SYMPOSIUM F
Defect- and Impurity-Engineered Semiconductors and Devices III
April 1 – 5, 2002

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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, DDILTS, 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, nSi-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 & Measure 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

Chair: Hiroshi Okada and Mario Capizzi

Tuesday, March 4, 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. Inoue, H. Higayama, Y. Aoyagi, RIKEN (The Institute of Physical and Chemical Research), Saitama, JAPAN; A. Kinoshiba, Waseda Univ, Dept of Chemical Engineering, Tokyo, JAPAN.

Realization of high-conductive p-type GaN and AlGaN is important for optical and electrical devices using nitride compounds. Co-doping is proposed to get high hole concentration in p-type GaN and AlGaN. 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 TMGaN 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 alternate supply of TMGaN 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 TMGaN 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 the 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 TMGaN and NH3, Mg and Si cannot 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 cm-3. 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.


9:00 AM F1.2 CARBON DOPING IN MBE GROWTH OF WURTZITE AND ZINCBLENDE Gn. Rob Armitage, Henning Sieck, Qing Yang, Eike 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 MOVPE and MBE-grown GaN.

Secondly, intentional carbon doping has found practical application in the growth of high structural quality semi-insulating wurtzite GaN. Although p-type wurtzite GaN-Ch is not yet fabricated, several groups growing on GaN substrates obtained carbon-doped wurtzite GaN with exceptional p-type conductivity (~5x1017 holes/em3 and hole mobility ~100 cm2/V·sec). We study carbon-doped GaN thin films grown by CVD on indium-tinted MBE. Several gaseous dopant sources are investigated (carbon tetrachloride, carbon tetrabromide, chlorosilane, carbon disulfide) in a comparative study of incorporation efficiency, compensating impurities, and parasitic etching of GaN. Dopant studies of carbon with Mg, O, and As are also included. Several types of substrate (MOVPE GaN templates, sapphire, GaN, MgO) are
used 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
MICROSTRUCTURAL 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; Carine Fornes, 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 SiC-Si 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 nanocrystalline 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 modification 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 layers. The 2θ rocking curve of 0.14° was obtained from high-resolution x-ray diffraction, with an FWHM of 12.5 seconds. The smooth surface of GaN with roughness (rms) of 0.71 nm was obtained with growth on P-SiC substrate. The X-ray rocking curve FWHM of 1.3 arcmin for [012] and 1.7 arcmin for [102] diffractions were recorded for the two submonochromatic GaN films grown on P-SiC. Optical properties studied by photoluminescence at 15 K demonstrated an excitation peak FWHM of 14 meV, with high quantum efficiency and relatively low yellow luminescence. Growth mechanisms of GaN on top of the porous-SiC surface were suggested from TEM and AFM analysis.
MULTIPLE TUNERS IN ZnO SUBSTRATES. K. Theunke, N. Kerwer, A. Halbleibert, Paul Maguire, B. Thang, G. Grinter, A. V. Wohlgemuth, R. A. B. Khan, and H. G. Schaff, University of Ulm, Germany. 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 excitons at ~3.56 eV. Zeeman measurements allow the identification of the two strongest lines from two different lines in between as donor and acceptor. From the measured two-electron satellite line we determine the binding energy of the donor states. However, ZnO:Sn and ZnO:Cu exhibit ~30% with Cu:GaSe and can be doped easily, more than twice the dopant. Cu:GaSe is added to Cu-InSe, the doping becomes problematic, and the solar cell efficiency deteriorates. We find that this can convert these materials to n-type due to two possible mechanisms. (a) Our first step calculations show that interstitial hydrogen in both Cu-InSe and Cu:GaSe acts as a donor, yielding an enhancement also for conductivity type conversion. (b) Another explanation for n-type behavior is the generation of copper vacancies by hydrogen. We will show formization and lattice structure for H, H, and H in Cu-InSe and Cu:GaSe. We find that H goes into the Cu Se bond while H and H remain interstitial. Doping chalcogenides by hydrogen could be a new way to overcome bandgap.

THEORETICAL INVESTIGATION OF NITROGEN-DOPING EFFECT ON NATIVE DEFECT AGGREGATION PROCESSES IN SILICON. Hiroaki Kageyama, Akiko Takayama, Tatsuya Taguchi, NTT Basic Research Labs, NTT Corporation, Atsugi, Kanagawa, Japan; Kurumia War, Massachusetts Institute of Technology, Cambridge, MA.

Nitrogen-doping in Si has 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 growth. In order to shed light on the nitrogen-doping effect, we investigated interactions between nitrogen atoms and these native defects by using first-principles calculations with an ultracold 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 (N=V). This complex is very stable because all bonds of the N=V complex are strong 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 interaction with N=V 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 occurred 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 complexes based on first-principles calculations.
problem resulting from the non scaling of the transport time of electrons in conventional metal interconnects. The optimum approach is to exploit the movement of an efficient light emitting diode 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 E5.2
DEFECT ENGINEERING IN CCD IMAGE SENSORS

CCD image sensors provide an excellent example of the interaction of product to defects and the use of defect engineering to manipulate and control defects. Defect engineering for imagers starts with the epitaxial silicon layer chosen for the uniformity of its electrical properties. The underlying substrate can then be tailored to optimize the impurity and 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 or unregulated contaminants in the epitaxial and substrate film, which 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 on a p+ silicon 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 scheme. This may also be occurring. In these experiments, we measured iron level as low as $5E+7$ cm$^{-3}$ for an estimated gettering efficiency of 99.95%. The final iron concentration was not as low as expected from solubility arguments. We conclude 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 E5.3
TRAPPING AND DETRAPPING OF H IN Si: IMPACT ON DIFFUSION PROPERTIES AND SOLAR CELL PROCESSING
Bhaskar Sengupta, Yi Zhang, Robert Reed, Kim Jones, National Renewable Energy Laboratory, Golden, CO; N.M. Ravindra, New Jersey Institute of Technology, School of Physics, Computing & Mathematics, G. Sano, S. Ledean, School of Engineering, University of Surrey, Guildford, Surrey, UNITED KINGDOM.

Hydrogenation is used as a standard process step in fabricating all commercial silicon 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 studies to analyze 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 silicon substrates. These results allow us to 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 other processes. Diffusion profiles from these experiments 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 nitration, which is a very common process in the photonic industry. In this paper, we show that a model involving 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 E5.4
RADIATION HARDNESS OF AlGaN/GaN BASED HEMTs
S.A Virosicic, N. Klein, S.V. Danyluk, Forschungszentrum Jülich, Germany.

SESSION E5. DEFECTS IN DEVICES
Chair: S Ashok and Reinhard Job
Wednesday Morning, April 3, 2002
Sands 1/2 (Merrick)

8:00 AM E5.1
EFFICIENT SILICON LIGHT EMITTING DIODES MADE BY DIELLOCATION ENGINEERING: K.P. Kosek, M.A. Laurence, Wai Lok Ng, R.A. Frey, R. Sullivan, School of Physics, Computing & Mathematics, G. Sano, S. Ledean, 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 (Moores Law) beyond the next five to ten years. This is needed to overcome the fundamental interconnect
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 are very different sizes, 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 the effect of area variations but species migrating over large unirradiated 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 opto-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
SEM NANOSPECTROSCOPIC STUDY OF DEFECTS IN SEMICONDUCTORS. Koji Mueda, Akira Hida and Yutaka Men, 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 optical absorption spectrum of even a single defect embedded in the crystal with a spatial resolution as high as nanometer in scale. The method was applied in HEMsurface 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 photoluminescence spectral peak of the defect. Another scheme using a continuous light of variable wavelength was applied to midgap centers, supposed to be anemic amine defects, densely populated in low-temperature-grown GaAs epitaxial layers. 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 non-resolved 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.


10:45 AM F6.3
NITROGEN-STABILIZED H\sb{\sb{\gamma}} DEFECTS IN DILUTE GaN. A. Junge, S.B. Zhang, and Sh-Huai Wei, National Renewable Energy Laboratory, Golden, CO.

III-VN 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 H\sb{\sb{\gamma}} defect complexes in GaP. The H\sb{\sb{\gamma}} 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 local vibration modes for H\sb{\sb{\gamma}} are in very good agreement with the experimentally observed infrared spectrum.

11:00 AM AM F6.4
CHARACTERIZATION OF DEEP LEVELS IN 3C-SiC BY OPTICAL CAPACITANCE-TRANSIENT SPECTROSCOPY. Yohei Nishikura, Masahiro Kato, Masayoshi Ichimura, Eisuke Arui, 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 wafer warps can be produced at low cost. However, at the 3C-SiC/Si
interface, defects are generated due to differences in thermal expansion coefficient and lattice constant. The defects would be extended to epitaxial films and so the investigation of defects in micrystals 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 photoionization energy and optical cross sections for defect. The sample used in this study was a 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 experiment, we observed the resistance change caused by changing reverse bias under a monochromatic light with a constant photon flux. The energy range of the incident monochromatic light was from 0.5 to 2.5 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 N1 center, which was also observed by deep level transient spectroscopy (DLTS) and found to have a thermal activation energy of 0.3 eV. Localized electronic states with increasing photon energy up to 0.6 eV and then decreases with increasing photon energy. The apparent photon ionization threshold energy is about 0.45 eV, which is about 1.5 eV larger than the thermal activation energy. This difference is supposed to be the Frank-Condon shift.

