SYMPOSIUM E

Semiconductor Defect Engineering–Materials, Synthetic Structures, and Devices

March 28 - April 1, 2005

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* Invited paper
Semiconductor Heterojunctions—Properties and Photoelectronic Characterization

Monday March 29, 2005
1:30 PM - 5:00 PM
Room 2006 (Moscone West)

TUTORIAL

This tutorial will cover basic concepts of semiconductor heterojunctions and their properties as well as many applications of a wide variety of electronic and optoelectronic devices. A broad range of material systems, with special emphasis on III-V alloys, will be used as examples to illustrate the types of band alignment and band-offset determination, and their electrical and photovoltaic characterization. A brief introduction to various methods of preparation, and a review of modern techniques to modify the properties of heterojunctions will also be included. The recent emergence of semiconductor heterojunctions in applications such as organic light-emitting diodes will be discussed in order to carry out a critical comparison with conventional inorganic semiconductor heterostructures.

Instructor:
Yashowanta N. Mohapatra, Indian Institute of Technology, Kanpur

SESSION E1: Dopant/Defect Issues in Wide Bandgap Semiconductors

Chair: J. Chevrier; Co-Chair: P. Mau Yu
Tuesday March, 29, 2005
Room 2006 (Moscone West)

8:00 AM *E1.1
Doping Strategies and Doping Rules in Difficult-to-Dope Semiconductors
Alex Zunger, National Renewable Energy Laboratory, Golden, Colorado.

In the past, some well-known "difficult to dope" systems were largely treated as isolated cases by isolated communities. Thus, n-type doping of diamond, or p-type doping of ZnO, or n-type doping of Chalcopyrites (CuGaSe2) were studied as isolated cases by these three respective communities in their respective disciplines (transparent conductor people, and photovoltaic people). Yet, it is now becoming clear, largely because of better inter-field communication and theoretical work (which is intrinsically more transferable to other systems than experiment, where investments in specific growth methods are required), that there are some common features and common "rules" concerning doping in semiconductors. I will describe those rules and results, formulating some general "design principles" which should help experimentalists to navigate in this multi-parameter space of optimizing doping in difficult cases. These rules do not address all cases, and do not provide simple cures. But they tell you in which direction you should concentrate your efforts. See recent paper: A. Zunger Appl. Phys. Lett. 83, 57 (2003) and references therein.

8:30 AM *E1.2
Grown-in and Radiation-Induced Defects in SiC
Thomas Eberle1, Robert Jones1, Patrick Bridillon2 and Sven Oberg2; 1School of Physics, University of Exeter, Exeter, United Kingdom; 2School of Natural Sciences, University of Newcastle upon Tyne, Newcastle upon Tyne, United Kingdom.

SiC is a material that seems ideal for high-power, high frequency and high temperature electronic devices. It does not suffer from large reverse recovery inefficiencies typical for silicon when switching. In contrast to silicon, SiC is however difficult to dope by diffusion, and instead ion-implantation is used to achieve selective area doping. The drawback of this technique is that irradiating the crystal with dopant atoms creates a great deal of lattice damage including vacancies, interstitials, antisites and impurity-radiation defect complexes. This becomes a very severe problem if the resulting defects are electrically active, resulting in a reduction of the carrier lifetime. It is even possible that the irradiation reduces the electrically active donor concentration. Although many of the point defects can be eliminated through thermal annealing, some however, e.g. the PL D1 and Z1/22 centers in 4H-SiC, are stable at high temperatures. In this polype type, D1 and the related Alphabet lines are the most prominent photoemission (PL) signals. The latter can be seen directly after low energy irradiation while D1 usually dominates the PL spectrum of implanted and irradiated SiC after annealing. Another important irradiation defect is the Si vacancy. In contrast to the C vacancy which is well characterized by EPR there is still an ongoing debate regarding the spin state of the neutral Si vacancy. While EPR measurements clearly favor a spin triplet ground state, PL measurements find a spin singlet. Not only implantation but also irradiation with energetic Si ions by CVD methods leads to a deterioration of the crystal quality with an increase in electrically active grown in defects. Among these, the Z1/22 defects are dominant in n-type 4H-SiC, as well as material that has been exposed to radiation. We use first principles density functional calculations to investigate defect models for the above mentioned defects in 4H-SiC and relate their electrical and optical activity to experiments.

9:00 AM E1.3
Defect Studies in Wide Bandgap Semiconductors such as Vanadium Doped 4H-SiC Using Optical Admittance Spectroscopy
Wonwoo Lee1 and Mary E. Zvanut2; 1 Materials Science, University of Alabama at Birmingham, Birmingham, Alabama; 2 Physics, University of Alabama at Birmingham, Birmingham, Alabama.

Semi-insulating SiC is an excellent candidate for a variety of applications, including microwave field effect transistors and other devices for high power and high temperature applications. Vanadium doping is one way to make a semi-insulating (SI) material. Vanadium impurity in SiC is important because it cannot only possess multiple charge states but can also play a role as an efficient carrier trap and recombination center. Vanadium acts as an amphoteric impurity in 4H-SiC with a V2+/3+ acceptor level thought to be within 1 eV of the conduction band edge and a V4+/5+ donor level known to be 1.6 eV below the conduction band edge. Optical admittance spectroscopy (OAS) is a technique which measures the AC capacitance and conductance in the depletion region of a Schottky diode under illumination as a function of photon energy. We studied vanadium doped 4H-SiC with the OAS technique at room temperature. The 4H-SiC samples were found to exhibit two OAS peaks at photon energy (Eph1) 1.89 ± 0.02 eV and (Eph2) 2.80 ± 0.02 eV. We observed peak broadening from our OAS data. The values of the full width at half maximum were 0.12 eV for the peak at 1.89 eV and 0.27 eV for the peak at 2.89 eV. Because we believe that peak width is due to thermal broadening, we interpret the threshold of each peak as a phonon-assisted optical transition and the peak energy as a Frank-Condon transition. The threshold energies may be compared with defect levels measured with thermal techniques. Compared with other data reported in literature, our results show that the defect level E1 -1.5 eV is fairly close to the vanadium donor level and the other level E2 -0.05 eV also falls into the range below 1 eV which many believe to be the vanadium acceptor level. At the conference, we will more thoroughly discuss the relevance of our spectra to the deep defect levels of vanadium doped 4H-SiC. We thank Dr. Bill Mitchell for providing samples. Program is funded by Dr. Colm Wood, ONR.

9:15 AM E1.4
Important Grown-in Defects in Novel Dilute Nitride (Al,Ga)N/GaN: Ga Intersitials. N. Q. Thinh1, I. P. Voronai2, I. A. Buyanov1, Wonly M. Chen3, Sukti Limpijumnong2, S. B. Zhang2, Y. G. Hong2, H. P. Xin2, C. W. Tu1, A. Utsunomia2, Y. Furukawa2, S. Mahalingan2, A. Woki2ar and H. Haen2; 1Dept of Electrical and Computer Engineering, University of California, La Jolla, California; 2Dept of Electrical Engineering and Computer Science, University of California, Los Angeles, California; 3Department of Electrical and Electronic Engineering, Tokyo University of Technology, Tokyo, Japan.

Novel (Al,In)GaN1-xPnx at-x, alloys have recently attracted increasing attention due to their fascinating physical properties as well as potential applications in optoelectronics that can be lattice matched to Si substrates. Unfortunately, epitaxial growth of these alloys remains as a great challenge and the crystal quality is known to depend on N incorporation leading to degradation of optical and electrical properties, which is commonly attributed to formation of defects. We provide the first identification of important grown-in defects in (Al,Ga)N-based alloys, from optically detected magnetic resonance (ODMR) studies. Based on the characteristic hyperfine structure, two Ga-interstitials (Ga1 and Ga2) defects are positively identified as being common grown-in defects in GaN and AlGaN grown by molecular beam epitaxy. The observed strong and nearly isotropic hyperfine interaction reveals an electron wave function of A 1 symmetry that is highly localized at the Ga1 and thus a deep-level nature of the defects. Based on comparison with important grown-in calculations, both defects are suggested to be complexes involving a Ga2. Taking advantage of the freedom in altering compositions of both Al and N of the novel alloy, compositions dependence of electron localization has been obtained that sheds light on the possible location and local surrounding of the defects in the lattice. Introduction of these defects is shown to be largely promoted by incorporation of N. In quaternary alloys, concentrations of the defects are found to critically depend on the group III atoms that
Role of the Substrate Doping in the Activation of Fe$^{2+}$ Centers in Fe Implanted InP. 
Tristina Cesca, Andrea Gasparotto, Adriano Vena, Beatrice Fraboni, Giuliana Impellizzeri and Francesco Priolo. 
Physics Department, INFEM and University of Padova, Padova, PD, Italy; 2Physics Department, INFEM and University of Bologna, Bologna, BO, Italy; 3Physics and Astronomy Department, INFEM and University of Catania, Catania, CT, Italy.

