increasing irradiation temperature. Three distinct thermal recovery stages have been identified, including a stage below room temperature.

SESSION F12: SEMICONDUCTOR INTERFACES, SUPERLATTICES

Chairs: Carleton H. Seager and William C. McColgin
Thursday Afternoon, April 4, 2002
Salon 1/2 (Marriott)

2:15 PM *F12.1

CHARGES AND DIPOLES AT SEMICONDUCTOR INTERFACES. Raymond T. Tung, Research Center for Quantum Effect Electronics, Tokyo Institute of Technology, O-okayama, Tokyo, JAPAN.

The formation mechanism of the Schottky barrier height at metal-semiconductor interfaces and the formation mechanism of the band offset at semiconductor heterojunctions have been vigorously debated for several decades. A question which has often been asked, especially for apparently pinned Schottky barrier systems, is the role played by defects. In this talk, theoretical models which explicitly consider the effect of defects and other interface states, such as the metal induced gap states, will be analyzed. It will be argued that care must be exercised to distinguish between the net dipole and the net charge of an interface and that no simple relationships exist between these two quantities. Two methods, traditionally used by molecular chemists, will be shown to provide simple solutions to the general problems of Schottky barrier height and heterojunction band offset. By using the electrochemical potential equalization (ECPE) method to estimate the polarization of random metal-semiconductor interface bonds, the experimentally observed Fermi level pinning phenomenon can be quantitatively accounted for. In addition, the quantum theory of atoms-in-molecules (AIM) can be used to provide accurate predictions of band offsets at high quality epitaxial semiconductor heterojunctions. These results point to the importance of correctly handling the chemistry at semiconductor interfaces in order to understand their electronic properties.

3:15 PM *F12.2

AB-INITIO RESULTS FROM SiO₂ TO HIGH-k GATE OXIDES. Peter E. Blöchl, Clemens Först, Institute for Theoretical Physics, Clausthal University of Technology, Clausthal-Zellerfeld, GERMANY.

Conventional SiO₂ based gate oxides suffer from stress-induced tunneling currents (SILC) and breakdown. We investigated defects in silica, including oxygen deficiency and hydrogen related defects, in order to identify the source of SILC and dielectric breakdown. An estimate of the energy dissipation during two-step tunneling in silica

identified the hydrogen bridge, i.e. a complex of an oxygen vacancy with a hydrogen atom, as the defect responsible for SILC. The results are confirmed by EDMR experiments of SILC. However, breakdown appears not to be directly related to those defects. Ab-initio molecular dynamics unveiled a new oxygen-ion diffusion mechanism, that could result in an electrochemical decomposition of the oxide. This is one possible mechanism for breakdown of gate oxides. High-k oxides are an alternative for SiO₂ as gate oxide. High-k gate oxides can be deposited with a larger physical thickness, thus suppressing quantum mechanical tunneling though an otherwise ultrathin gate oxide. One of the major problems is related to the growth and chemical stability of such oxides on silica. First results on the growth processes will be presented.

3:45 PM F12.3

ENHANCED INTERDIFFUSION IN CVD AND MBE GROWN Si/SiGe SUPERLATTICES. Daniel B. Aubertine, Ann Marshall, Paul C. McIntyre, Stanford Univ, Dept of Materials Science and Engineering, Stanford, CA.

We present the results of interdiffusion measurements on epitaxial Si/SiGe superlattices grown by both chemical vapor deposition and molecular beam epitaxy. In films grown by both techniques, the interdiffusivity during the early stages of diffusion is enhanced by more than an order of magnitude over the long time value. Scaling techniques are further used to show that this behavior is consistent with a single activation energy of 4.1 ± 0.7 eV and 4.1 ± 1.5 eV for the CVD and MBE grown material respectively. While films produced by both growth techniques were examined in the same manner, there is a reproducible scatter in the MBE diffusion behavior that is not seen for the CVD grown material. This suggests that growth technique dependent defects can play a significant role in the diffusion behavior of this system. Measurements of misfit stress relaxation and its role in the kinetics of interdiffusion in Si/SiGe heterostructures will also be presented.