11:15 AM P6.5

A room-temperature photoluminescence (PL) mapping technique recently developed by Hitachi has been exploited for characterizing a variety of features in C2 silicon. Here we present PL studies of oxygen precipitate-related defects (OPD), stress relaxation related defect localizations (SRD), and dopant distributions in various highly doped silicon materials. The sample consists of a variety of dopant species, and the dopant concentration range covers several 10^{19} cm^{-3} to several 10^{20} cm^{-3}. PL intensity in this dopant concentration range is controlled by three basic recombination mechanisms: radiation recombination competing with multi phonon Shockley-Rendel-Hall (SRH) and Auger recombination. In addition, certain enhancement of nonradiative recombination due to localized lattice disorder is observed. In the case of a highly boron-doped, precipitation annealed silicon, intentionally metal-contaminated samples with different OPD levels revealed a metastable PL spectrum with OPD density. For the relatively low diffuser ion, the PL intensity increased with OPD density. In this case, PL is primarily controlled by highly SRH recombination active Fe dissolvod in the silicon lattice, not by the OPDs themselves. Higher OPD density led to progressive gettering of Fe and therefore dopant distribution is 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 Fe dissolution but rather by metal impurities which are enhanced by metal contaminated 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 dopant distributions, and thermal and cold defects, such as SRD, and in the case of heavily doped silicon. This technique 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 devices processed Si wafers. Examples include SRD analysis and assessment of relative cleanliness of epitaxial silicon to device regions. The detected localizations originated either from misfit strain at epi interfaces or local stress as 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 micron. The impact of added deep-level centers (due to heavy metal doping) on SRD density is also observed. At present, the actual threshold concentration levels of specific metals where a contaminating defect (such as SRDs or OPDs) becomes detectable by PL remain unknown. Nevertheless, a reasonable relationship between relative cleanliness of silicon beneath certain defect structures and actual device yield could be established. In other words, the impact of epi misfit-related and diffusion-induced SRD density on device yield is illustrated.

11:30 AM P6.6

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

The improvement of low-cost photovoltaic cells based on multicrystalline silicon requires the identification of efficiency-limiting grown-in and process-induced microdefects in the solar cell material. This identification is then used to develop optimized conditions for defect removal and relaxation electrical characterization with chemical analysis. For this purpose, novel synchrotron radiation analysis has been developed, X-ray Beam Induced Current (XBC), that can be used to map the distribution of defects and lifetime limiting defects in solar cells. XBC 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 XBC 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 XBC. 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 cells, some extended metal clusters which also showed strong contrast in XBC maps did not have any detectable metal contamination. The role of metals in the enhancement of recombination activity of lifetime defects in Si solar cells will be discussed in detail.

11:45 AM P6.7
MULTI-MODEL PARAMETERIZATION OF POINT DEFECT PROPERTIES IN SILICON. Thomas Frenzel and Tadé Siono, Dept of Chemical Engineering, University of Pennsylvania, Philadelphia, PA; Erih Dornberger, Christian Hoess, and Robert Hoeld, Wacker Siltronic AG, Burghausen, GERMANY; Harmut Bracht, Institut für Metallforschung, University of Minster, Minster, 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 of the evolution of defects and dopants during silicon crystal growth and device processing continue to be only semiquantitatively 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 crystal growth, crystal structure, defect selfdiffusion measurements, and metal (atom) (diffusion) profiles in wafers. Ozchukhsky (C2) crystal growth experiments are performed with controlled varying pull rates, leading to complex transient behavior for point defect diffusion and metal diffusion 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 fitting of SRH and SRD experimental results is performed using Simultaneous 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 somewhat limited by the number of evaluations, especially for two-dimensional transient finite element models of C2 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, April 3, 2002
Salon 1/2 (Marriott)
1:30 PM F7.1
FUNCTIONAL Voids BY GAS ION IMPPLANTATION FOR

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APPLICATIONS IN SEMICONDUCTOR PROCESSING. V. Raineri and E. Rumi, CNR-IMM, Catania, ITALY.

Vooids in semiconductor crystals can be induced by gaseous ion implantation and annealing. Depending on the implanted dose, environment, and/or thermal budget, gas bubbles can be formed already in the implanted layers. The diffusion of gaseous atoms in silicon is mainly by thermal transport and/or evaporation from the surface. To be used in semiconductor processing for void formation should not introduce contamination and ensure both the required integrity and the required processing should be demonstrated. To date, void formation based on He ion implantation is the most widely and deeply investigated, and its utility will be demonstrated. Voids and bubbles can also be formed by ion implantation of different gases. The relative void/bubble formation will be briefly discussed. Applications of voids in semiconductors for device fabrication are for enhanced materials, improved device performance, or even as in situ sensor structures. Examples are SMART-CUT, self-gettering semiconductors, polycrystalline layers with high thermal stability, lifetime engineering, risk-free devices and sensors for interstitials. The specific application requires the right combination of ion implantation, 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

Cavities induced by helium implantation can have many applications including the gettering of metallic impurities. The thermal growth of these cavities is, however, under study. 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 can retard the thermal exodiffusion of helium while the process is slower for deeper implantation. 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 facetted and bigger than they are when 1.55 MeV is used. These differences are critically discussed. The described results are the first ones to allow us to better understand the way the cavities are created and to better understand the role of helium in the growth of cavities. 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 Peena, Jorges Kuschny, Reinhard Koegler, Wolfgang Sokurum, Forschungszentrum Jena, 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^{17} cm^{-2} and 2×10^{18} cm^{-2}. 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} cm^{-2} where the projected range of the implanted 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 min in order to study their behaviour. No visible cavities are formed in the He-implanted state after the He anneal. An anneal at 700°C for 30 min TEM micrographs of both the reference sample only with He implant and the sample with He implant and the previously formed cavities show no presence of a cavity formed in the He regions after longer annealing at 700°C for 60 min the reference sample shows no cavities while in the sample with the cavities is seen. The cavities are found to be located in the areas where the pre-existing defects are observed. TEM micrographs show that the cavities are located in 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 observed by the cavities formed in the cavities. If a pre-existing sink is trapped at the cavity surface an epitaxial growth can occur, and the empty volume shrinks. The pre-existing cavities are surrounded by the preferred sites for the interstitials. The pre-existing cavities can get the interstitials which in the reference sample are trapped in the internal surface of the cavities, and prevent the cavity disappearance.

3:00 PM F7.4
COMPARATIVE RAMAN AND TEM ANALYSIS OF THE EVOLUTION OF PLATELET DEFECTS IN PLASMA HYDROGENATED AND ANNEALED CZOCZORLISI SILICON. Reinhard Job, Alexander G. Ulyanin, Wolfgang R. Fahrner, Univ. of Hagen [LGBE], Hagen, GERMANY; Marie-France Beaumont, Jean-François Barbot, Univ. of Poitiers, Futuroscope Chasseneuil, FRANCE.

By Raman spectroscopy the formation of H^2 molecules in platelets and their evolution upon annealing were studied. Transmission electron microscopy (TEM) was applied for complementary investigations of hydrogenated 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 in air. H^2 molecules did appear only as newly formed species in plasma-implanted Si wafers [1]. Raman spectroscopy confirmed the appearance of the H_2 vibration modes exhibited significant intensity modifications in dependence on the annealing temperature for both p- and n-type wafers. 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 substrate regions of the treated samples. The conclusions from Raman spectroscopy was proved by TEM investigations. In case of p-type substrates the Raman intensities were significantly higher than for n-type material. The higher H_2 Raman intensities in n-type Cz Si can be explained by the empty volume next to the hydrogenation defects and the driving force for the hydrogen migration is lower. In p-type material the region over-saturated by hydrogen is wider, resulting in higher total number of defects and therefore background. The defects 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 IG IMPLANTED AND HYDROGEN PLASMA TREATED SILICON. Alexander Ulyanin, Reinhard Job, Wolfgang Fahrner, University of Hagen, Dept. of Electrical Engineering, Hagen, GERMANY; Anatoli Frolovskii, Belarusian S t Polytechnical Academy, Dept. of Electronic Devices, Minsk, BELARUS; Alexander Usenko, Silicon Wafer Technologies Inc., Newark, NJ.