Fe is a key impurity in InP-based materials and technology. Thanks to its deep acceptor character, it is used to induce insulating behavior in both bulk and epitaxial materials; moreover, it has interesting optical properties in the mid-infrared spectral region. High densities of electrically and optically active Fe$^{2+}$ centers can be incorporated in InP crystals by high temperature implantation (1); by this method damage-related undesired reactions can be reduced and solubility limitations can be overcome, creating a high supersaturation of substitutional Fe atoms in a relatively undamaged crystal. Post-implantation annealing at temperatures in the range between 300 and 600 °C cause both a reduction of the residual damage and an Fe escape from substitutional sites (2). It is very important to study this process because it determines the final concentration of active Fe$^{2+}$ centers which in turn control the electrical and optical properties of the implanted and annealed samples. The dynamics of the Fe escape from the substitutional sites is influenced by the reactions with the damage-induced point defects occurring during the annealing, but also the substrate doping appears to play an important role. In this paper we present and discuss some results which help to clarify the role of the background doping of the InP substrate (n-type) in this Fe escape process. InP substrates with background doping densities of $5 \times 10^{15}$ and $1 \times 10^{16}$ cm$^{-3}$ were implanted at $200 \, \text{°C}$ at energies between 150 and 300 keV and fluences ranging from $1 \times 10^{15}$ up to $5 \times 10^{16}$ cm$^{-2}$. This wide range of experimental conditions allows us to use several characterization techniques, depending on the various fluence regimes, in order to study the different Fe-related properties. Damage production and annealing, and Fe lattice location were studied by means of RBS-FIXEL-channeling. Electrical properties related to the activation of Fe$^{2+}$ centers were studied by means of experimental and simulated I-V characteristics or DLTS-PIClTS depending on the resistivity of the sample. The results allow to distinguish between the role of the defects and that of the Fe centers in determining the electrical behavior, and show how the presence of background acceptors may severely influence the final location and electrical properties of the implanted atoms. A possible mechanism is discussed to explain the observed behavior at a microscopic level. (1) A. Gasparotto et al., Appl. Phys. Lett. 78, 668 (1999). (27). Cesca et al., Phys. Rev. B 68, 242113 (2003).

Electrical Activity of ZnO Grown by Closed Space Vapor Transport on Sapphire Substrates. 
Laboratoire de Physique des Solides et de Cristallogenie, CNRS UMR 8635, Meudon, France; 2INVESTAV, IPN, Mexico, Mexico.

The electrical activity of ZnO is an important issue for the development of ZnO-based optoelectronic devices. Indeed, both non-intentionally doped thin films and bulk crystals exhibit n-type conductivity. As most of the studies are still performed on films grown on sapphire substrates, the possible diffusion of Al from the substrate to the epilayer can generate a highly p-type conductive layer close to the substrate interface. This may cause difficulty in achieving a low level of carriers in non intentionally doped ZnO thin films. This could also be a difficulty for measuring p-type conductivity. We report on the electrical activity of ZnO films grown on sapphire substrate using the Closed Space Vapor Transport (CSVT) technique. The n-type conductivity of the epitaxially deposited films has been studied for thicknesses ranging from 0.1 to 60 μm. The carrier concentration, measured by Hall effect, is found to decrease linearly with the film thickness. This is explained by the presence of an interface layer to the measured conductivity in relation with Al diffusion from the substrate as demonstrated by Secondary Ion Mass Spectrometry (SIMS). This interface contribution dominates the electrical behavior of the films for thicknesses up to 10 μm. We show that this strong interface conductivity can be compensated on thin films using thermal annealing under oxygen atmosphere at 850°C. Under these conditions, a strong mobility enhancement of about 10$^3$ fold can be achieved. Furthermore, the effect of this annealing under oxygen is found to be completely reversible after a further thermal annealing under argon atmosphere at the same temperature. The creation of complex defects such as Al vacancy (acceptor) whose creation is favored by oxygen annealing is proposed to explain our results. These studies confirm the importance of oxygen treatments on the electrical activity of ZnO and indicate that a suitable thermal annealing can compensate n-type conductivity in thin ZnO films. The low level of carriers achieved after oxygen annealing suggests that the compensation phenomenon observed with Al is also effective for other n-dopants. However, this compensation effect is only observed on films below one micron. This indicates that, with our experimental conditions, Zn vacancies are only generated close to the surface. We conclude that it is possible to achieve and measure p-type conductive ZnO thin films by being conditioned by the mean of (i) an alternative substrate to sapphire or (ii) a specific buffer layer as barrier to the diffusion of Al.

Effects of Impurity Incorporation in Ni on Silicidation/Germanosilicidation Reactions and Structural/Electrical Properties of NiSi/NiSi$_2$(Ge). 
Dongchi Cui, R. T. P. Lee, Huibiao Yao and Soojin Chua; Institute of Materials Research & Engineering, Singapore, Singapore.

As the semiconductor industry approaches sub-90 nm technology nodes, the trend is to replace cobalt silicide with nickel monosilicide (NiSi) since the use of NiSi for contact metallization shows a number of technological advantages, including its line-width independent low resistivity, less Si consumption and low thermal budget for its formation, and compatibility with Si- and Ge-based substrate technology. However, NiSi has not been considered as a serious candidate until recently mainly due to its poor morphological/thermal stability. Recent studies have shown that the morphological/thermal stability of NiSi can be enhanced substantially through the addition of a small amount of impurities, resulting in much improved silicided shallow junction integrity. In addition to improving the morphological/thermal stability, it has also been demonstrated that the addition of certain impurities, such as Ti, effectively reduces the sensitivity of NiSi formation to oxygen (e.g., residual interfacial oxide). Other than the beneficial effects in enhancing thermal/morphological stability of NiSi as well as alleviating the sensitivity of NiSi to surface contamination for its formation, the incorporation of some elements has also been found to be effective in tuning the work function of NiSi, thus making it a suitable candidate material for the use as metal gate. This talk will present and discuss the details of these experimental results.

SESSION E2: Dopant/Defects in Silicon Technology
Chairs: J. Chevallier and Kin-Man Yu
Tuesday Morning, March 29, 2005
Room 2006 (Moscone West)
The extreme miniaturization of ultra-large-scale integration Si-based devices requires an ever increasing carrier density - especially for p-type doping. Engineering the coupling of acceptors with other impurities ("co-doping") may offer a route to improving the solubility and ionization, and ultimately the carrier density, for some dopants. Here we suggest that the substitutional-pair complexes found in silicon as acceptors, are not able to form p-acceptors, the latter giving the partially filled p-like states of the acceptor, pushing the latter down in energy. This should lead to a reduction of the formation energy as well as of the ionization energy. Ab initio density-functional calculations in In-C, In-Ge, B-Ge pairs confirm the soundness of the general scheme. The effect is sizable (and in good agreement with experiment) for In - whose 0.19 eV shift upon coupling to C - whereas it is less significant for B. We also investigated co-doping with other acceptors, considering the Ga-B and In-B pairs: but none of these is bound, so that the acceptor-acceptor co-doping is of no help.

11:30 AM E2.8 Study of the Pt – O Complex Formation in Platinum Doped Silicon. Wilfried Vervisch,1,2,3 Laurent Ventura1, Bernard Pichaud2, Gerard Duscher1 and Andre Lhorte3; 1LMP, Universite de Tours, Tours, France; 2Condensed Matter Science Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; 3Department of Materials Science, University of Wisconsin, Madison, Wisconsin.

In this work, we report experimental results demonstrating the formation of an oxygen complex with platinum. We model the reaction of this complex formation and propose a set of parameters according to our experimental results. When platinum is diffused at temperatures higher than 900°C in Cz and FZ n-type silicon samples which are then cooled slowly in the range [1-10]°C/min, a p-type doping leading to the formation of a p-n structure is observed by current spectroscopy. We have shown that this reaction occurs also in intrinsic and boron doped silicon materials, rejecting the reaction with phosphorus or boron acceptor, pushing the latter down in energy. This should lead to a reduction of the formation energy as well as of the ionization energy. Ab initio density-functional calculations in In-C, In-Ge, B-Ge pairs confirm the soundness of the general scheme. The effect is sizable (and in good agreement with experiment) for In - whose 0.19 eV shift upon coupling to C - whereas it is less significant for B. We also investigated co-doping with other acceptors, considering the Ga-B and In-B pairs: but none of these is bound, so that the acceptor-acceptor co-doping is of no help.

11:45 AM E2.9 New Additions to the Menagerie of Defects in Silicon. Gerd Drucner1,2, Alexander Kvít3, Donavan Leonardi1, Abdennaceur Karoui1 and Nathan G. Stoddard3; 1Materials Science & Engineering, North Carolina State University, Raleigh, North Carolina; 2Condensed Matter Science Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; 3Department of Materials Science, University of Wisconsin, Madison, Wisconsin.

Annealing of nitrogen doped Czochralski silicon has resulted in the creation of a number of new defect structures. The morphology is depth-dependent in the first tens of microns from the surface and features some structures with unusual shapes. Transmission electron microscopy using a combination of high resolution and Z-contrast imaging as well as electron energy-loss spectroscopy reveal that these defects generally consist of SiO2 and an silicon interstitial-rich region. To reconstruct the three-dimensional morphology of these defects, we investigated samples in different crystallographic orientations. The shape of the SiO2 region seems to be dependent on the N distribution within this region, because N is only present at the interfaces that seem to be terminating the defect in its growth directions. The SiO2 region can be easily identified as a dark region in Z-contrast images while the Si interstitial-rich region will appear brighter than the matrix. The interstitial-rich region did not collapse into stacking faults, but seems to be dependent on the depth within the sample. The shape of the interstitial region follows crystallographic directions, ultimately causing the highly symmetric shape in three dimensions. Unexpectedly, O is present in this interstitial rich region. Their characteristic shapes distinguish these defects. We identify umbrella, dragonfly, jellyfish, scissors and simple rod defects. All of these defects have a typical length of 100-200 nm. The depth of the interstitial-rich region of these extended defects is beneficial for gettering of metal impurities, effectively increasing the trapping volume.