4:00 PM F12.4

THE IMPORTANCE OF SCREENING AND CLUSTERING OF DOPANT ATOMS IN THE ROUGHNESS OF ELECTRONIC P-N INTERFACES IN GaAs. N.D. Jäger^a, K. Urban^a, E.R. Weber^b, and Ph. Ebert^a; ^aInstitut für Festkörperforschung, Forschungszentrum Jülich, Jülich, GERMANY; ^bDept. of Materials Science, University of California, and Materials Science Division, Lawrence Berkeley Laboratory, Berkeley, CA.

The functionality of semiconductor devices is critically depending on the ability to achieve a precise spatial and energetic positioning of the Fermi energy in nanoscale semiconductor structures by suitable incorporation of dopant atoms. The smaller the devices get, the sharper the changes between differently doped sections or layers in the device structure need to be. We address here the physics governing the electronic properties of interfaces between differently doped layers by analyzing the roughness of interfaces in GaAs p-n multilayers using cross-sectional scanning tunneling microscopy. We demonstrate that the electronic p-n interface exhibits a much larger roughness than the underlying essentially perfect 'metallurgical' interface, due to the individual long range electrostatic screening fields around each dopant atom near the interface and due to a clustering of dopant atoms. The clustering and the inherently connected local lack of dopant atoms gives rise to charge carrier depletion zones extending locally through entire nominally homogeneously doped layers once the layer thickness is close to the cluster dimensions. Thus, local variations in the dopant atom distribution limit the precision of the spatial and energetic positioning of the Fermi energy in nanoscale semiconductor structures and a further miniaturization eventually requires the control of the spatial location of dopant atoms.

SESSION F13: POINT DEFECTS, IMPURITIES, DIFFUSION IN SEMICONDUCTORS

Chairs: Yoshowanta N. Mohapatra and Vito Raineri
Friday Morning, April 5, 2002
Salon 1/2 (Marriott)

8:00 AM *F13.1

DEFECT AND IMPURITY ENGINEERING IN ZnO.
Chris G. Van de Walle, Xerox PARC, Palo Alto, CA.

ZnO is a fascinating material that is already in use for a wide range of electrical and electromechanical applications. Its properties also make it a candidate for light emission in the blue or near-UV range of the spectrum – the same type of applications that are currently being addressed with gallium nitride. Unlike GaN, however, ZnO is available in the form of bulk crystals that can be used as substrates. One serious obstacle remains, though: as-grown ZnO frequently exhibits n-type conductivity, and p-type doping has so far not been achieved. Because of its prevalence, the n-type conductivity has traditionally

been attributed to native defects. First-principles investigations reveal, however, that none of the native defects has characteristics consistent with a high-concentration shallow donor. In particular, the widely discussed oxygen vacancies are actually deep rather than shallow donors. I will present detailed results about their negative-U character and configuration coordinate diagram, which allow a reinterpretation of numerous results in the literature. If the prevailing n-type conductivity is not due to native defects, then unintentional impurities must be responsible. Hydrogen is an excellent candidate for such an impurity. While hydrogen in other semiconductors is amphoteric, always assuming a charge state that counteracts the prevailing doping of the material, hydrogen in ZnO behaves exclusively as a donor. I will discuss the consequences of these results for past and future experimental work, and address the prospects for achieving p-type ZnO with nitrogen acceptors. More broadly, I will show how our conclusions impact the understanding of the behavior of hydrogen in semiconductors and insulators in general.

¹C.G. Van de Walle, Phys. Rev. Lett. **85**, 1012 (2000).

8:30 AM *F13.2

THERMOCHEMICAL DECOMPOSITION IN GaN: LASER LIFT-OFF AND NOVEL DEFECT FORMATION. E.A. Stach, C. Kisielowski, National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, CA; W.S. Wong, Xerox Palo Alto Research Center, Palo Alto, CA; Y. Cho and T. Sands, Department of Materials Science and Engineering, University of California at Berkeley, Berkeley, CA.