The onset for surface blistering and exfoliation of thin layers at different temperatures were studied for n- and p-type Cz-Si implanted by He or He ions (100 keV doses 1E16 - 1E18 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 process is responsible for the onset of blistering for low-dose H_2 implantation and then hydrogen plasma treated samples. The complete layer transfer for silicon samples, joined to a supporting wafer was realized for low-dose implanted (~1E16 cm^{-2}) Si samples. It was found that 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.
CAVITY FORMATION IN SI-COVERED Ge ISLANDS
M. Kummer*, F. M. Ross, R. M. Tromp and R. Hall, University of Virginia, Department of MSE, Charlottesville, VA; IBM T.J. Watson Research Center, Yorktown Heights, NY.

In our ultrahigh 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 extended and self-assembled islands and the motion of defects such as dislocations during chemical vapor deposition carried out in the microscope polype. We are now applying this technique to the study of other self-assembled systems, including CNTs. 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 Ge island. The ability to control the location 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.

SESSION F8 POSTER SESSION
Chang-Juan Cho and S. Ashok
Wednesday, April 3, 2002
8:00 PM
Salon 1-7 (Merriot)

E8.1 IMPURITY EFFECTS ON THE DISLOCATION ACTIVITIES IN Si, Ichiro Yonemoto, 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 in such large diameter Si crystals 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 Okochi-dislocation 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 x 10^{16}cm^{-2} in comparison with those in undoped and O-doped Si crystals. Suppression of the generation of dislocations from surface scratch is found for Si doped with B, P and As to a concentration higher than 1 x 10^{16}cm^{-2} and the critical stress for dislocation generation increases with the impurity concentration, which is interpreted in terms of dislocation locking due to a density segregation. The velocity of dislocations in B, P and As doped crystals increases with increasing the concentration.

E8.2 INTRINSIC POINT DEFECTS AND OXYGEN INTERACTION IN HEAVILY DOPED SILICON, Pierre Liewen, Peter Werner, Norbert Engler, Gerhard Gerth and Ulrich Gosele, 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 [1]. As a result, a diffusion process at high C concentration causes a large self-interstitial (Si) generation. This behavior can lead to 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 heterostructures have been grown by molecular beam epitaxy (MBE) to investigate the corresponding influence of 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 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 basis of the simulations of diffusion.

E8.3 ELECTRICALLY ACTIVE BORON-HYDROGEN COMPLEXES IN IRRADIATED SILICON, Nikola Yarykin, Olga Fedkova, Inst. Microelectronics Technology NAS, Cherepovetsk, 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 irradiated 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 100 K. Creation of the new defects exceeds those of other prominent radiation defects and always follow the depth distribution of the pre-irradiated boron-hydrogen pairs. The new radiation defects are not detected in non-irradiated 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 was shown to reveal 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 rate and kinetics of the transformation of different silicon crystals with different contents of oxygen and carbon impurities. The possible reactions of irradiation-induced interstitial boron in silicon are discussed.

FS.4 HYDROGEN PENETRATION AND REDISTRIBUTION DURING AND AFTER CHEMICAL ETCHING OF SILICON. Nikolai Yarinskii, Oleg Fedorov, and Oleg Fedorov, Institute of Solid State Physics, Academy of Sciences of Ukraine, Chernogolovka, RUSSIA; and 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 diffusion of hydrogen in different charge states as a function of its interaction with other defects. It is established that the unknown conditions at the etching surface prevent the unambiguous determination of hydrogen diffusivity from the fitting of the simulated depth profiles to the final hydrogen 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 electrolysis 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 p-type silicon is much shorter than expected from the currently accepted structure of the energy levels of isolated hydrogen in silicon.


(111) Oriented silicon samples were implanted at room temperature with 1.55 MeV He+ ions in the dose range of 5x10^{15} to 5x10^{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 1x10^{16} ions/cm² and during subsequent high temperature annealing. The dislocation loops were moved and aligned away from the defect layer by the movement of He bubbles in the buried layer acting as the source 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 relaxation behavior 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 forming at high dose. The results are qualitatively discussed. Key words: silicon, He implant, XTEM, bubbles, dislocation loops, vacancy-like defects.

FS.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; Yoshiaki Iwasa, 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 study, we present data on the effects of hydrogen implantation on hole traps produced in p-type silicon by boron implantation which have been studied by deep level transient spectroscopy (DLTS). Schottky contacts were fabricated by evaporation of Ti on implanted surfaces for DLTS measurements. When a dose of 1x10^{16} cm⁻² is used, 4 hole traps with thermal emission activation energies of 0.21, 0.35, 0.46 and 0.55 eV. Subsequent hydrogen implantation was performed to a dose of 5x10^{16} cm⁻² at 80 K. The measured activation energies of 0.60, 0.90, 1.20 and 1.50 eV. 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 K boron implantation. The peak position of the 1x10^{16} cm⁻² in dependence for the trap (0.46) after boron implantation decreased to the concentration of 7.0x10¹⁰ cm⁻² after subsequent hydrogen implantation with the energy of 120 keV. This partial annealing is attributed to the reaction of precipitating 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, 1032 (1997).

FS.7 INVESTIGATION OF SUBSTRATE DAMAGE UNDER DIFFERENT MODES OF HYDROGEN PLASMA IMMERSON ION IMPLANTATION RICKY R. Paul, V. G. Y. 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-selected and focused in a well-defined hydrogen ion-energy distribution. Plasma immersion ion implantation (PII) 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 H⁺, H₂⁺ and H₃⁺ are formed in the plasma and co-implanted into the wafer, thereby causing not only broadened hydrogen ion-energy distribution but also different degree of surface damage compared to beam-line implantation. To compare the damage and defects created by hydrogen PII, we conducted experiments using three modes: (1) 30 mA short pulse PII, (2) 500 mA long pulse PII, and (3) current direct current PII. Dynamic secondary ion mass spectrometry (SIMS) is employed to determine the hydrogen depth profiles and surface doses. The crystal damage of the implanted samples is examined by grazing incidence X-ray scattering (GIXS). The SIMS results show that the DC mode yields the least crystal damage, followed by long pulse PII. 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 induced by ion-impact bombardment and atom displacement due to nuclear stopping near the substrate surface. Our data suggest that the DC PII mode is more preferred provided that there is sufficient surface cooling.

FS.8 PHOTOCARDED DISSOCIATION AND OPTICAL CROSS SECTION OF SiH AND SiH COMPLEXES IN GaAs AND AlGaAs. M. Barbe, P. Buly, J. Chevallier, Laboratoire de Physique des Solides et de Cristallinite, CNRS, Meudon, FRANCE; S. Sièvelre, D. L. Rodier-Bernard, L. Kurovskii, E. Constant, Institut d’Electronique et de MicroElectronique du Nord, CNRS, Villeneuve d’Ascq, FRANCE; M. C. Guillaud, Laboratoire de Spectroscopie Infrarouge et Rayonnement, CNRS, Université des Sciences et Technologies de Lille, Villeneuve d’Ascq, FRANCE.

The excitation of dopant 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 phenomenon is to find out efficient dopant activation 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 SiH complexes in GaAs at 300 K, as well as in H₂. Low energy bandgap illumination induces a much smaller dissociation effect. In this work, we present a determination of the optical cross section of SiH complex in GaAs for different wavelengths by modeling of the photon density dependence of the extrinsic carrier concentration induced by illumination in the range 1x10¹⁶ cm⁻², 1x10²² cm⁻² of.
photon densities. The sheet carrier concentrations have been measured either by Hall effect and conductivity experiments or by Hennan, scanning 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 unbinding state of Si-H bonds in GaN. We also show that a UV induced dissociation of Si-H and Si-F complexes occurs in AlGaNs and in 2D AlGaNs-GaN 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 empty states as the excess energy is re-emitted. In AlGaNs and in 2D AlGaNs-GaN heterostructures, the replacement of hydrogen by deuterium in the complexes shows that the Si-D and Si-F complexes are significantly more stable than the Si-H and Si-F complexes as previously found in GaN Si-H.

**P8.9**

**INFLUENCE OF HIGHLY DEFECTED 4 LAYERS ON P-N STRUCTURE PROPERTIES.** B.S. Skokovskii, V.K. Pyusvetovskii, R.M. Kovtun, Ivan Franko National Univ., Dept. of Physics, Lviv, UKRAINE.

It has been developed an analytical model describing the influence of highly defects 4-layers located in the base region of p-n structure on reverse branches of current-voltage characteristics. The highly defects 4-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 defect 4-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 monotonically 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 defect 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.

**P8.10**

Abstract Withdrawn.

**P8.11**

**DEEP LEVEL STUDY IN EPITAXIAL 4H-SiC GROWN ON SUBSTRATES INCLINED TOWARD \( < 11 \theta > \).** Masahide Kata, Masayoshi Inoue, Nisshin Electro-Engineering, Nisshin Electro-Engineering, Nagoya Institute of Technology, Dept. of Electronics and Information Science, Nagoya, JAPAN, and Nisshin Electro-Engineering, Nisshin Electro-Engineering, Nagoya Institute of Technology, Dept. of Electronics and Information Science, Nagoya, JAPAN.