SESSION E3: Interfaces and Strain-Induced Defects

Chair: T. Tsushima and Wai-Shing Lau

Tuesday Afternoon, May 3, 2006
Room 2006 (Moscone West)

1:30 PM E3.1 Experimental Observation of Formation Processes in Si/SiO2 Interface Defects using in-situ UHV-ESR System. Satoshi Yamada1,2, W. Futako3 and Norikazu Mizuno1,3; 1AIMT, Daimon Research Center, Tsukuba, Japan; 2Graduate School of Pure and Applied Science, University of Tsukuba, Tsukuba, Japan; 3Institute of Physics and Information Science, University of Tsukuba, Tsukuba, Japan.

As a typical point defect at the Si/SiO2 interface affecting electrical properties, a three-fold coordinated silicon atom with a neutral charge, the so-called P3 center, has been widely investigated. Electron spin resonance (ESR) is one of the most powerful tools available for investigating P3 centers. However, these studies have been limited to the high oxygen concentration region of Si/SiO2 interface. For oxygen concentrated silicon material, information about the dynamic oxidation mechanism is required. For above purposes, we have developed an ultra-high-vacuum (UHV)-ESR system, which is a combination of an ESR system and a UHV chamber, and reported the dynamic oxygen and hydrogen termination processes on Si clean surface. In this talk, we focus on the process of P3 center generation during silicon oxidation following oxygen termination on a clean Si surface. Based on which we discuss the microscopic origin of P3 center formation [1].

2:00 PM E3.2 Efficient Quantitative Detection of Oxygen Vacancy Double Donors in Capacitors with Ultra-Thin Tantalum Oxide Films for Future Nano Applications Using a-BiThio-Tannate Current Spectroscopy. Wai-Shing Lau1, Linbin Zhong1, Taejoon Han2 and Nathan P. Saddler3; 1School of EEE, Nanyang Technological University, Singapore, Singapore; 2Lam Research Corporation, Fremont, California.

8 nm tantalum oxide was deposited onto (100) heavily doped p-Si or n-Si wafers by LP-MOCVD. Post-deposition anneal of samples was done by RTP (rapid thermal processing) in O2 or N2O at 800°C for 30 s. Current measurements were performed at a ramp rate of 0.5 K/s as before [1-2]. Our old method to fill the defect states was UV illumination at about 90 K. The energy level of the defect was estimated using $E_T = 23kT_m$, where $T_m$ is the peak temperature and $k$ the Boltzmann constant. The first ionization state of the oxygen vacancy deep double donor (VO2+) is also known as defect D and is the deepest electron trap detected in the temperature range of 100-100 K [3]. Smaller leakage current can be easily correlated with lower ZBTSC signal from D (0.3 eV) [3]. However, the ZBTSC signal from D is pretty weak such that it is almost buried by a parasitic current which is due to the presence of a very small parasitic voltage. We agree with Ullman [4] that defect D, the first ionization state of the oxygen vacancy deep double donor (VO2+) is an electron trap with an electron-repulsive energy barrier such that its electron capture cross section is thermally activated and is very small, especially at low temperature. Thus it is very inefficient to use UV illumination at about 90 K to fill defect D. We tried the most efficient way to fill defect D with electrons is to use the optical illumination and soft X-ray radiation during electron beam evaporation of metal to form the top electrode for sample preparation.

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The sample actually became slightly hot and since the capture cross section is thermally activated the electron capture became much faster. In addition to the electron drift in the built-in fields, when the metal was thin such that its light blocking effect is much smaller, to the end of the electron beam evaporation process. With this innovation, defect D was detected as a strong ZBTS peak at about 580 K. By performing a simple integration, we found that the concentration of oxygen vacancies is of the order of 1E17 cm\(^{-3}\) in decent samples. Thus we demonstrated that ZBTS can detect O vacancy double donors efficiently and quantitatively for tantalum oxide using oxygen implanted metal oxide semiconductor field-effect transistor (MOSFET) and the old filling method (UV illumination at 90 K) is more useful for the detection of Si and C contamination. We can predict that ZBTS can also be applied to other high-k dielectric materials for next generation memory technology [1]. W. S. Lau et al., Jpn. J. Appl. Phys., 34, 737 (1995). [2] W. S. Lau et al., Appl. Phys. Lett. 71, 500 (1997). [3] W. S. Lau et al., Appl. Phys. Lett. 83, 2855 (2003). [4] F. G. Ullman, J. Phys. Chem. Solids. 28, 279 (1967).

2:15 PM E9.3
An Investigation on the Band Offsets of GaNAsSb/GaAs and GaInAsSb/GaAs by New Charge-Pumping Technique. Kraszynska Ryckiao, Seeth. B. Hahn1, Mark A. Wistey1, Hopil Bae1, Jan Misiewicz1 and James S. Harris1; 1Solid State & Photonics Laboratory, Stanford University, Stanford, California; 2Institute of Physics, Wroclaw University of Technology, Wroclaw, Poland.

The addition of small amounts of N into InGaAs has allowed for growth of dilute-nitride materials which have much lower energy bandgap than previously attainable on GaAs. GaNAs has enabled the development of lasers at the important fiber communication wavelength of 1.3 μm. However, the incorporation of N into (In)GaAs degrades the optical properties of the material due to non-radiative traps, phase segregation, and/or relaxation. To improve the material quality and reduction of band gap, by adding Sb, has enabled the development of GaAs-based laser diodes at 1.55 μm. Although dilute-nitride-antimonide lasers have been shown to have great potential telecommunication applications, several issues, including the band offsets, are not well known. Since these materials are relatively new, there has not been any detailed study of the band structure. A better understanding of the heterojunction band offsets and effective masses would allow for better design of lasers and understanding of the physical processes in these new semiconductor active regions. One powerful method of determining band offsets is photoelectron spectroscopy (PES). By simulating the spectra obtained from PES, a model of the band offsets, energy levels, and effective masses are obtained. There have been many studies on GaNAs and GaAs band offsets, however there have been none for GaNAsSb and only a few for GaNAsSb. Before this study, it was unclear what effect the addition of Sb would have on the GaNAs and GaNAsSb band offsets. In the dilute-nitrides, it was not known if Sb would affect the valence band or if there would be a more complex interaction of the valence and conduction bands due to effects such as band anti-crossing. To investigate the band structure of GaNAsSb and GaNAsSb materials, we performed PES measurements on GaNAsSb/GaAsSb/GaAs quantum wells. These samples were grown by solid-source molecular beam epitaxy utilizing a N flow of 100 sccm. Second-order high-resolution x-ray diffraction were performed to obtain the compositions of the samples. We find that for the technologically important compositions, Ga\(_0\)N\(_{0.06}\)As\(_{0.94}\)Sb\(_{0.02}\)Se\(_{0.02}\)SB\(_{0.02}\)/GaAs has a band offset ratio of ΔEc/ΔEv= 0.9 and Ga\(_0\)Sb\(_{0.22}\)As\(_{0.47}\)Sb\(_{0.31}\)/GaAs a ratio of ΔEc/ΔEv= 0.5. Other results from these samples will also be presented to provide a better understanding of Sb’s role in dilute-nitride band structure. The results suggest that the addition of Sb affects the band structure of dilute-nitride devices by mostly only affecting the valence band. With a greater understanding of the band structure, more advanced GaNAsSb laser devices can be obtained.

2:30 PM E8.2
Direct Measurements of Trap Density in a SiGe/Si Hetero Interface by New Charge-Pumping Technique. Toshiaki Tsuchiya1, Masao Sakuraba2 and Junichi Murota1; 1Shinshu University, Matsumoto, Japan; 2Tohoku University, Sendai, Japan.

Strained-Si and SiGe/Si-hetero CMOS structures are highly promising materials for the construction of advanced high-performance Si CMOS devices. To exploit the advantages of SiGe heterostructures effectively and to establish a good device design methodology, it is important to clarify the relationship between device characteristics and the introduced heterostructures, and to understand the electrical properties of the hetero-interface. However, to our knowledge, there are very few (if any) reports on the direct measurement of interface trap density in such semiconductor heterostructures. The charge pumping technique [1] and the temperature-dependent method of evaluating interface traps between the gate oxide and the semiconductor surface in MOSFETs. In this study, we propose a new charge pumping technique, i.e., low-temperature charge pumping (LT-CP), to measure the interface trap density in the SiGe/Si heterostructure introduced into the channel region of MOSFETs, without interference from the interface traps between the gate oxide and the semiconductor surface [2]. The devices used in this study were a strained SiGe/Si MOSFET, which has a wide range of Ge fractions of 0.2-0.7, and SiGe thickness of 2-14 nm. These devices were fabricated using low-temperature, high-quality, epitaxial heterostructure growth of 180-μm thick Si-buffer layer, strained-SiGe layer, and Si top layer. All of the annealing processes were performed at temperatures below 700 C to prevent degradation of the heterostructure surface flatness and of the Ge profile in the channel region at high Ge fractions. We also measured the low frequency noise power in the drain current flowing in the SiGe-channel [4], and showed a good correlation between the measured hetero-interface trap density and the low frequency noise level, which also indicates the accuracy of the measured hetero-interface trap density. Moreover, we investigated hot carrier reliability of the SiGe/Si-hetero-interface utilizing the LT-CP technique, and it was found for the first time that interface traps are generated by hot carriers in SiGe/Si heterostructures [5]. We estimated the density of the generated hetero-interface traps. References [1] G. Groeseneken, H. E. Maes, N. Beltran, and B. F. De Keersmaecker, IEEE Trans. Electron Devices, vol. ED-31, no. 4, pp. 52-53, 1984. [2] M. Takahashi, K. Arahata, Y. Inada, and J. Murota, IEEE Trans. Electron Devices, vol. 50, no. 12, pp. 2507-2512, 2003. [3] J. Murota and S. Oto, Jpn. J. Appl. Phys., vol. 33, Part I, no 4B, pp. 2290-2299, 1994. [4] T. Tsuchiyu, T. Murota, J. Murota, and M. Sakuraba, Jpn. J. Appl. Phys., vol. 40, no. 9A, pp. 5290-5293, 2001. [5] T. Tsuchiyu, M. Sakuraba, and J. Murota, Proc. of IEEE Int'l Reliability Physics Symp., pp. 449-454, 2004.