In this presentation, we will focus on a number of interesting phenomena that occur in gallium nitride as a result of thermochemical decomposition at elevated temperatures. It has been known for quite some time that when gallium nitride is held at temperatures in excess of about 850°C (exact temperature depending on the vacuum level), nitrogen may desorb preferentially. This fact can be exploited to create freestanding layers of GaN by a process known as laser lift-off. Here, an excimer laser with a wavelength above the absorption edge of GaN is used to selectively decompose the GaN / sapphire interfacial layer [W.S. Wong, et al., Appl. Phys. Lett. **72**, 599 (1998)]. In this presentation, we will present some of our recent results which indicate that for MOCVD films, the process is largely controlled by this thermochemical decomposition alone, whereas for HVPE films it appears to be both thermochemical and thermomechanical in nature. Additionally, it is possible to study in real time and at high resolution how this thermochemical decomposition occurs in "bulk-like" GaN. This is accomplished by heating freestanding GaN crystals within the objective lens of a transmission electron microscope and imaging the process in real time. In particular, we find that desorption proceeds along the {10T0} prism planes and results in strong hexagonal faceting of the crystal. Desorption is found to occur preferentially along the cores of dislocations with a screw component, resulting in the formation of nanopipe defects, but does not occur along pure edge dislocations, even at temperatures in excess of 1150°C. Finally, we will discuss how thermal decomposition is accompanied by the formation of a new type of defect which we call "wormholes". These are an internal defect that we believe may be caused by burrowing of the remaining metallic Ga through the bulk crystal.

9:00 AM F13.3

COMPARISON OF DEEP LEVEL SPECTRA OF MOCVD- AND MBE-GROWN InGaAsN. R.J. Kaplar and S.A. Ringel, Ohio State University, Department of Electrical Engineering, Columbus, OH; A.A. Allerman, J.F. Klem, and Steven R. Kurtz, Sandia National Laboratories, Albuquerque, NM.

The quaternary semiconductor InGaAsN has attracted interest as a candidate for use in 1.30 and 1.55 μm optoelectronics and in multi-junction solar cells. Unfortunately, to date InGaAsN has exhibited poor electronic quality, although this has been observed to improve following thermal annealing. It is possible that deep level defects are partially responsible for this behavior, and deep levels have in fact been observed previously in InGaAsN grown by MOCVD. However, it has been unclear whether these levels are due to intrinsic sources (e.g. N-related) or to extrinsic sources (e.g. related to dopants, impurities in the precursor gases, etc.) To investigate the physical sources of deep levels in InGaAsN, we have used deep level transient spectroscopy (DLTS) to perform a comparative study of MOCVD- and MBE-grown InGaAsN. Three 1.05 eV n-type InGaAsN layers were studied. Two of the samples were grown by MOCVD and were doped with Sn and Te, respectively, and the third sample was grown by MBE and doped with Si. All three samples were subjected to post-growth thermal annealing. The majority-carrier DLTS spectra of the three layers exhibited a number of universal features. The first of these was a broad distribution of states located just below the conduction band edge, the presence of which is consistent with the predicted bandstructure of InGaAsN. A narrower distribution of states was present between 0.3 and 0.4 eV below the conduction band edge, and a deeper state exhibiting unusual capture kinetics

(thermally activated cross section, long saturation time) was observed at roughly 0.45 eV. Additionally, a minority-carrier hole trap was observed at approximately 0.35 eV above the valence band edge. The presence of these states in each of the three layers demonstrates that deep levels in InGaAsN are likely attributable to intrinsic, as opposed to extrinsic, sources.

9:15 AM F13.4

INJECTION OF POINT DEFECTS BY OXIDATION OF $\text{Al}_x\text{Ga}_{1-x}\text{As}$. D.R. Chamberlin, S.A. McHugo, D.R. Burke, T.D. Osentowski, and S.J. Rosner, Agilent Technologies, Palo Alto, CA.