4H-SiC epitaxial layers are generally grown on (0001) face substrates inclined toward \( < 11 \theta > \) direction. Recently, it has been reported that good epitaxial layers can be grown even on substrates inclined toward \( < 11 \theta > \) 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 \( < 115 \theta > \) and \( < 11 \theta > \) directions by the cold wall chemical vapor deposition method. Source gases were SiCl, Ar, and H, with H, 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 annealed in order to form the ohmic contacts. The Au was evaporated on the Si face of the Schottky contacts. From the capacitance voltage (C-V) measurements of the samples we have donor concentrations of 3 x 10^15 cm^-3 and 3 x 10^15 cm^-3. The 6 μm thick sample 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 donor of 10^15 cm^-3 and 10^15 cm^-3, and the sum of the deep level concentrations is of order of 10^15 cm^-3 by 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 less than 10^15 cm^-3, which is in the 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.

**P8.12**

**INFLUENCE OF SUBSTRATE SURFACE MORPHOLOGY ON DEFECT GENERATION DURING SILICON CARBIDE SINGLE CRYSTAL GROWTH.** Myeong Yoon Um, Joe Kyeong Jeong, Bum Soon Kim, Hoeon Ju Na, In Rek Seng, and Hyoeng Joong 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 have focused our efforts on getting a better understanding of substrate preparation and 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 gluing 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 Raman and MOKE characterization. The 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 0.25μm diamond paste showed uniformly distributed small scratches with RMS roughness of 10.8Å while substrate polished by 6 μm diamond paste had nonuniformly large scratches with RMS roughness of 66.7Å. 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 0.25μm diamond paste and by 6μm diamond paste, mounted side by side. The SiC grown on a substrate polished by 0.25μm diamond paste had a edge/screw dislocation density of 6.1 x 10^5/cm^2 without microstip. The edge/screw dislocation density of 7.3 x 10^5/cm^2 without microstip. On the other hand, the SiC grown on a substrate polished by 6μm diamond paste had an edge/screw dislocation density of 5.1 x 10^5/cm^2, two orders of magnitude lower than the hydrogen etched sample and four microstip in this sample.

**P8.13**

**NiSi:ION BEAM MIXING INTO SiC FOR STABLE LOW TEMPERATURE OHMIC CONTACT.** A.M. Elezadny, D. Iba, R. Zimmerman, M. Vora, J.J. Weimer, J.K. Byrson, J.D. Demnenci.

We have used Ion Beam Mixing in introducing a Nickel-Silicide NiSi) in Silicon Carbide substrate. Formation of Nickel Silicide NiSi) is investigated as possible ohmic contacts to high temperature n-type 4H-SiC and p-SiC. 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 (NiSi). We enhanced the ohmic property by electron gun evaporation of (NiSi) on the Substrates surface. SIMS code was used to predict the depth of the Ion Mixing zone. The (NiSi) contacts were formed at room temperature by Rutherford Backscattering Spectroscopy (RBS) and Auger Electron Spectroscopy (AES) were used for depth profiling of the (NiSi), Si, and C X-Ray Photoemission Spectroscopy (XPS) was used to study the chemical structures of the (NiSi)/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.

**P8.14**

**Transferred to F9.7**

**P8.15**

**HEAT AND FIBER STUDIES OF SILICON CARBIDE SUBSTRATE DAMAGED BY HEAVY ION IMPLANTATION.** Claudia L. Muntele, Julia C. Muntele, Darusha Isb., Center for Irradiation of Materials, Alabama A&M University, Normal, AL; David M. Pocker, Dale K. Hendry, 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 radiation recovery after annealing in a high purity argon environment between 600 and 1600°C. We implanted silicon carbide with 30 and Au ions at levels between 1014 and 1016 ions/cm2, and used micro-Raman and FTIR techniques for investigating the lattice parameters and stess states 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 exclude the possibility of using 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 were stable in a broad range of temperatures, and, since the signal is less uniform than in the case of deposited sensors, because the p-n junction created by ion implantation has a lower 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 in this major study. Research sponsored by the NASA Grant No. NSG2392, and partially by the Center for Irradiation of Materials at Alabama A&M University and U.S. Department of Energy under contact DE-AC05-00OR22725 with the Oak Ridge National Laboratory, managed by UT-Battelle, LLC.

PS.16
CHARACTERIZATION OF SILICON CARBIDE IMPLANTED WITH EITHER B OR AI USING THERMAL ADMITTANCE SPECTROSCOPY. S.R. Smith, M.A. Capone, A.O. Enevage, 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+ epilayers. The implantation plus annealing produced p-type layers that were acceptable for characterization. The specimens were annealed at 900°C, 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 proceeded. Some of the specimens showed bandbending, which 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 AI. From this, we conclude that at least one shallow donor level is introduced into the bandgap by implantation damage. Further, more defects associated with these shallow levels may affect the device performance by interfering with the lattice occupation of the implanted species, and limit the lifetime of the carriers.

PS.17
OPTICAL METHODS FOR DEFECT CHARACTERIZATION IN LIGHT ION IMPLANTED SILICON CARBIDE. J. Muntele, Chaiu I. Muntele, Doru V. Ciobulea, Center for Irradiation of Materials, Alabama A&M University, Normal, AL. James Thompson, Department of Chemistry, Alabama A&M University, Normal, AL, David B. Baker, Dale K. Henley, 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 (AI doped) and n-type (Ndoped). Conventional Micro-Raman (MR) and Fourier Transform Infrared (FTIR) techniques have been used for monitoring the structural properties of amorphous silicon (380 to 540 cm⁻¹) and carbon (1300 to 1600 cm⁻¹). Broad peaks in some of the regions because of silicon and carbon atoms relocated as interstitials, transforming into a locally stressed crystalline lattice. The locally relaxed lattice of the amorphous carbon- and silicon-terminated regions also suggests a broadening of the characteristic Raman peaks of each type of material (976, 797, 789, and 767 cm⁻¹ for 6H silicon, and 965, 748, and 726 cm⁻¹ for 4H). Furthermore, if any of the oxygen vacancies in the other then a shift of the peak towards higher or lower wave numbers is observable. UV/VIS Optical Absorption (OA) Spectroscopy has also 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 will be collected from virgin samples, as implanted, and after annealing at various temperatures between 500°C and 1600°C. MR and FTIR spectra, and EPR results will be presented. Simulated vacancies, primary and secondary ionisations 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. NAG1-2123. 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.

PS.18
ELECTRICAL CHARACTERIZATION OF LASER-IRRADIATED 4H-SiC WAIFER. L. Salhah, School of Optics/CREOL, Department of Mechanical, Materials, and Aerospace Engineering, University of Central Florida, Orlando, FL; H. Quick, Quick 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 ablation write technique. The substrate and interstitial sites are governed by reactions that transfer the solute from one site to another. Highly ordered compounds, has been shown using the law of mass action that, in the absence of interactions among defects and solutes, sites fractions of solutes are not only by energies of the solute and the various sites but also by concentrations of intrinsic elementary point defects (vacancies, interstitial 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 a substitution or Schottky defect formed by removal of a removal unit of the compound, leaving behind vacancies. As a consequence, simulation of such 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 with none possible by structure 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 neighbour interaction models. – This work was supported in part by the NSF under grant DMR-0129101. [1] Gary S. Collins and Matthew O. Zucarre (submitted.)

PS.19
PASSIVATION OF THE NATIVE POINT DEFECTS IN LOW-TEMPERATURE-GROWN GaAs. V. V. Chkhalovsky, A.E. Kunytsyn, D.A. Vasyukov, Ifo Institute, St. Petersburg, RUSSIA; V.A. Kaganov, Research Institute of Semiconductor Devices, Tomsk, RUSSIA; D.I. Frolov, Institute of High Current Electronics, Tomsk, RUSSIA; V. V. Prechker, Institute of High Current Electronics, Tomsk, RUSSIA; A. B. Sevminyan, 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 × 10¹⁸ cm⁻². These deep donors are 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 intentionally doped with Si or Be. The treatment in atomic hydrogen was performed at various temperatures and with different durations. Two main phenomena have been observed, which are essentially correlated with hydrogenation. The one of them is the 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.

PS.20
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. Morco, Virginia Commonwealth Univ., Richmond, VA; J. Name, Getir, Inc., Atlanta, GA; Gene Cantwell, Electronic Design Tecnoologies, LLC, Mimi, OK; H. Paul Manski, CPT Crystal Photonics, Inc., Sanford, FL; C.W. Litton, Air Force Research Laboratory [AFRL/MLPS], Wright Paterson 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 high-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. Sapphire is a growing 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 our investigation we investigated several 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 on a thickness of film in the temperature range of 610–650°C, on SiC, ZnO (0-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 demonstrated the chemical etch front for growth on ZnO and LiGaO₂. X-ray rocking curve measurements showed the best FWHM for GaN films to be 0.02°, and that for GaN films grown on SiC, Preliminary photoluminescence measurements at 15K showed the FWHM’s 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.  