3:30 PM E8.3
Ultra-Shallow Junctions for the 65nm Node Based on Defect and Stress Engineering. Victor Moroz1, Majeed Foad2, Houda Grai2, Farahnour Nouri2, Dipu Pramanik1 and Susan Felch2; 1Synopsys, Inc, Mountain View, California; 2Applied Materials, Sunnyvale, California.

The co-implantation of germanium, carbon, and boron with the optimum implant energies and doses makes it possible to create p+/n junctions with the sheet resistance of less than 620 Ohm/sq and the slope of less than 3 nm/dce. The narrow process window is based on careful engineering of the amorphization, point defects, and stresses and includes standard 1050C spike annealing. The germanium pre-amorphization suppresses the ion channeling for the subsequent boron implant. The tensile stress induced by the substitutional carbon atoms and the compressive stress induced by the substitutional germanium atoms slow down hole movement in the junctions shallower. The stress gradient in the transition region from the strained carbon and germanium doped layers to the relaxed silicon underneath creates an uphill boron flux that mixes the junction slope shallowest. The optimum amount of carbon is placed in between the implanted boron and the implant damage, which is located below the amorphized layer. During the annealing, the carbon atoms capture silicon interstitials that are coming from the implant damage and form carbon-interstitial clusters. The analysis demonstrates that it is possible to capture over 95% of the interstitials this way before they reach the boron-doped layer. This completely suppresses the transient-enhanced boron diffusion (TED) and drastically reduces the amount of boron that is deactivated in boron-interstitial clusters (BICs). In fact, the point defect engineering with an optimized carbon profile allows to remove all non-equilibrium silicon interstitials that are generated by the following three sources: the implant damage before the rapid thermal anneal, the interstitials generated by boron at high concentrations (due to the effect known as boron-enhanced diffusion (BED)). The latter effect leads to significant increase of the apparent boron activation level beyond the well-characterized solid-state solubility level. We explain this effect as a reduction in formation of BICs due to the lack of interstitial supersaturation. In carbon-free silicon, high concentration boron is always accompanied by the non-equilibrium interstitials, coming from either the implant damage or the BICs even if boron is introduced into silicon by pre-deposition instead of the implantation. Extensive experiments and theoretical analysis based on simulation of the interaction of Ge, C, I, and B atoms, as well as the stress effects, point to the optimized process flow that improves the shape and parameters of the p+/n USJs.

3:45 PM E8.8
In a strained-Si/SiGe/Si sub-system, the properties of strained-Si layer depend on the state of SiGe strain-relaxed-buffer (SRB). The stress exerted on Si capping layer is directly correlated with the SRB relaxation. In this work, we examined two techniques to improve the relaxation degree of SiGe SRB. The SRB was grown on the highly boron-doped substrate (P+-wafer) and the SRB was annealed several times in the middle of its growth. The SRB relaxation degree increased with dislocation density in SiGe graded layer and the surface etch pit density became lower for Strained-Si prepared by these two techniques than for conventional low-temperature annealed SRB. Relaxation of SRB layer reduces the driving force for dislocation movement from the graded layer to the strained Si layer in spite of high dislocation density. The induced dislocations in the SRB, the thick boron in Si substrate can diffuse into the SRB graded layer, which results in high misfit dislocation density (relaxation of SRB) since the boron doped SiGe have a different stress-strain behavior compared with undoped SiGe. Finally, low surface defect density can be formed as a suitable channel Si layer. In order to prepare a high quality strained-Si layer, we investigated the effect of both annealing and boron doping on SiGe SRB.

4:00 PM E5.7
N+/-P and P+/N Junctions in Strained Si on Thin Strain Relaxed SiGe Buffers: the Effect of Defect Density and Layer Structure. Geert Enenlaen, Benny Perez Rodriguez, Eddy Sinloen, Ronlain Delvingne, Delphine Delhougne, and Peter Verheyen. 1.1, 1.3.4, Eddy Sinloen, Ronlain Delvingne, Delphine Delhougne, and Peter Verheyen. 1.1, 1.3.4, Eddy Sinloen, Ronlain Delvingne, Delphine Delhougne, and Peter Verheyen.

Downscaling of transistor dimensions has led to an important performance increase in microelectronics, combined with a decreasing cost per logical function. To obtain the highest possible gain in performance, several changes of the standard technology are investigated. One of these changes is the use of silicon under a tensile strain (Strained Si) in the channel, grown on a Strained Buffer (SRB) of silicon-germanium: strained Si can lead to high-performance devices, which can be scaled down in the future. The presence of Ge in strained Si channel layer causes the relaxation of silicon and simultaneously help reducing the number of threading dislocations. In this experiment, the threading dislocation density in the layers was varied, as well as the distance of the C-rich layer to the surface, allowing to study the effect of these parameters. The best junctions were found in SRBs with lowest defect densities and with the largest distance between the C layer and the junction. The leakage increase, as compared to the reference silicon junction, was about 2-3 orders for SRBs lower defect density as well as bringing the carbon-doped layer closer to the junction sharply degrades the junction quality, leading to 7-8 orders of leakage increase w.r.t. silicon. It was found that the number of defects plays a different role for the two types of junctions (n+-p and p+-n). The effect of increasing the defects, as well as changing the thickness of the defect-rich carbon-doped layer, on the current characteristics at elevated temperatures is investigated.

4:15 PM E5.8
Morphology, Defects and Thermal Stability of SiGe Grown on SOI. Qinghua Xie, Mike Korte, Xianglei Wang, Mike Canonicco, Deb White, Binh-Yen Nguyen, Alex Barr, Shawn Thomas, and Linh Le. 4 Physical Analysis Laboratory, Freescale Semiconductor Inc., Tempe, Arizona; 5 Advanced Process Research and Development Laboratory, Freescale Semiconductor Inc., Austin, Texas; 6 Cirove-2, Freescale Semiconductor, Creles, France.

We present a systematic study of the strain, defect and morphology of SiGe (Ge composition from 20-40%) layers grown on silicon on insulators (SOI). For low Ge composition, the strain relaxation in SiGe layer is minimal as determined by Raman spectroscopy (delayed by the increased critical thickness for dislocation formation in SiGe on SOI). The misfit dislocation density is below the detect limit of transmission electron microscopy (TEM). For higher Ge content, the tensile stress in a Si capping layer grown on top of SiGe/SOI is 0.46% to 0.65% (a stress of 0.81 GPa to 1.17 GPa). The misfit dislocation linear density observed in cross sectional TEM is 17 μm and 23 μm which is consistent with the strain relaxation of the SiGe layer as determined by elastic thermal annealing, increased surface roughness, dislocation density and strain relaxation in the SiGe layer are observed. TEM also reveals that the misfit dislocations are confined mostly at SiGe/SOI interface and moves down to the Si/oxide interface. Based on this, a new compositionally downgraded scheme having a higher-Ge (upto 40%) buffer layer grown first has been devised. This buffer adsorbs most of the misfit defects and is partially relaxed. Then a thin layer of SiGe of lower Ge composition (20-25%) is grown on this artificial sublayer achieving high strain relaxation and low defect density in this layer. This stack serves as the substrate upon which a tensely strained silicon capping layer can be grown to realize strained Si CMOS devices.
We report on the preparation and optical spectroscopy of diffusion doped Cr: ZnSe and Cr: CdTe windows. Cr2+ doped II-VI semiconductors have recently emerged as a new class of room temperature operated and widely tunable (2-3 µm) mid-infrared (MIR) solid-state lasers. The demonstration of efficient lasing from diffusion doped polycrystalline Cr: ZnSe windows provides an attractive method for producing MIR laser materials at low cost. For the advancement of current Cr2+ chalcogenide lasers, however, it is critical to gain a better understanding of the Cr2+ incorporation and infrared optical properties in II-VI hosts. In this work we present results on Cr diffusion experiments performed on commercial ZnSe and CdTe windows. Compared to Cr: ZnSe, Cr: CdTe offers the advantage of an extended MIR emission with a larger emission cross-section of >3000 cm. Cr doping was achieved in both window materials through a thermal diffusion process controlled by temperature (750-850°C) and time (0.25-6 days). Commercial CrSe powder (99.5% purity) was used as the dopant source. Various samples of Cr: ZnSe and Cr: CdTe were prepared with Cr2+ peak absorption coefficients ranging from 1 cm-1 to 25 cm-1. The estimated Cr2+ concentrations ranged from 5x1017 cm-3 to 3x1019 cm-3, with a Cr2+ peak at 2.018±0.002 eV for Cr: ZnSe and 1.1x1018±0.1 cm-3 for Cr: CdTe. For low Cr2+ concentrations (1x1018 cm-3) the room-temperature decay time varied between 5-6 µs for Cr: ZnSe and 2-3 µs for Cr: CdTe. Based on low temperature (15 K) lifetime data, the emission efficiencies were estimated to be 75% for Cr: CdTe and 95% for Cr: ZnSe. The effect of Cr concentration quenching on the MIR emission was observed for doping concentrations above 1x1018 cm-3. A more detailed discussion of the absorption and MIR emission properties of Cr: ZnSe and Cr: CdTe windows as a function of Cr concentration will be presented at the conference.