Injection of point defects into GaAs/ $\text{Al}_x\text{Ga}_{1-x}\text{As}$ heterostructures by oxidation of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ is investigated. The blueshift of the PL emission from GaAs quantum wells is measured as a function of rapid thermal annealing conditions in as-grown and thermally oxidized samples. Contrary to published data for point defect injection by oxidation of GaAs, oxidation of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ appears to reduce the interdiffusion of the quantum wells, indicating that vacancies are not injected by the oxidation process, but are rather annihilated. The effect of Al concentration in the oxidation layer on the point defect injection is investigated.

9:30 AM F13.5

COMPARATIVE STUDY OF TRAP LEVELS OBSERVED IN UNDOPED AND Si-DOPED GaN. C.B. Soh^a, D.Z. Chi^b, H.F. Lim^a and S.J. Chua^{a,b}; ^aCentre of Optoelectronics, Department of Electrical and Computer Engineering, National University of Singapore, SINGAPORE; ^bInstitute of Materials Research and Engineering, SINGAPORE.

In this paper, the deep level defects in undoped and SiC doped GaN has been studied using digital deep level transient spectroscopy (DLTS). The alternative isothermal technique offered by the DL8000 system is used to complement the conventional temperature scan technique. Common trap levels at $E_c-E_t \sim 0.15\text{eV}$ and $E_c-E_t \sim 0.6\text{eV}$ were detected for both doped and the undoped samples. For the doped samples, additional trap levels at $E_c-E_t \sim 0.37\text{eV}$ and $E_c-E_t \sim 0.48\text{eV}$ was detected which we tentatively attributed to Si C related defects. The $E_c-E_t \sim 0.15\text{eV}$ trap level is believed to be related to nitrogen vacancy¹, V_N , while the trap level at $E_c-E_t \sim 0.60\text{eV}$ is probably associated with carbon or hydrogen that are incorporated into the methyl radicals of trimethylgallium (TMGA) during growth². The trap level at $E_c-E_t \sim 0.15\text{eV}$ shows an exponential carrier capture kinetic as expected for a point like defects. In contrast, the trap level at $E_c-E_t \sim 0.37\text{eV}$ and $E_c-E_t \sim 0.60\text{eV}$ exhibit a logarithmic capture behavior, indicating that they are probably related to extended like defects. The capture barrier heights were also determined for the trap levels identified. ¹Z-Q. Fang, J.W. Hemsley, D.C. Look, and M.P. Mack, Appl Phys. Lett. 72, 448, 1998. ²C.D. Wang, E.T. Yu, "Deep level defects in n-type GaN grown by molecular beam epitaxy", APL, 72, 1211-1214, 1998.

10:15 AM F13.6

THE ISOTOPIC DEPENDENCE OF THE RATE OF ELECTRON BEAM DISSOCIATION OF Mg-H COMPLEXES IN GaN. C.H. Seager, S.M. Myers, and B. Vaandrager, Sandia National Laboratories, Albuquerque, NM; J.S. Nelson, Uniroyal Optoelectronics, Tampa, FL.

Using infrared optical spectroscopy we have studied the effect of Low Energy Electron Beam Irradiation (LEEBI) on the stability of acceptor-hydrogen complexes in Mg-doped GaN. Mg-H pairs begin to break apart under 25 keV electron beam exposure at doses of a few mC/cm^2 . However we find that, even after long exposures, approximately 60% of the acceptor - hydrogen pairs appear to be unaffected by the electron exposure. By vacuum annealing and then re-charging some of our samples in D_2 or H_2 gas, we are able to show for the first time that there is a large (~ 5) isotopic shift in the beam-induced debonding rate of these acceptor hydrogen complexes. Preliminary measurements of this debonding rate as a function of the electron beam dose rate show little, if any dependence. Post electron-irradiation thermal annealing at 200°C causes the Mg-H(D) infrared absorption to return to as-received conditions, demonstrating that H and D remain in the material during electron beam exposure and move back to the acceptor site at quite low temperatures. Based on these observations and other data we suggest that the interstitial H_2 molecule is a logical candidate for the state of the hydrogen which is removed from the acceptor by an electron beam. The implications of these observations for understanding the nature of the debonding process and the competing H/D interactions in the GaN lattice will be discussed.