FS. 22 CORRELATION OF SURFACE MORPHOLOGIES WITH MC COMPOSITION OF GaN 

FS. 23 PROBING THE ALLOY DISTRIBUTION IN Al₀.₃ Ga₀.₇ N 

FS. 24 EFFECT OFAlUMINUM COMPOSITION ON EXTENDED DEFECTS IN Al₀.₃ Ga₀.₇ N 

FS. 25 THE EFFECT OF DISLOCATIONS AND DEFECTS ON THERMAL CONDUCTION IN GaN FILMS
structural materials for fabricating those devices above. Employing low pressure metalorganic chemical deposition, Si- and In-doped GaN/AlGaN MQWs with well (MQWs) and In-doping levels, respectively, have been grown. Photoluminescence (PL) measurements have been performed on Si- and In-doped GaN/AlGaN MQWs in the temperature range of 77–300 K. In these two kinds of doping, there were 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.

**FS.27**

**INTEGRATION AND HIGHLY DOPED GA**

**N AN P-TYPE HETEROEPITAXY**


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 splitting 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 the concentration of active Fe atoms into the lattice; in order to reduce the damage production and avoid Fe-defect reactions we heated the substrate at a temperature \(T \geq 200^\circ\text{C}\) before the implantation. With this method local electrical compensation and semi-insulator formation in substrates with n-type 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-channelling 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 \(^\circ\text{C}\) 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.

**FS.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 semiconductor materials. We have investigated the Raman scattering in Be-implanted GaN epilayers. (a) In Be implanted GaN, the Raman bands at \(\approx 310\), \(\approx 350\), \(\approx 370\), 660 cm\(^{-1}\) appeared. From phonon dispersion curves for hexagonal GaN, the \(\approx 310\) cm\(^{-1}\) and 660 cm\(^{-1}\) bands were assigned to the highest acoustic-phonon branch and the optical-branch, respectively. Comparing with Raman spectra from GaN sample implanted with other species, such as Mg and C ions, we discuss the origins of the \(\approx 350\) and \(\approx 370\) cm\(^{-1}\) peaks. (b) Two sharp bands at \(118\) and \(199\) cm\(^{-1}\) were observed in Raman spectra of Be-implanted GaN after post-implantation annealing treatments. We attentively assign these two bands to Be-related local vibrational modes.

**FS.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 density of the defects depends on the ECR gas type, sample 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.

**FS.30**

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

The addition of indium to the 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 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 Pb Te single crystals, grown in the Cadmium Telluride technique: (a) p-type PbTe, doped with 1 \(\times\) 10\(^{16}\) \text{ cm}^{-3}, (b) offstoichiometric 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 vacancy centers 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 anneals) was determined using a photoluminescence technique, whereby the location of the change of sign of the Seebeck coefficient is determined within a resolution of 0.1 \(\mu m\). 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\(^\circ\text{C}\) 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: \(D_x = \text{exp}(E_d/k_B T)\) with \(E_d = 1.4\pm 0.1\) eV, \(D_x = (9.21) \times 10^{-9}\) cm\(^2\) s\(^{-1}\). The effective diffusivities of In in PbTe(Na) are lower by a factor of 20 at 25\(^\circ\text{C}\) and 2 in the range of 25 to 200\(^\circ\text{C}\) with a similar decrease in 0.1 eV. 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 Pb lattice sites in offstoichiometric PbTe with excess Te.

**FS.31**

**NATIVE DEFECT FORMATION AND IONIZATION ENERGIES IN CdMnTe TELLURIDE.** John E. Jaffe, Mary Blas, 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 electron structure calculations, these features have been attributed to the second ionization level of the Cd vacancy, while the Te vacancy, possibly combined 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 vacancy 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 this 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.

**FS.32**

**BEHAVIOR OF COPPER IN CdGeAs\(_2\), CRYSTALS.** Volodya G. Vorobiof, Olga V. Vasilenko, Svetlana A. Berezhnoya, Zoya V. Korotchenko, Siberian Physico-Technical Institute, Tomsk, RUSSIA; C. Gomer, Jonathan T. Goldstein, Nils C. Berringa, 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 CdGeAs\(_2\). Cu was found to be an acceptor, its introduction in the melt controlled the introduction of holes into CdGeAs\(_2\) with a rate of 10\(^{16}\) cm\(^{-3}\) to -1 \times 10\(^{18}\) 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\(^\circ\text{C}\) to 600\(^\circ\text{C}\), obeying the equation \(N_s = N_0\text{exp}(-\Delta H/kT)\) with the parameter \(N_0 = 6 \times 10^{15} \text{ cm}^{-3}\), \(\Delta H = 0.3\) eV, and \(k\) is the Boltzmann constant. From 600\(^\circ\text{C}\) to 650\(^\circ\text{C}\), the saturation solubility was found to shape decrease exponentially with temperature.

**FS.33**

**CONTROL OF VALENCE STATES FOR ZnO AND ZnS WITH A WIDE-BAND GAP BY A CO-DOPING METHOD.** Tetsuya Yamamoto, Kode Univ. of Technology, Dept of Electronic and Photonic Engineering, Kode, 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-structure calculations, and the thermal properties which is characterized by using the solid compounds, Zn$_2$N$_2$. Nitrogen doping gives rise to localized impurity states at the top of the valence band for ZnO and ZnS while it causes a delocalized states for ZnTe. Hole in the narrow bands for ZnO and ZnS are localized and regulations in the Madelung energies for the three N-doped semiconductors are found to be increased. For ZnTe, based on the calculation 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 enthalpies between the materials and the Zn$_2$N$_2$ 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 in a donor concentration. The delocalizing effect of the donors is essential for the delocalization of the impurity states as 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-play because acceptors activate p-type, i.e., the reactive co-dopant. Based on theoretical calculations, Ga or Al species is suitable for the use as reactive co-dopants for ZnO and Ga or In for ZnS. We will discuss the experimental data of the two semiconductors.

FS.34 PERTURBATION OF COPPER SUBSTITUTIONAL DEFECT CONCENTRATIONS IN CdS/CdTe HETEROJUNCTION DEVICES. D. Aliev, T. Osepchenko, V. Abiyan, A. Asher, and S. Johnston, National Renewable Energy Laboratory, Golden, CO.

The efficiency of implementing terrestrial-based photocell artisans is dictated by trade-offs in device performance, cost, and reliability. Presently, the highest efficiency polycrystalline CdS/CdTe supercell solar cells utilize backcontacted copper as an intentional dopant. Accelerated stress data correlates copper diffusion from this contact with performance degradation. The use of nitro-phosphoric 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 (E_C + 0.28 to 0.34 eV). These levels are believed to be associated with Cu$_2$ substitutional defects and are localized in the vicinity of the backcontact.

FS.35 LASER ENGINEERING OF BARRIER STRUCTURES BASED ON SOLID SOLUTION ZnCdHgTe. Galina Khlypay, State Pedagogical University, Drohoby check, 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 COS-laser radiation on the practical 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 textellated structure observed on the as-grown samples. The detailed numerical analysis of the experimental measurements and morphodynamic investigation which is the formation enthalpy of 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.


The role of imperfections on the initiation and propagation of buckle driven deformations 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 Atomic Force Microscopy (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 results for the effect of imperfections on the energy release rate.

FS.37 FIRST-PRINCIPLES SIMULATION OF HYDROGEN INTERACTION IN AMORPHOUS SILICON NITRIDE. Peter Krull, 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 β-Si$_2$N$_4$ and the crystal phase Si$_3$N$_4$.A thin film between N-H bond vibrations at surfaces and in the bulk shows that within the bulk the frequency of N-H bond stretching (≈ 3000 cm$^{-1}$) is considerably lower than at the surface (≈ 3300 cm$^{-1}$). We attribute this decrease of the force constant for this vibration to secondary interaction through space of hydrogen with nearby interatomic hydrogen. This influence is also responsible for the asymmetric peak shape. Casimir-Polder molecular dynamic simulations at elevated temperatures showed hopping of bulk hydrogen between typically two binding sites. Moreover, the preferential migration of hydrogen atoms occurs through interaction with adjacent N atoms.

FS.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 (COSD&F) & Department of Physics and Materials Science, City University of Hong Kong, Hong Kong SAR, CHINA; U. Gosede, Max-Planck-Institute of Microstructure Physics, Halle, GERMANY.

Experimental results showed that most silicon nanowires (SNW) grown using Si monoxide source materials are oriented in the (112) direction, some in the (110) direction, but hardly any in the (100) or (111) directions. These SNW growth directional features may be understood by considering 4 mechanisms based on criteria that concerns with the stability of 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 dislocation in providing [111] surface steps. Analyses of SNW growth in accordance with these criteria showed that <112> and <110> are the preferred SNW growth directions, but <111> and <100> are not.