E4.2 GaN Films Grown on (11-20) Sapphire Substrates under Various V:III Ratios. Wei-Tsai Liao1, Jyh-Rong Gong1, Yu-Li Tsai1, Cheng-Liang Wang1, Keh-Chang Chen1 and Tai-Yuan Lin3; 1Department of Materials Science and Engineering, Feng Chia University, Taichung, Taiwan; 2Department of Optoelectronics, National Chung Cheng University, Chiai, Taiwan; 3Institute of Optoelectronic Sciences, National Taiwan Ocean University, Keelung, Taiwan.

GaN films were grown on (11-20) sapphire substrates at 1000 °C under various V:III ratios. Growth was conducted by exposing the (11-20) sapphire substrate alternatively to ammonium-reactant (AH) and ammonia(NH3) fluxes carried by purified H2 gas. An AlN buffer layer, 75 Å in thickness, was deposited at 500 °C followed by the deposition of a 0.8 µm-thick GaN film at 1000 °C. In this case, the V:III ratios of TMG and NH3 were 4100, 5200, 6900, 8000, and 10400, respectively. It appears that the OM surface morphology of the GaN film grown on a (11-20) sapphire substrate improves with the increment of V:III ratio. Room temperature (RT) PL spectrum of the GaN film grown under a V:III ratio of 5200 shows strong near bandedge emission along with prominent yellow luminescence. An increment of V:III ratio up to 10400 was found to enhance near bandedge emissions and to quench yellow luminescence. It is believed that the amount of reactive N-H radicals may not be high enough to support sufficient overpressure on the grown surface at a V:III ratio of 5200 presumably due to the existence of a pulse time between successive NH3 exposures. As a result, point defects like Ga vacancies as well as complexes between Ga vacancies and impurities may easily be created. These defects have been reported to be responsible for the yellow luminescence near 2.25 eV[1,2]. Thus, the prominent yellow luminescence of the GaN film under a V:III ratio of 5200 can be attributed to the high density of the above-mentioned point defects. It is known that high quality GaN films grown on (0001) substrate have growth rate under high V:III ratio at a growth temperature higher than 1000 °C by the MOCVD process owing to the fact that high dissociation efficiency of NH3 occurs at very high temperature and high desorption rate of surface adsorbates can only be suppressed under high V:III ratio. Thus, it is believed that sufficient supply of the reactive N-H radicals at a V:III ratio of 10400 is crucial for the growth of high quality GaN films on (11-20) sapphire substrates in this study. A plot of the linewidth of the RT near band edge PL emissions of GaN films versus V:III ratios revealed that an increase of V:III ratio from 5200 to 10400 tends to reduce the linewidth of near bandedge PL emission from 220 to 120 meV. Such a near bandedge emission linewidth decrement is attributed to the pronounced reduction of point defects in the GaN film because of the sufficient replenishment of N-H radicals. This explains the improved optical properties of the GaN films grown on (11-20) sapphire substrates under high V:III ratios.

E4.3 Characteristics of GaN Films Grown on Wet- Etched GaN. Yi-Chi Tsai1, Jyh-Rong Gong1, Kun-Ming Lin2, Wei-Tsai Liao1, Cheng-Liang Wang1 and Tai-Yuan Lin3; 1Department of Materials Science and Engineering, Feng Chia University, Taichung, Taiwan; 2Institute of Opto-Mechatronics, National Chung Cheng University, Chiai, Taiwan; 3Institute of Optoelectronic Sciences, National Taiwan Ocean University, Keelung, Taiwan.

It is well known that the reliability of light-emitting devices, particularly laser diodes, can be greatly deteriorated by the presence of structural defects such as dislocations. Many approaches including epitaxial lateral overgrowth process [1] and patterned substrate techniques [2] have been reported to improve the quality of GaN films remarkably. However, the employment of dry etching process makes the fabrication process less cost-effective. In this study, we report the improvement of optical properties of GaN films by using a simple wet-etching technique. Typically, a GaN sample was prepared by growing a 2 µm-thick GaN underlayer on the c-plane Al2O3 substrate with a subsequent wet-etching treatment. GaN films were overgrown on the etched GaN underlayers at 245°C for 25 min. H3PO4/H2SO4 etching solutions having H3PO4/H2SO4 ratios of 1/3, 1, 2, and 3, respectively, were employed to develop etch pits on the GaN surface. Growth of the etched GaN underlayers, an 1.5 µm-thick GaN film was grown afterward. For comparison, a GaN film, 1.5 µm in thickness, was also grown on the 2 µm-thick GaN underlayer without wet-etching treatment. All the overgrown GaN films were etched again by molten KOH at ∼260°C for 10 min to reveal the etching pit densities (EPDs) of the GaN films. The grown samples were characterized by using optical microscopy (OM), scanning electron microscopy (SEM), photoluminescence (PL) spectroscopy, and transmission electron microscopy (TEM). Room temperature (RT) PL measurements of the overgrown GaN films show a remarkable increment in PL intensity and a considerable reduction in emission linewidth of the near bandedge (BE) luminescence when GaN film were grown on the wet-etched GaN underlayers. In addition, the RT PL intensity ratio (Ig/IY) of near BE emission to yellow luminescence (YL) of a GaN film grown on an etched GaN underlayer having an average pit size of 2.9 µm increases by one order of magnitude when compared with that of the GaN film grown on a GaN underlayer without wet-etching process. OM images of the etched overgrown GaN films indicate that the EPD of the film reduces from 1.7x1014 cm-2 to 3.1x1013 cm-2 when the pit size of the underlying etched GaN increases from 0 to 2.9 µm. Cross-section TEM observations show that the improved optical characteristics of the GaN films grown on the etched GaN underlayers are due to the selective blocking of threading dislocations at the locations of etch pits, which with few dislocations were observed to be embedded in the laterally overgrown GaN areas. Results: [1] T. S. Zheleva, O. H. Nan, M. D. Brosser, and R. F. Davis, Appl. Phys. Lett. 71 (1997) 2472. [2] A. Bell, R. Liu, F. A. Ponce, H. Amano, I. Akasaki, and D. Cherns, Appl. Phys. Lett. 82 (2003) 549.

E4.4 On the Properties of GaN Films Grown on (111) Si Substrates using Intermediate Temperature AlGaN Buffer Layers. Cheng-Liang Wang1, Jyh-Rong Gong2, Chung-Kwel Lin1, Wei-Tsai Liao1, Yu-Li Tsai1 and Tai-Yuan Lin3; 1Department of Materials Science and Engineering, Feng Chia University, Taichung, Taiwan; 2Department of Opto-Mechatronics, National Chung Cheng University, Chiai, Taiwan; 3Institute of Optoelectronics, National Taiwan Ocean University, Keelung, Taiwan.

Recently, there has been a considerable interest in the growth of GaN films on (111) Si substrates for applications in AlGaN/GaN high...
power electronics and GaN-based LEDs [1, 2]. However, because of the large difference in lattice structure and thermal expansion coefficients, the quality of high-quality GaN films remains to be a great challenge [3]. GaN films were grown on (111) Si substrates at 1000°C using Al0.5Ga0.42N buffer layers, deposited at 800°C, with the thickness of Al0.4Ga0.6N layers being 150 nm, 180 nm, and 200 nm, respectively. In this case, a 0.4 μm-thick HT GaN film was deposited with the admittances of TMG and NH3 being 34 μmol/min and 0.2 μmol/min. 6-29 X-ray diffraction (XRD) measurements were used to identify the orientation relationship among GaN and Si. Significant changes in the XRD intensity of (002) GaN were observed, in the case of 0.4 μm-thick HT GaN film.

In the growth of GaN films, a nucleation layer is used to improve the film quality. This layer is usually a chemical composition similar to GaN but with a large difference in lattice structure and thermal expansion coefficients. The quality deterioration of GaN films was studied with XRD. The results of X-ray θ-2θ scan of all the grown samples clearly revealed that the films had good crystallinity. The diffraction peaks along with the (111) Si diffracted peak at 28.4°. There is no other diffraction peak from the GaN film grown on the Al0.4Ga0.6N-coated (111) Si substrate. The additional peaks correspond to the peak and the linewidth of the near edge band emission being 3.49 eV and 100 meV, respectively. Such a PL result is superior to that obtained in previous studies.