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-ACO4-94AL85000.

10:30 AM F13.7

ISOELECTRONIC DEEP TRAPS AND GIANT BANDGAP BOWING PHENOMENA IN III-V SEMICONDUCTOR ALLOYS. M.J. Seong, A. Mascarenhas, National Renewable Energy Lab., Golden, CO.

The novel properties exhibited by $\text{GaAs}_{1-x}\text{N}_x$ where it was observed that the incorporation of just 3% N reduced the band-gap by 400meV bringing it close to 1eV has thus generated a recent flurry of research activity because of the exciting possibility of fabricating very high efficiency solar cells as well as synthesizing VCSEL s for use in fiber optic communications based on a single step growth process on GaAs substrates. However, that incorporation of just 1% N into GaAs results in severe degradation of its electronic properties and so there has thus been an intense effort devoted to understanding the reasons for the giant band gap reduction and the poor transport properties of $\text{GaAs}_{1-x}\text{N}_x$. The mechanisms for the giant band-gap reduction and the abnormal conduction band effective mass have become the subject of extensive theoretical and experimental investigations. Quite an analogous situation exists for $\text{GaP}_{1-x}\text{N}_x$. The recent research in this area will be reviewed with respect to: Spectroscopic studies on the nature of the E_0 and $E_0+\Delta_0$ critical points using, photoluminescence, modulated reflectivity, resonance Raman, high pressure, and transport studies. Current models that have been constructed to explain the abnormal behavior of dilute III-V-N alloys appear inadequate for describing their unusual properties. It will be shown from experimental evidence that the reason for this is that $\text{GaAs}_{1-x}\text{N}_x$ and $\text{GaP}_{1-x}\text{N}_x$ are better described as heavy N isoelectronically doped semiconductors as opposed to dilute N containing alloys.

10:45 AM F13.8

DEFECTS IN SEMICONDUCTING DIAMOND: THE USE OF BLACK DIAMOND FOR ELECTRONIC APPLICATIONS. Oliver A. Williams, Richard B. Jackman, Christoph E. Nebel.

To date, black diamond has been considered a "thermal management grade" material not suitable for device applications. This paper demonstrates hall effect measurements on the hydrogen surface conductivity layer on numerous films of low quality black diamond. It will be shown that black diamond can yield mobilities comparable to that of white and even single crystal diamond when hydrogenated. Devices have also shown similar characteristics. This exciting and unexpected result has led us to question the nature of the defects that give rise to the black nature of this material. PL and CL results along with Raman and electron microscopy will be presented to show the near surface region of well faceted black material may not be as defective as expected. Moreover, photoconductivity of suitably treated black diamond films reveal strong UV conductivity with little apparent in the visible region of the spectrum. This is again an unexpected result and relates to both the inhomogeneity of the defects responsible for the blackness of the film and the influence that post growth film treatments can have on the defects within the surface region of these films. The implications for device applications are exciting, as black diamond is considerably cheaper than high quality polycrystalline diamond due to the significantly faster rate at which it can be grown. Substrate costs of only a few dollars can be envisaged. The impact of this on potential applications for diamond devices will be discussed.

11:00 AM F13.9

FORMATION AND PROPERTIES OF THREE COPPER PAIRS IN SILICON. S.K. Estreicher, D. West, Texas Tech Univ, Dept of Physics, Lubbock, TX; J.M. Pruneda, Univ. of Oviedo, Dept of Physics, Oviedo, SPAIN; P. Ordejón, Inst. de Ciencia de Materials-CSIC, Univ Autònoma de Barcelona, Bellaterra, SPAIN; S. Knack, J. Weber, Technical Univ of Dresden, Dept. of Physics, Dresden, GERMANY.