FS.39 SIEN RELAXATION AND DISLOCATION DENSITY OF SiGe FILMS IN MICRON SIZE WINDOW WITH DIFFERENT MASK MATERIALS GROWN BY MBE. Xiang-ju Zhang, Hai Xiong, Jihang Hu, Zuming Jiao, Yangfang Fan, Dongzhi Hu, Jun Lin, Yong Chen, Surface Physics Laboratory, Fudan University, Shanghai, P.R. CHINA.

Many authors reported that for heteroepitaxial growth the misfit dislocation density in thin film is proportional to the strain relaxation and the dislocation density of the SiGe films in microns sized 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$_3$N$_4$ and the combined mask made by SiO$_2$ andSi$_3$N$_4$ films. Si$_3$N$_4$Ge$_2$ films of 298 nm 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 affected by the window size and the mask. 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 30x20 μm$^2$ 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 30x30 μm². For the samples with different mask materials but same mask windows, the strain relaxation and the strain 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 SiN₄ mask was highest, and that in the windows of combined mask was the lowest. Annealing effect for these samples was also studied. Samples were annealed successfully at 620°C, 670°C, 720°C and 870°C for 30 minutes. The strain relaxation and the dislocation density in the SiGe films grown on Si were increased greatly but that in the SiGe films in the windows of 3x3 μm² was less changed. Especially for the sample with the combined mask material of SiO₂ and SiN₄ 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.

**FS.40**

**THE ROLE OF INTERFACES IN THIN FILM SOLAR CELLS.**


Thin film (LiV) 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 Cu(In,Ga)Se₂ solar cells fabricated by the three-stage process. Although these developments are very promising, further improvements in device efficiency will require a deeper 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 I-V and II-VI thin films exhibit grain boundaries, which might be understood as homointerfaces. Heterointerfaces such as CuTe/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 discuss the role of both internal and external interfaces in the functionality of thin film solar cells. For CuTe/CdS, a detailed study of the effects of grain boundaries and the Te/CuTe or ZnTe/CdTe/CdTe interfaces for back contact have been conducted. On the other hand, for Cu(In,Ga)Se₂ 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 interface is indeed critical in the definition of the mechanisms for carrier collection.

**FS.41**


Polycrystalline silicon thin film transistors (poly-Si TFTs) crystallized by reactive ion etching method; amorphous (ELA) of [100], [110] are promising devices for active matrix displays (AMOs). 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 ion-polycrystalline TFT with large lateral grain 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 laser annealing of active silicon film. The crystallization of Si and the doping activation were simultaneously accomplished by single ELA process. We have observed 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 of magnitude compared to conventional poly-Si TFT with small grain boundaries and residual implantation damage at the drain junction. The proposed poly-Si TFT, of which mobility is over 170cm²/Vs, exhibits a large on/off current ratio exceeding 4 × 10⁶ 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.

**FS.42**

**STUDY OF E-RELATED DEFECTS IN n-Si:H FETs USED IN LIGHT-PICTIONION HETEROSTRUCTURES.** A. Narendra, J. Uslick, V. Lysenko, Institute of Semiconductor Physics, NASU, Kyiv, UKRAINE; O. Konev, E. Terentev, 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 the performance degradation of hydrogenated amorphous silicon films used in crystalline-aminosilicon hydrogenated (a-Si:H) light emitters. The n-Si:H/Fet films were deposited on Si by chemical vapor deposition (CVD) or magnetron deposition (MASD). The defects were evaluated by thermally stimulated current spectroscopy (TSCS) and high-frequency (1 MHz) capacitance-voltage (CV) characteristics measured at 77K. For charging of the traps, visible light illumination was used at high temperatures and thermal bias stress at high temperatures. Observed TSC spectra display no dependence on the film growth technique, and no signal came from the material. The origin of the observed deep levels at high temperatures is discussed.

**FS.43**

**LOW-TEMPERATURE PROPERTIES OF COMPENSATED GE FILMS USED FOR CRYOGENIC THERMOMETERS.** V.F. Mitin, V.V. Khlopkov, Inst of Semiconductor Physics, NASU, Kiev, UKRAINE; V.K. Dugan, M. Vieira, Dept of Electronics and Communications, STL, Lisbon, PORTUGAL.

Ge films are obtained by thermal evaporation of Ge in vacuum on semi-insulating GaAs substrates, and the temperature microscopes 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 dependencies 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 strong dependence on both temperature and magnetic field at ultralow temperatures. At T ≤ 0.5K the magnetoresistance is small and positive over the whole range of applied fields. At lower temperatures the magnetoresistance is negative. At T ≤ 0.1K, 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 have made the scaling theory of localization, matching the 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 and magnetic field dependencies 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.

**FS.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 nano crystalline carbon (n-c-S) thin films grown on molybdenum substrates by hot-flamelet chemical vapor deposition (HFCVD) techniques from methane-hydrogen (CH₄/H₂) and sulfur-hydrogen (H₂S/H₂) gas feedstocks. All of the films were grown for 24±0 minutes and the thicknesses were around 0.5 microm. The structural bondings in thin films are studied as a function of substrate temperature [500-900°C] and sulfur concentration (10-500 ppm of H₂S) 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, fullwidth at half maximum 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 to a network. The in-plane correlation length $L_c$ which is related to the D band intensity is also a function of both substrate temperature and sulfur concentration and found to decrease with increasing both the process variables. The XPS Cls 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 S$_2$ and AFM results support the conclusions drawn on the losses of RS and XPS investigations. This is a new and important development in engineering the carbon-based material through defects and impurity incorporation as visible cold cathodes.

SESSION F9: HYDROGEN-DEFECT INTERACTION WITH SEMICONDUCTORS

Chairs: Noble M. Johnson and Jacqueline P. Chevalier
Thursday Morning, April 4, 2002
Session 1/2 (Marriott)

8:00 AM *F9.1
HYDROGEN PASSIVATION AS A TOOL TO ENGINEER PROPAGATION COUPLED Circuits ON InP, E.V.K. Rau, B. Theys, and B. Theron, "CNRIS/SP, Bignoux, FRANCE, "CNRIS/LPSM, Meudon, FRANCE, "OPTO+ALCATEL, Massy, FRANCE.

The photonic circuits (PCs) 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, V junctions, etc.) monolithically integrated on one common 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 present 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 particularly 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.

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 transition (IVBT). In the second part, the optical and electrical properties of deliberately hydrogenated p-InP and InGaAsP/InP double heterostructures (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 multiplexing) 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 which 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 crystal. Hydrogen effectively passivates point defects acting as nonradiative centers but not dislocations. On the other hand, point defects due to hydrogen incorporation may not yield 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 released centers produce a broad emission around 540 nm in wavelength. Since homoeptaxial diamond films are usually grown in hydrogen plasma enhanced chemical vapor deposition, hydrogen is incorporated in the subsurface region of the films. Such hydrogen is not only not a nonradiative center but also a further emission from 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, UK, FEDERICK M. HOGG, C.P. Ewels, C.PES, University of Southampton, Palmer, Brighton, UNITED KINGDOM PR. Bridgdon, Department of Physics, University of Newcastle upon Tyne, Newcastle upon Tyne, UNITED KINGDOM S. Oberg, Department of Mechanics, 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 intention is given to the single isolated species, hydrogen dimers and complexes with important donors, acceptors and extended defects. It is found that H$_2$ is highly mobile and H$_3^+$ is the most stable dimer. Hydrogenation in bulk diamond is readily trapped by B, N and P. We assign the 31.07 cm to a N-H pair. The role of surface hydrogenation with regards to the presence of surface hole conduction in diamond is also discussed.

9:30 AM *F9.4
REVERSIBLE NITROGEN PASSIVATION BY HYDROGEN IN III-N COMPOUNDS, M. Capigari, A. Polimeni, G. Balandari H. R., M. Biazzii, A. Augeri, INFM and Dept. of Physics, U. of Rome I, Rome, ITALY; A. Amore Bonnafous, CNRS-CNAM, Monterotondo, ITALY; Fen Jinjin, M. Stewa, Dept. of Physics, Lehigh Univ., Bethlehem, PA; M. Fischer, A. Forchel, Universit"at W"urzburg, Technische Physik, Würzburg, GERMANY.

Hydrogen is present in most of semiconductors growth and device processing and, because of its high diffusivity and strong chemical activity, it may simply 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 (In,Ga)As at 4K and GaN 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 $y < 0.01$, photo-luminescence lines due to exciton complexes are fully quenched under hydrogenation; (ii) in the alloy limit ($y < 0.01$) and for increasing H dose, the (In,Ga)As 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 (In,Ga)As 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 was pre-irradiated. The samples were analyzed by thermally annealing the samples. These results are the first example of H as an isoelectronic impurity. They highlight the strong point character of the N wavefunction maintained in (In,Ga)As for values of yN 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 (In,Ga)As. This suggests a mechanism for N-H bond formation by H. Finally, preliminary results on the H irradiation show on other isoelectronic systems, as GaP-N and Zn(Se), will be presented.