Ferroelectricity in the Diluted Magnetic Semiconductor Phase of ZnO:Co: Marco Aurelio Boselli 1, Itsuo C. da Cunha Lima 2, and A. Ghazali 3, 1Departamento de Física, Universidade Federal de Ouro Preto, Ouro Preto, MG, Brazil; 2Instituto de Física, Universidade de Estado do Rio de Janeiro, Rio de Janeiro, RJ, Brazil; 3Groupe de Physique des Solides, UMR 7688-CNRS, Universités Paris 6 et Paris 7, Paris, France.

Mean field theory using indirect exchange between magnetic impurities in semiconductor predicts ferromagnetism in ZnO:Mn with high transition temperature [1]. Despite the recent interest in high-transition-temperature diluted magnetic semiconductor, the case of ZnO is still under investigation. Co has shown to be more interesting than Mn in what concerns the magnetism of this compound. As in other ferromagnetic semiconductors, two key issues are the occurrence of clustering and the presence of free carriers [2,3]. These two factors are determined, in principle, by the Co concentration in the growth process. We have adapted a spin-polarized quasi-2D RKKY formalism [4] to treat the wurtzite structure. The indirect exchange matrix resulting of this indirect interaction is then used in a temperature dependent Monte Carlo simulation to obtain the average magnetization and the magnetic susceptibility. The Co concentration and the density of free carriers providing the interaction between the magnetic moments are treated as independent parameters. Therefore, we do not have to assume a definite origin for the carriers mediating the interaction, neither effects like compensation. Every Co atom participates of the interaction, either being ionized or not. The Co distribution is assumed to be homogeneous allow the sample. In terms of the in-plane simulation, it is equivalent to assume that a Co atom is equally likely to occupy any Zn site in the structure. Samples containing 5%, 15%, and 25% were simulated both for a thin film and a layered system. The magnetization curve as function of temperature shows the typical shape appearing in other 2D DMS systems [5]. We show how the transition temperature varies with the Co concentration and the density of free carriers. [1] T. Dietl, H. Ohno, and F. Matsukura, Phys. Rev. B 63, 195205 (2001) [2] Jung H. Ohno, and F. Matsukura, Phys. Rev. B 63, 195205 (2001) [3] A. Dadgar, M. Poschenrieder, J. Biasing, and K. Fehse, A. Dadgar, J. Appl. Phys. 80 (2002) 3670. [4] R. Gong, M. F. Yeh, and C.L. Wang, J. Crystal Growth 247 (2004) 261.

A Method for Finding Potential N-type and P-type Impurities for Wide Band-Gap Materials such as Diamond: Adrian E. Mendez and Mark A. Prelas; Nuclear Science and Engineering Institute, University of Missouri-Columbia, Columbia, Missouri.

Wide band gap materials such as Diamond and Diamond-like Carbon DLC are promising materials with a wide variety of potential applications due to their unique properties. Several applications that include high hardness, low friction coefficient, mechanical and electrical properties can be achieved doping diamond crystals with impurities. Two basic processes, dopant diffusion and ion implantation, are the main methods to study the diffusion of impurities in diamond. The introduction of impurities such as B, Li, and Na may change the structure of diamond crystal and the electronic and physical properties such as resistivity, strength, and heat capacity. Our research focus is on the study of a new method of diffusion, the study of elements that can be introduced into the diamond crystal lattice and its characterization. Author: Adrian E. Mendez, Ph.D student. Advisors: Mark A. Prelas Ph.D., Tushar Ghosh Ph.D.

Structural Characterization of GaN Epilayers Grown on Porous Silicon Substrates: Yiting Sun 1,2, Byung-Sung Lee 1,2,3,4, Su-Jeong Jung 1,2,3,4, Byung-Sung O'2 and Jay P. Song 1; 1National Research Laboratory, Materials Evaluation Center, Korea Research Institute of Standards and Science, Taejon, South Korea; 2Photonic Device Group, Samsung Electro-Mechanics, Suwon, South Korea; 3Department of Physics, Chungnam National University, Taejon, South Korea; 4SongHee Industrial Corporation, Sungnam, South Korea.

The structural properties of GaN epitaxial layers grown on PSS(patterned substrate) by MOVCD have been investigated using HRXRD(high-resolution X-ray diffraction), GIXRD(grazing incidence X-ray diffraction), PL(photoluminescence) and TEM(transmission electron microscopy) techniques. The low-temperature GaN nucleation layer and a 0.4 μm-thick GaN layer were grown on both patterned and unpatterned (001) sapphire substrates. For X-ray characterizations rocking curves for GaN (10 0), (00 2), (1 1 0) reflections for which incident angles of
X-rays are 30, 17, 11 and 0.3°, respectively, were measured. For (110) reflection which is perpendicular to the sample surface, GIXRD technique was applied. (105) for (105) reflection, the variation of FWHMs of the rocking curves for patterned substrate were broader than those for unpatterned substrate, for (110) reflection, however, FWHM for patterned substrate was much narrower than that for unpatterned substrate. The normalized FWHM for all reflections decreases as the incidence angle of X-ray decreases. The results suggest that the crystallinity quality in the surface region of the epilayer on patterned substrate was especially improved because the penetration depth of X-ray depends on the wavelength at the depth for (110) reflection is about 40 nm. The improvement of the crystallinity in the surface region is attributed to the reduced dislocation density which was confirmed by TEM image. The intensity of FPL peak of the epilayer for patterned substrate increased compared to that for unpatterned substrate and the result is consistent with the XRD results. A mechanism for the reduction of dislocation density at the surface region will be discussed.

E4.9  
**Defect Modification in GaInNAs Growth with Insertion of GaAs Prewedge.**  S. H. Kang, Mark Wistey, Homan Yuen, Rupel Bae, Lynford Goddard and James S. Harris; Solid State and Photonics Laboratory, Stanford University, Stanford, California.

GaInNAs and GaInNAsSb, grown on GaAs, have emerged as promising active layer materials for lasers covering the entire low-loss fiber bandwidth from 1.2-1.6 μm, but lasing at 1.55 μm has remained illusive. We present an important growth optimization that illustrates the importance of the carrier-extended and point defects in the generation of high-quality dilute-nitride layers by molecular beam epitaxy. A rf plasma cell was employed to generate reactive nitrogen, as is typical for dilute-nitride growth. Substantial defect generation and surface roughness are accompanied by increased optical losses. The results of high-quality dilute-nitride layers by molecular beam epitaxy. A rf plasma cell was employed to generate reactive nitrogen, as is typical for dilute-nitride growth. Substantial defect generation and surface roughness are accompanied by increased optical losses.

E4.10  
**Structural Properties of Thin Oxide Films (ZnO and SnO2) Deposited on Glass and Silicon Substrates.**  Serekkol Zharlygapp-ul Tokmoldin, Bulat N. Mukashev, Nurjan B. Beisenkhanov, Azamat B. Aimgambetov and Irina V. Ovcharenko; Solid State Physics, Institute of Physics and Technology, Almaty, Kazakhstan.

Gas sensitive layers of SnO2 are perspective for making chemical sensors due to their high sensitivity and low cost. Preparation of SnO2 films by RF sputtering from stoichiometry and on the microstructure. The SnO2 films 250-400 nm thickness were deposited on glass substrates using ion-beam deposition technique. Pure oxygen ion beam were formed in a ring-like electrode system with crossed electric and magnetic fields. Discharge power was 300 Wt (3 V, 100 mA), the substrate temperature was 200 C. Pure (99.99%) Sn target was used for the sputtering. Samples and in-situ scanning cathodoluminescence R. but lasing at 1.55 μm for dilute-nitride growth. Substantial defect generation and surface roughness are accompanied by increased optical losses. The results of high-quality dilute-nitride layers by molecular beam epitaxy. A rf plasma cell was employed to generate reactive nitrogen, as is typical for dilute-nitride growth. Substantial defect generation and surface roughness are accompanied by increased optical losses.

E4.11  
**RHEED Oscillation Study of GaAs(311)B Surface.**  Vahid H. Yazdapanah, Z H. M. Wang, S. H. Seydmohamadi and Greg Salamo; Physics, University of Arkansas, Fayetteville, Arkansas.

RHEED oscillations have been intensively studied for the control of growth rates and growth conditions. The oscillation is generally observed under growth conditions that lead to layer-by-layer two-dimensional (2D) growth. During the 2D growth, the surface morphology is dynamically modified by the surface-reaction and coalescence of 2D islands in the growing front. In this work, the surface morphology and growth dynamics of the GaAs(311)B surface has been studied by both in-situ RHEED and in-situ scanning tunnelling microscopy (STM) in the first time. The growth of GaAs(311)B facet is shown at the bottom of the paper. RHEED oscillation is reported on high index GaAs(311)B facet surface with (110) and (111)B facets. The RHEED oscillation was observed only along the [-1-16] direction. Absence of any RHEED oscillations along [1-10], [1-10], and [1-10] indicates a growth model for the GaAs(311)B in which the surface is growing only along (111)B facets although the (110) facets have the same chance to receive the Ga and As atoms. In another word, all deposited material on (110) facets move toward [-1-16] direction in order to form a 2D island. This helps us to better understand the nature of RHEED oscillation on high index GaAs.