Copper is a feared contaminant in Si device processing. It diffuses quickly as an interstitial and forms electrically active precipitates which are difficult to dissolve. Several complexes assigned to copper-copper pairs have been observed by EPR, DLTS, and PL, but have yet to be unambiguously identified and fully characterized. We present the results of joint theoretical and experimental studies of different pair structures. The theoretical work involves ab-initio molecular-dynamics simulations. The results include the configurations, binding energies, electronic structures, local vibrational modes, and formation dynamics. Three distinct Cu-Cu pairs are found to be stable. The experimental studies combine DLTS, PL, and local vibrational mode (LVM) spectroscopy. One characteristic of the PL spectra is the presence of phonon replicas which implies low-frequency modes. Calculations reproduce the observed local modes and allow the identification of at least two of these complexes.

11:15 AM F13.10**DOPANT AND SELF-DIFFUSION IN EXTRINSIC N-TYPE SILICON ISOTOPICALLY CONTROLLED HETERO-STRUCTURES.**

H.H. Silvestri^{a,b}, I.D. Sharp^{a,b}, H. Bracht^c, S.P. Nicols^{a,b}, J.W. Beeman^b, J.L. Hansen^d, A. Nylandsted Larsen^d, E.E. Haller^{a,b}, ^aDepartment of Materials Science and Engineering, University of California, Berkeley, CA; ^bLawrence Berkeley National Laboratory, Berkeley, CA; ^cInstitut für Materialphysik, Universität Münster, Münster, GERMANY; ^dInstitute of Physics and Astronomy, University of Aarhus, Aarhus, DENMARK.

Dopant diffusion in silicon is mediated by interstitial silicon atoms and/or lattice vacancies. A Fermi level shift caused by extrinsic doping changes the concentration of native point defects that are charged and whose charge states are Fermi level dependent. We present experimental results of dopant- and self-diffusion in extrinsic silicon doped with the n-type impurities P, As, and Sb. Multilayers of isotopically controlled ²⁸Si and natural silicon enable simultaneous analysis of ³⁰Si self-diffusion into the ²⁸Si enriched layers and dopant diffusion throughout the multilayer structure. In order to suppress transient enhanced dopant- and self-diffusion caused by ion implantation, we adopted a special approach to dopant introduction. First, an amorphous 260 nm thick Si layer was deposited on top of the Si isotope heterostructure. Then the dopant ions were implanted to a depth such that all the radiation damage resided inside this amorphous cap layer. These samples were annealed for various times and temperatures to study the impact of P, As, and Sb diffusion and doping on Si self-diffusion. The Si self-diffusion coefficient and the dopant diffusivities for various extrinsic n-type conditions were determined over a wide temperature range. We observed increased diffusivities that we attribute to the increase in the concentration of the native defect promoting diffusion.

11:30 AM F13.11**SELF- AND DOPANT DIFFUSION IN EXTRINSIC BORON DOPED ISOTOPICALLY CONTROLLED SILICON MULTILAYER STRUCTURES.**

I.D. Sharp^{a,b}, H. Bracht^c, H.H. Silvestri^{a,b}, S.P. Nicols^{a,b}, J.W. Beeman^b, J.L. Hansen^d, A. Nylandsted Larsen^d, E.E. Haller^{a,b}, ^aDepartment of Materials Science and Engineering, University of California, Berkeley, CA; ^bLawrence Berkeley National Laboratory, Berkeley, CA; ^cInstitut für Materialphysik, Universität Münster, Münster, GERMANY; ^dInstitute of Physics and Astronomy, University of Aarhus, Aarhus, DENMARK.