10:15 AM F9.5
DOPING OF OXIDIZED FLOAT ZONE SILICON BY THERMAL DONORS - A LOW BUDGET BUDGET DOPING METHOD FOR DEVICE APPLICATION, Robert J.W. Lea, Alexander G. Uyeda, Wolfgang R. Fahlman, Univ. of Hamburg (THB), Hamburg, GERMANY; Eddy Simoen, Cor Cleva, IMEC, Leuven, BELGIUM; Franz-Josef Niedermeier, Hans-Joachim Schulz, Infineon AG, Munich, GERMANY; Guido Tonelli, IFN, Pisa, ITALY.

Hydrogen enhanced formation of thermal donors (TDs), i.e. oxygen related voids) TDs, can be observed in Czochralski [Cz] silicon after annealing in a plasma hydrogenation at 250°C (60 min), and subsequent annealing at 540°C in air for (15 min) [1]. By such processes deep p-n junctions were created in p-type Cz Si wafers due to counter doping
by T0Ds [1]. In the present study TD formation was studied also in oxygen
enriched high resistivity float zone (FZ) silicon. Such substrates are used to study long
lived defects and bulk volume effects. RF plasma hydrogcnation (110 MHz, 50 W) was
carried out at 250°C for 1 h. Subsequent annealing was done at 450°C for up to 5 h.
The plasma treated and annealed oxidized FZ Si samples were analyzed by
scanning resonance luminescence (SRL), C-V measurements and Raman
measurements. Also Raman measurements and scanning
electron microscopy were applied for the analysis. SRL measurements show that
doping by TDs occurs up to deep wafer regions, i.e. 5000.
5000. Due to the high C-V measurements one can state that the FZ material is not
dominated by the formation of T0Ds [as in similar treated Cz Si [1]], but also a
significant shallow thermal donor concentration seems to exist in the
5000. In the FZ material TD formation is lower than in Cz Si, since despite the oxidation the interstitial oxygen concentration is rather low (1015 cm-3). Therefore, in FZ Si S1Ds are of comparable importance like the TDs. Due to the higher Oi concentration in Cz Si the S1Ds play a negligible role in comparison
with the TDs. Finally, the low thermal energy necessary on base of hydrogen supported TD formation and some high voltage test

10:30 AM F0.6
HYDROGEN PLATELET LAYER IN SILICON FORMED FROM HYDROGEN TRAPPED ONTO MICR0BUBBLES OF GASES.
Alexander Ustenski, 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 hydrogcnation are described. The process involves first making a
buried layer, then implanting carbon or hydrogen into the wafer to form the trap layer. The traps are microbubbles that appear along the
buried layer plane of implanted ions. Results for argon, helium, and hydrogen implantation are compared. Wafer thus processed with an initial
implant to levels below 2 x 1018 cm-2 are then hydrogenated with a RF plasma. During hydrogcnation, 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 plateau-like extension to the microbubbles. The extensions grow preferentially along the buried layer plane (i.e. < 100 > plane). A silicon layer above the layer of grown platelets were delaminated through post-bonding cut/post-bonding sequence as in the
Smart-cut process. The plasma hydrogcnation 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 hydrogcnation process allows
self-consistent extended hydrogen platelet from the microbubbles. Mechanisms of nucleation of platelets as extensions of inert gas
microbubbles are suggested. Other effects of hydrogen outdiffusion from platelet growth with thermal trajectory during plasma
cleaning is discussed.

10:45 AM F0.7
THERMAL EVOLUTION OF DEUTERIUM IN 4H-SiC BY NUCLEAR METHODS.
Romain Delcarne, Esidor Nseneck, Thierry Sauvage, CERL-CNRS, Orleans, FRANCE; Andrei Shiryaev,
A. van Veen, HIL-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 passivate donors. 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 deuteriem in SiC. 4H-SiC was implanted with 30 keV D+ at room temperature with a fluency of 1018 cm-2. Deuterium was measured by both the nuclear reaction (NRA) 14N(d, pγ)13C and SIMS. To investigate the thermal evolution of deuterium, we applied thermal annealing with temperature up to 1500°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 with a tail toward the surface. In addition Rutherford back scattering (RBS) and ion channeling experiments were used in order to study the evolution of defects in the matrix and the position of deuterium. Implantation of deuterium induces small clusters at Rg but with annealing, cationics can be found in the sample. We will also discuss how these affects the deuterium moving.

11:00 AM F0.8
ELECTRON-BEAM-INDUCED REACTIVATION OF SI DOPANTS IN HYDROGENATED AND DEUTERIUM- AND DIALKYLAMMONIUM HETEROSTRUCTURES. APPLICATION TO THE FABRICATION OF NANOSTRUCTURES.
Ludovic Kurovsky, Sarah Silvestre, Dorothée Lorrain-Beard, Eugene Constant, Institut d’Electronique et de Microélectronique du Nord, Villeneuve d’Ascq, FRANCE, Michel Revel, Sorbonne Universités, UPMC, CNRS, Laboratoire de Physique des Solides et des Cristallinologies, Meylan, FRANCE, Marcia Constant, Laboratoire de Spectrochimie Infrarouge et Raman, Villeneuve d’Ascq, FRANCE.

Hydrogen incorporation in n-type Si-doped GaAs epilayer 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 Si-doped GaAs epilayer and 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 cm) and Si phosphorus-doped AlGaAs/GaAs/InGaAs heterostructures exposed to a hydrogen beam with different injection energies (10 to 50 keV). On one hand, we observe that the reactivation of Si dopants is weaker when deuterated. On the other hand, the study of this reaction versus injection energy of electrons suggests an energetic electron excitation effect more than a minority carrier generation effect. Moreover, for the 0.2 cm 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 phosphorus-doped AlGaAs/GaAs/InGaAs heterostructures are particularly interesting to reactivating dopants, with a good contrast, using an electron beam irradiation. Also, it could open the fabrication of high mobility 2D mesoscopic structures for electronic or optoelectronic applications.

SESSION F1.0 10:00 AM - 11:30 AM
ION IMPLANTATION

11:15 AM *F1.0.1
VACANCY IMPLANTATION—NO LONGER JUST A MYTH.

In spite of the fact that interstitials and vacancies are produced in equal numbers in 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 quantified, they are only the intermediate step in the overall process of vacancy formation. 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 potential of vacancy-rich environments in silicon such as the energetics and kinetics of vacancy clustering and cluster dissociation. In addition, new effects resulting from implantation through interstitial channeling directions have been discovered. This presentation will discuss significant technological implications of these results for dopant activation and strain engineering.

11:45 AM F1.0.2
CREATION OF INTERNAL POINT DEFECT SOURCES IN SILICON BY CARBON IMPLANTATION.
Mark Huberlen, Jürgen K. Linder, Bernd Strunk, 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 self-interstitials and vacancies. In this contribution it is demonstrated by cross-sectional and energy-filtered TEM that amorphous SiC nanocrystallites, which are formed during low-temperature high-dose implantation of
carbon into silicon, constitute such sources or drains. The formation of amorphous SiC nanochannels in silicon is the result of both the negligible mobility of solubility in crystalline silicon and the stopping of carbon ions in silicon. The implantation conditions at which such nanochannels are created have been extensively studied. Since the atomic density of silicon in amorphous SiC is significantly reduced compared to the atomic density used for crystalline silicon, the nanochannel formation involves emission of Si self-interstitials. Vice versa, crystallization of these nanochannels into SiC crystals is 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 the interstitials can be provided by edge-type dislocations which are formed as a primary defect at elevated implantation temperatures.

**SESSION F11: ION IMPLANTATION**

Chair: Esidor N. Nieschulz and Wolfgang Skorupa

Thursday Afternoon, April 4, 2002

Sakon 1/2 (Marriott)

1:30 PM F11.1

ELECTRICAL SIGNATURES OF ION IMPLANTATION INDUCED DEFECTS IN ULTRA-HIGH DENSITY CLUSTERING STUDIED USING DLTS AND ISOThERMAL TRANSIENT SPECTROSCOPIES. Sunandendra P. Singh, Vinod Rao, V.N. Mohapatra Dept. of Physics, Indian Institute of Technology Roorkee, INDIA; Sunjay Rangan, S. Ashok, Dept. of Engg Science and Mechanics, Pennsylvania State University, University Park, PA.

There is 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 28keV 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 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 gave up its charge to deeper levels for longer filling times. The activation energy of the dominant trap (appearing at all temperatures between 200K-270K) deepens from 0.43 to 0.65eV increasing linearly with logarithm of filling time varying from 10ms to 1s. A similar trend appears above 270K with a lower temperature dependence.