E4.12  
**Structural and Electrical Characterization of Fe Implanted GaInP: Interaction of Fe with Ion Induced Defects and Deep Trap Activation.**  Tiziana Cesca 1,  Andrea Gasparotto 1, Adriano Verna 1, Beatrice Fraboni 2, Giuliana Impellizzeri 1, Francesco Priolo 1, Dominico Tarricone 4 and Massimiliano Longo 4; 1Physics Department, INFM and University of Padova, Padova, PD, Italy; 2Physics Department, INFM and University of Bologna, Bologna, BO, Italy; 3Physics and Astronomy Department, INFM and University of Catania, Catania, CT, Italy; 4Physics Department, INFM and University of Parma, Parma, PR, Italy.

Fe is one of the most important transition metal impurities in InP-related materials. Thanks to its mixig deep acceptor character...
it is widely employed to produce highly resistive layers for leakage current blocking and electrical insulation in optoelectronic devices. Moreover, Fe has peculiar optical properties, interesting from both a fundamental and an applicative point of view, related to luminescent emission in the mid-IR region of the electromagnetic spectrum; these can be potentially exploited to produce mid-IR emitter devices, LEDs or laser diodes. In order to display these properties, high concentrations of Fe atoms have to be introduced in substitutional sites in the semiconductor lattice. It has been shown recently that high densities of electrically and optically active Fe centers can be incorporated in InP by high temperature ion implantation and proper post-implantation annealing treatments: by this method both solubility limitations and damage-related undesired redistribution phenomena can be overcome and avoided, creating a supersaturation of substitutional Fe atoms in a slightly damaged crystal (1). Despite the technological interest, the knowledge about the Fe related electrical and optical properties in ternary (and quaternary) InP related materials is still fragmentary. Aim of this work is to extend the results obtained for Fe implantation in InP to these compounds. The main goal is to understand the mechanisms leading to the final location of the Fe atoms and to correlate the structural information (with regard both to the electronic configuration of the Fe) with possible interactions with implant-induced defects) to the Fe-related electrical properties. In this preliminary report we examined single GaN layers, grown by MOVPE lattice matched to GaAs. The role of the implantation damage and dose in determining the crystal damage, and the recovery of this damage by the following high temperature annealing treatments is investigated mainly by RBS-channeling measurements. Channeling is used again, in conjunction with X-ray diffraction (XRD) and High Resolution XRD (HRXRD) to establish the local configuration around the implanted Fe atoms and its modification after the annealing treatments. SIMS depth profiling and HRXRD were also employed to complete the structural characterization. The electrical properties related to Fe implantation are studied by current-voltage measurements on mesa devices, and related to the different implantation and annealing conditions. The deep level properties of the Fe centers were studied by means of Photoinduced Current-Voltage Spectroscopy (PICTS). The results allow a first analysis of the similarities and differences showed by the Fe implanted InGaP with respect to the InP case. (1) T. Cesca et al., Phys. Rev. B 68, 224113 (2003).

E4.14 Transmission Electron Microscopy Study of Nonpolar a-Plane GaN Grown by Penndeo-Epitaxy on (1120) 4H-SiC.


Recent studies have shown that (1120) (a-plane) GaN layers demonstrated polarization free behavior along the growth direction. Such polarization existed in GaN samples grown along [0001] direction. This polarization led to high interface charge densities and spatial separation of the electronic and holes wave functions in GaN-based quantum well structures. Our transmission electron microscopy investigations performed on a-plane GaN grown by organometallic vapor phase epitaxy at 1015°C on 4H-SiC substrate with 10nm AlN barrier layers reveal the high density of threading dislocations 4.0×10^10 cm^-2 and basal stacking faults (BSFs) 1.6×10^7 cm^-2. We applied pendeo-epitaxy (PE) growth on such substrates in order to decrease density of these defects.

Uncoalesced and coalesced a-plane GaN layers with thicknesses 2µm and 12µm, respectively have been studied. Our results show decrease of threading dislocation density from 4.4×10^10 cm^-2 to 2.0×10^9 cm^-2 and BSFs from 1.0×10^9 cm^-2 to 2.3×10^8 cm^-2 in need and twing areas, respectively. These dislocations are mainly partial dislocations which terminate BSFs. Prismatic stacking faults are also observed. Cross-section images reveal cracks and voids at the areas where two coalesced wings meet each other. Formation mechanism of these defects will be discussed in conjunction with epitaxial growth process.


The subsurface damage generated by mechanical polishing of silicon carbide seed wafers was investigated and quantified by plan view transmission electron microscopy (TEM) and atomic force microscopy (AFM). Damage consisting of basal plane dislocations is punctured out up to 400 nm along the scratches during mechanical polishing and up to a total dislocation density of 5×10^10 dislocations/cm^2 is produced. TEM analysis of the Burgers vectors indicates that the initial perfect dislocations have a Burgers vector of ½/√3 a/3 < 1 1 2 0> type then diffuse into a stacking fault bounded by two partial dislocations with Burgers vectors of ½ a/3 < 1 1 1 0> type. The depth of damage was estimated to be up to 50 nm and was confined by AFM on a KOH etched surface. High purity CVD grown 4H-SiC epitayer grown on mechanically polished substrates exhibits threading dislocation pairs along scratches on the surface of the epitayer. The linear dislocation density along the scratch is 8 dislocations/micron.

E4.16 The Influence of Stoichiometry on Growth-in Point Defects and Impurities in PVT Growth 4H-SiC Single Crystals.

Qiang Li, Alexander Poljakov, Mark Paxton and Marek Skowronski 1, 2Center for Electro-Optics Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, Pennsylvania; 2Pennsylvania State University Electro-Optics Center, Freeport, Pennsylvania.

Effects of adding hydrogen into the growth atmosphere during physical vapor transport growth of bulk SiC were studied. It is known that addition of 4-10% of hydrogen decreases the concentration of residual nitrogen donors in SiC boules. It also greatly decreases the concentration of major electron traps with activation energy of 0.4 eV, 0.5 eV, 0.65 eV, and 1 eV. Growth in the presence of hydrogen makes it easier to obtain undoped semi-insulating SiC. The results are explained by enhancement of the carbon transport efficiency by hydrogen and subsequent change in the stoichiometry of the grown crystals toward more C-rich conditions.

E4.17 Engineering of EL2 Related Defects in SI-GaAs using High Energy Light Ion Irradiation. Debdulal Kabiraj and Subhasis Ghosh, 1Nuclear Science Centre, New Delhi, Delhi, India; 2Jawaharlal Nehru University, New Delhi, Delhi, India.

EL2, which is the most extensively studied intrinsic defect in GaAs, has very interesting properties, such as transformation to metastable configuration under sub-band gap light, known as photo-quenching. It is also the most technologically important defect for the production of semi-insulating GaAs. Recently, the interest in EL2 has been revived because several new models have been proposed for the microscopic origin and to settle certain fundamental issues related to EL2. We have shown (1) the existence of several metastable levels related to EL2, providing evidences to support the four-level model (2). Here, we report the effect of high energy light ion irradiation on EL2 and on their related to metastable transformation. Semi-insulating GaAs samples have been irradiated by 50 MeV Li ions with different fluences. The thickness of the GaAs samples and the energy of the irradiated ions are such a way that (i) the range of the ions (200 micron) is more than the sample thickness (150 µm), so the defects are created by the electronic energy loss only, (ii) the samples are not damaged with extended defects which are produced by nuclear energy loss process dominated at the end of the ion range, (iii) mostly native point defects (vacancies, interstitials and antinities) are produced by this method and the irradiation is of sub-band gap, and (iv) the defects are produced uniformly throughout the sample. The defects have been characterized by thermally stimulated current spectroscopy (TSCS) and thermally stimulated Hall voltage spectroscopy (TSHVS) under sub-band gap and above band gap light. We have found that (i) EL2 is a defect complex, most probably composed of three components giving rise to several metastable and stable energy levels, and (ii) it is possible to control the EL2 conduction and hence the semi-insulating property of GaAs by varying the ion fluence. References. [1] D. Kabiraj, Subhasis Ghosh, Appl. Phys. Lett., vol. 84, pp 1713-1715, 2004. [2] A. Fukuyama, T. Ikari, Y. Akashi, and M. Suenitani, Phys. Rev. B, vol. 67, pp 113202-113205, 2003.


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Cadmium Telluride (CdTe) has been successfully employed as room temperature x-ray and gamma-ray detector material in many applications such as medical and industrial imaging, security and monitoring, nuclear safeguards, non-destructive testing, and astrophysics. In order to provide stronger absorption and higher detection efficiency, investigators CdTe samples have been doped with heavy elements such as Bi, Yb, Ge, Yb, Tl, and Hg of different concentrations. However, dopants often form defect complexes, for example vacancy-impurity complexes, which act as carrier trapping and recombination centers and deteriorate the device performance. For this work, defect complexes were characterized by x-ray topography and transmission electron microscopy (TEM) in order to understand the formation, distribution and effect of these complexes on the electrical properties of the material.
spectral shifts, a slight broadening of the absorption and emission was observed in systems CdTe and ZnTe. Moreover, the Cr$^{2+}$ emission dynamics of Cr$^{2+}$ doped samples exhibited the characteristic IR absorption band peaking either in-situ doping or through a thermal diffusion process. All the emission energy between the 5T$_2$ ground state and 5E excited state of Cr$^{2+}$ is observed in ternary Cr: CdZnTe compounds compared to the binary observed spectral blue shift of the Cr$^{2+}$ absorption and emission is due to the decrease in bond-length when going from CdTe to CdZnTe. Based on the work presented in this paper, we present compositional changes in the structure and luminescence properties of a variety of doped samples of Cr$^{2+}$ ions entering into substitutional Zn and Cd lattice sites. The obtained results will be discussed in terms of possible applications of Cr: CdZnTe in IR solid-state lasers and for passive optical Q-switches.