Isotopically controlled silicon multilayer structures were used to measure the enhancement of self-diffusion in extrinsic B doped silicon. ³⁰Si was used as a tracer through a multilayer structure of alternating natural Si and enriched ²⁸Si layers. Low energy, high resolution secondary ion mass spectrometry (SIMS) allowed for simultaneous measurement of self- and dopant diffusion profiles of samples annealed at temperatures between 850°C and 1100°C. A specially designed ion-implanted amorphous Si surface layer was used as a dopant source to suppress excess defects in the multilayer structure. Self- and dopant diffusion coefficients, diffusion mechanisms, and native defect charge states were determined from computer-aided modeling, based on differential equations describing the diffusion process. Self-interstitials are known to be the dominant native defects mediating B diffusion at the annealing temperatures under investigation, but their charge states and individual contributions to Si self-diffusion have not been determined so far. We present a quantitative description of B enhanced self-diffusion in silicon and conclude that the diffusion of both B and Si is mainly mediated by neutral and singly positively charged self-interstitials under p-type doping conditions. Significant contributions of vacancies to both B and Si diffusion are not evident. The diffusion coefficient of B reduced to intrinsic conditions is in excellent agreement with corresponding data reported in the literature. This reveals that B and Si diffusion are not enhanced by transient diffusion phenomena which may be associated with the crystallization of the B implanted amorphous Si surface layer. Fitting of the simultaneous diffusion profiles of B and Si in the Si isotope structure yields accurate results not only for the enhancement of Si self-diffusion under heavy B doping but also for the temperature dependence of the individual contributions of neutral and singly positively charged self-interstitials to Si self-diffusion. The contribution of neutral self-interstitials is independent of the Fermi level, but B doping increases the contribution of singly positively charged self-interstitials, thereby enhancing Si self-diffusion. The sum of the individual contributions of self-interstitials to self-diffusion reduced to intrinsic conditions is in good agreement with recent results from self- and metal diffusion experiments indicating the overall consistency of our results.

11:45 AM F13.12**TRACE ANALYSIS OF COPPER IN SILICON USING TRANSIENT ION DRIFT IN COMBINATION WITH RAPID THERMAL ANNEALING.**

Thomas Heiser, Assia Bellayachi, Etienne Pihan, Laboratoire de Physique et Applications des Semiconducteurs, CNRS,

Strasbourg, FRANCE; Stephane Bourdais, Bachir Semmache, J.I.P. ELEC, Meylan, FRANCE; Armin Kempf, Peter Bloechl, Alois Huber, Wacker Siltronic AG, Burghausen, GERMANY.

Transient Ion Drift (TID) combined with a Rapid Thermal Annealing (RTA) process is shown to be a sensitive tool for detecting copper contamination of bulk silicon and silicon surfaces. A double impulse method is introduced in order to allow for the identification of TID signals with a high signal to noise ratio. The RTA system, which is used to indiffuse Cu during a high temperature step, is equipped with a fast cooling stage in order to keep the copper atoms interstitially dissolved and detectable by TID after the quench. Measurements are performed immediately after the quenching using a mercury probe as a Schottky barrier. Surface contamination of silicon wafers is done by spin-on of a copper contaminated solution and controlled by Total-X Ray Fluorescence measurements. A good agreement is obtained between the surface contamination level and bulk Cu concentration as measured by RTA/TID. A sensitivity of the order of 10^{11}cm^{-3} (or $5 \cdot 10^{10} \text{cm}^{-2}$) is reached, with a 0.8mm lateral resolution. Capacitance transients, originating from hole emission processes, are separated from copper drift induced signals by the response of the Schottky barrier to a double voltage pulse. This allows an unambiguous identification of the signal origin even at the lowest copper concentration and ensures the reliability of the method. Finally, a low temperature annealing is performed in order to induce copper precipitation or outdiffusion prior to TID measurements. It is found that subsequent RTA/TID analyses still allows the detection of the total initial copper concentration. The method is used to estimate the amount of trapped copper atoms and to study precipitate dissolution kinetics.