Contrary to the above results, few dominant point defects are observed electrically in presence of ion-implantation induced defect clusters, our results show that the band gap may be depleted with bands of trap states, however their occupation and hence observation depends critically on experimental conditions like capture rate 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


The shape of ion range profiles obtained by channeling implantation depends strongly on the implanted dose. This behavior is caused by enhanced depletion 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. 70keV channeling implantation of Ge into Si and 30keV SiC was performed, using doses between 5 x 10^12 and 8 x 10^13 cm^-2. The implantation temperature varied between 87 and 580°C. The use of a focused ion beam system enabled the application of two very different dose rates (10^12 and 10^13 cm^-2 s^-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 intrasurface 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 computer simulations yields Ge depth profiles which agree well with the measured data.

2:00 PM F11.3

DIELECTRIC BREAKDOWN 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 6H-SiC(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 amorphous single crystal. 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.

Isothermal 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 process. The disorder accumulation for all ion species is consistent with a combined direct-impact and defect-stimulated (DID) model for amorphization. A lower level of disorder on both the Si and C sublattices is observed along the <1102>, and along the <1120> and <1012> 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**

Chair: 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. R. Wang, 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 has been extensively 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 paper, we will present experimental results as well as theoretical considerations of metal-semiconductor interface. We will consider the effect of defects and other interface states, such as the metal induced gap states, will be analyzed. It will be argued that the energy-band diagram for metal-semiconductor interfaces is a result of the difference between the Fermi level in a metal and the Fermi level in a semiconductor. The results present the importance of correctly handling the chemistry at semiconductor interfaces in order to understand the electronic properties.

3:15 PM F12.2

AB-INITIO RESULTS FROM SiO_2 TO HIGH-K GATE OXIDES. Peter E. Blöchl, Clemens Frits, Institute for Theoretical Physics, Clausthal University of Technology, Clausthal-Zellerfeld, GERMANY.

Conventional SiO_2 based gate oxides suffer from stress-induced tunneling currents (SILC) and breakdown. We investigated defects in silicon, including oxygen deficiency and hydrogen relaxed defects, in order to identify the source of SILC and dielectric breakdown. An estimate of the energy barrier between two-step tunneling in silicon
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 consistent with previous experiments of SILC. However, breakdown appears not to be directly related to those defects. A-bulk model 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 gate oxides can be deposited with a larger physical thickness, thus surpassing quantum mechanical tunneling though an otherwise ultra-thin gate oxide. One of the major problems that arise due to high-k growth is the contamination of interfacial oxides on silicon. First results on the growth mechanisms will be presented.

3:45 PM F123
ENHANCED INTERDIFFUSION IN CVD AND MBE GROWN Si/SiGe SUPERLATTICES. Daniel B. Asherline, 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 0.11 ± 0.18 eV and 0.15 ± 0.18 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 material. This is a result that is of significant interest. It indicates that the interdiffusivity of the two deposition techniques depends on the underlying interface. Environments of misfit strain relaxation and its role in the kinetics of interdiffusion in Si/SiGe heterostructures will also be presented.

4:00 PM F124

The functionality of semiconductor devices is critically dependent on the ability to limit the spatial and energetic position 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 GaN 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 large range electronic 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 the entire nominally homogeneously doped layers once the layer thickness is close to the cluster dimensions. Thus, local variations in the dopant atom distribution result in the precision of the energetic and spatial position of the Fermi energy in nanoscale semiconductor structures and a further miniaturization especially requires the control of the spatial location of dopant atoms.

SESSION F13: POINT DEFECTS, IMPURITIES, DIFFUSION IN SEMICONDUCTORS
Chair: Yoshikawa N., Mohapatra A., Ruo P.  Friday Morning, April 5, 2002  Salon 1/2 (Marriott)

3:00 PM 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 – a new opportunity to address the 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 major 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. Instead, the widely discussed oxygen vacancies are actually deep rather than shallow donors. I will present detailed results about their negative charged configuration and find that they are responsible for the defect nature of the nitrogen vacancies. More broadly, I will show how these conclusions impact the understanding of the behavior of hydrogen in semiconductors and insulators in general.


8:30 AM F13.2
THERMOCHEMICAL DECOMPOSITION IN GaN. LASER LIFT-OFF AND NOVEL DEFECT FORMATION. E. A. Shchekin, 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 nitride treatment. First, a novel 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), nitridation may occur preferentially. This fact can be employed 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.  J. Appl. Phys. Lett. 72, 5074 (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. Additionally, it is possible to study in real time and at high resolution how this thermochemical decomposition occurs in individual 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 the description proceeds along the (100) twin planes and results in strong hexagonal faceting of the crystal. Description is found to occur preferentially along the cores of dislocations with a screw component, resulting in the formation of nanorope 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 that we call nanorope defects. These are an internal defect that we believe may be caused by boring 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. E. A. Shchekin, S. A. Ringel, Ohio State University, Department of Electrical Engineering, Columbus, OH, A. Allerman, J. P. Keane, Steven R. Kurtz, Sandia National Laboratories, Albuquerque, NM.

The quaternary semiconductor InGaAsN has attracted interest as a candidate for use in the 1.3 and 1.55 µm optoelectronics and in multijunction 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, some of which 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 1.85 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 postgrowth thermal annealing. Temperature-dependent spectra of the three layers exhibited a number of unique features. The first of these was a broad distribution of levels located just below the conduction band edge, the presence of which is consistent with the proposed bandstructure. A minor contribution of states was present between 0.3 and 0.4 eV below the conduction band edge, and a deeper state exhibiting unusual capture kinetics.
10:30 AM F13.1
ISOELECTRONIC DEEP TRAPS AND GIANT BANDGAP BOWING PHENOMENA IN III-V SEMICONDUCTOR ALLOYS.
M.J. Seong, A. Messerhans, National Renewable Energy Lab., Golden, CO.

The novel properties exhibited by GaAs$_{1-x}$N$_x$, where it was observed that the incorporation of just 3% N reduced the band-gap by 400meV bringing it close to 4eV 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 other optoelectronic devices. However, this incorporation of just 1% N into GaAs results in severe degradation of its electronic properties and so there has been an intense effort devoted to understanding the reasons for the giant band gap reduction and the poor transport properties of GaAs$_{1-x}$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 GaP$_{1-x}$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$_0$+A$_0$ 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 GaAs$_{1-x}$N$_x$ and GaP$_{1-x}$N$_x$ are better described by heavy N iso-electronically 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 that the effects of four major defects in 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 been shown to exhibit similar performance. This exciting and unexpected result has led us to question the nature 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 considerable, as black diamond is considerably cheaper than high quality polycrystalline diamond due to the significant improvement in the cost of the material.

11:00 AM F13.9
FORMATION AND PROPERTIES OF THREE COPPER PAIRS IN SiC-ON: S. K. Estreich, 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 Materiales-CSIC, Univ Autonoma de Barcelona, Bellaterra, SPAIN; S. Knick, J. Weber, Technical Univ of Dresden, Dept. of Physics, Dresden, GERMANY.

Copper is a feared contaminant in Si device processing. It diffuses quickly from any intentional or accidental active precipitates which are difficult to dissolve. Several complexs 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. In the results include the configurations, bonding energies, electronic structures, local vibrational modes, and formation energies. 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 photon replicas which implies low-frequency modes. Calculations reproduce the observed local modes and allow the identification of at least two of these complexes.
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 $^{28}$Si and natural silicon enable simultaneous analysis of $^{28}$Si self-diffusion into the $^{28}$Si-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 $200\,\text{nm}$ thick Si layer was deposited on top of the $^{28}$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 ISOPTICALLY CONTROLLED SILICON MULTILAYER STRUCTURES.**

D. Sharp$^a$, H. Bracht$^b$, H. Silvestrin$^c$, S.P. Nicol$^d$, J.W. Beeman$^e$, J.L. Hansen$^f$, A. Nylander Larsen$^g$, E.E. Haller$^h$, "Department of Materials Science and Engineering, University of California, Berkeley, CA; Lawrence Berkeley National Laboratory, Berkeley, CA; Institut für Materialphysik, Universität Münster, Münster, Germany; Institute 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. $^{28}$Si was used as a tracer through a multilayer structure of alternating natural Si and enriched $^{28}$Si 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. 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 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 $^{28}$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 Højér, Assad Brillaghi, Etienne Pilote, Laboratoire de Physique et Applications des Semi-conducteurs, CNRS, Strasbourg, FRANCE; Stephane Bourdais, Bichir Semmache, J.F. ELEC, Meylan, FRANCE; Armin Kempf, Peter Biechel, 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 implanter method is introduced in order to allow for the identification of TID signals with a high signal to noise ratio. 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 $10^{-15}$ cm$^{-3}$ (or $5 \times 10^{10}$ cm$^{-2}$) is reached, with a 0.8 mm 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.