### E4.19 Composition Changes in the Infrared Optical Properties of Cr Doped CdZnTe Bulk Crystals

We are currently investigating the infrared (IR) optical properties of transition metal doped ternary CdZnTe Chalcopyrides for solid-state laser applications and for passive optical Q-switches. In this paper, we present compositional changes in the IR optical properties of Cr$^{2+}$ doped CdZnTe bulk crystals with x = 0, 0.05, 0.1, 0.2, and 1 (ZnTe). Undoped CdZnTe crystals were grown by vertical Bridgman technique. ZnTe was prepared by the physical vapor transport method. Cr doping of CdZnTe was achieved through either in-situ doping through a thermal diffusion process. All the samples exhibited the characteristic IR absorption band peaking between 1800-1900 nm due to the 5T$_2$->5E transition of tetrahedrally coordinated Cr$^{2+}$ ions. The corresponding Cr$^{2+}$ IR absorption and emission shifted to shorter wavelengths with increasing Zn content. This blue shift is due to the decrease in bond-length when going from CdTe to CdZnTe.

### E4.20 Relaxation Mechanism of SiGe Thin Film on SOI Substrate

Zengfeng Di1,2, Miao Zhang 2, Weili Liu 2, Ming Zhu1,2, Chenglu Lin 2; 1School of EEE, Nanyang Technological University, Singapore, Singapore; 2Lan Research Corporation, Fremont, California.

Tantalum oxide films have attracted world-wide interest for memory dielectric in DRAM. However, the leakage current has to be reduced. We used zero-bias thermally stimulated current (ZBTS) spectroscopy to study defect states in tantalum oxide samples. We also performed current-voltage (LV) measurements for the same samples. In this way, we observed several different approaches to reduce defect states and their leakage current.

### E4.21 Phase Field Simulation of Alloying Effects on Metal Silicide

We used zero-bias thermally stimulated current (ZBTS) spectroscopy to study defect states in tantalum oxide samples. We also performed current-voltage (LV) measurements for the same samples. In this way, we observed several different approaches to reduce defect states and their leakage current.

Over the last decade, lasers, detectors and other optoelectronic devices exploiting the unique electronic properties of heterostructures and superlattices have been developed. In many cases, these devices contain extremely thin layers composed of just a few atomic layers of semiconductor material. For example, TiN tends to produce less defect states than Al. Another way to reduce leakage current is by Ti doping.
lowest-energy configuration for the many-electron superlattice. We consider a two-component superlattice made up of a material A and a material B. For this purpose, we self-consistently solved the valence electrons interacting with the bulk A-core lattice, arriving at a self-consistent potential for the material A. Next, using the identical method, we solved for the self-consistent many-electron potential for the material B. Finally, we combined the self-consistent many-electron superlattice potential by solving the many-electron problem on the superlattice ion-core lattice made up of alternating A and B cores; this result represents the true potential of the superlattice. We then used the SEPM prescription, as well as the calculated A potential and the B potential to form the SEPM approximation to the true superlattice potential. Upon comparing the SEPM result with the true potential of the superlattice, we found excellent agreement.\[1\] G. C. Dente and M. L. Tilton, J. Appl. Phys., Vol. 86, no. 3, 1420-1429, (1999).


The diminishing of the size of integrated circuit elements results in an increasing influence of point defects on their electrical parameters and reliability. It has been shown that the vacancy-type defects electron paramagnetic resonance (EPR) signal intensity dependence on the oxidation time is not synchronous. On the other hand, the signal intensity dependence on the oxide thickness reveal a minima or a maxima depending on the oxidation ambient (impurity content). Surface states Ec-0.4eV are identified as interstitial Si atoms. We suggest that the formation of the Si-O-Si bond and the extra free electron in the upper conduction band indicates the creation of a new structural and electronic state which is characterized by an increased electron and hole mobility expected in strained channels.


Admittance spectroscopy measurements on Metal-Oxide-Semiconductor (MOS) devices allow the determination of electronic states at the oxide/silicon interface. The contribution of the AC conductance on the measurements allows the calculation of the interface traps density and the relevant time constant. As shown in recent articles, two equivalent model approaches can be applied in order to explain the experimental results. One model is the classical statistical model based on the Shockley-Read-Hall (S-R-H) recombination statistics and the other one is a model based on the quantum tunneling effect. Recent evidence suggest that the tunneling model can be equivalent to the statistical one when extended to the modeling of the MOS device, creating a so called extended tunneling model. In the present paper, a further investigation on the extended tunneling model is attempted, where the shape of the barrier and the tunneling mechanism are considered as part of the model. Thus, the interface states for MOS devices on Si substrates were studied.

E4.26 A Pulsed EDMR Study of Charge Trapping at P3 Centers. Felice Friedrich, Christoph Boehme and Klaas Lippe; Silizium-Photovoltaik, Hahn-Meitner-Institut, Berlin, Germany.

P3 defects at the (111) oriented crystalline silicon (c-Si) to silicon dioxide (SiO2) interface are strongly localized, paramagnetic point defects whose energy level is distributed in the band gap. Because of this, P3 defects are important trapping and recombination centers of the c-Si/SiO2 interface in this study. In present work, low temperature pulsed electrically detected magnetic resonance (pEDMR) measurements of charge trapping and recombination at paramagnetic P3 centers. The results show that when a conduction electron is trapped, a strongly coupled spin pair consisting of the conduction electron and the defect electron forms prior to their recombimation into the charged P3 ground state. While the ground state is known to exist in singlet spin configuration only, the intermediate state of the electron pair before recombimation can exist in any of four spin eigenstates (three singlet state, and one triplet state) and thus, they can be paramagnetic. This data reveals that the Landé factor difference of the two electrons within these pairs are almost vanishing in X Band (< 50 µT) and that they are, within the measurement accuracy, identical to the Landé factor of the uncharged, singly occupied P3 center. We conclude that trapping and recombination at P3 defects is dominated by direct charge capture and not by tunneling or hopping transitions from other localized states. Different cross sections attributed in previous studies to different interface defect states were identified and the nature of the traps time constant.

E4.27 Strain Relaxation in Semiconductor Thin Films on (001) Oriented Semiconductor Substrates via use of Defected Sub-Surface Layers. Atul Konkar, Materials Science, University of Southern California, Los Angeles, California.

Strained and relaxed Si and SiGe thin films are expected to play an increasingly important role in CMOS in the near future due to the intrinsic mobility expected in relaxed material. The major limitation to the implementation of this strategy has been the high densities of threading dislocations. Amongst the various methods employed, in recent times growth on low-temperature buffer layers followed by annealing has been shown to be the most promising. Both of these methods rely upon creation of engineered sub-surface defect layer. The defected layer is presumably responsible for relaxation of the layers that reside on top; however the exact mechanism of the relaxation is not clear. We will present a structural analysis which clarifies some of the aspects of the relaxation mechanisms. The analysis assumes that the entire relaxation process of the strained layer is due to formation of dislocations and their interaction. The major limitations mentioned above will be diminished if the silicon in the SiGe/Si(001) structures will be clarified. Influence of the defected layer due to its structurally heterogeneous nature and its ability to act as a source and sink for various types of defects will be examined.

E4.28 The Influence of Stress on the Formation of Boron Interstitial Clusters. Michelle Chu and Kevin Jones; University of Florida, Gainesville, Florida.

Stress has become an increasingly important parameter in semiconductor devices. It has been used to tailor mobility of carriers and bandgap engineering. Yet, the effect of stress on front-end process has not yet been sufficiently characterized. This study is undertaken to investigate whether tensile or compressive stress has an effect on Boron Interstitial Clusters. The Interstitial Clusters are inactive immobile species which decrease the active concentration of carriers in semiconducting devices. 300mm n-type CZ grown silicon wafers were implanted with boron at a dose of 1x10^14 cm^-2 and energy of 150keV. The wafers where cut into 1cm x 1cm sample strips and were subsequently subjected to a 4 point bend
which induced 150-250 MPa of tensile or compressive forces in the implanted layer. The strained samples were then annealed in temperatures ranging from 500-700°C for time ranging from 10-60 minutes under N2 ambient. This temperature range is within the region where reverse annealing phenomenon occurs in boron and BIC formation is predominant. Hall Effect measurements will be used to support SIMS data. Plan-view Transmission Electron Microscopy will be used to study how the interstitial population changes with applied stress.

**E4.29** Modeling of Germanium/Silicon Interdiffusion in Silicon/Silicon Germanium Heterostructures.

Mohammed Hasanuzzaman and Yaser M. Hoddara, Department of Electrical and Computer Engineering, McMaster University, Hamilton, Ontario, Canada.

Intermixing at heterointerfaces and the broadening of the SiGe layer in a Si/SiGe/Si single quantum well (SQW) structure can be detrimental to device performance. Thus it is important to develop predictive models for interdiffusion phenomena in heterostructures. In this work, the vacancy flux model [1] is implemented using the FLOOPS-ISE process simulator and used to simulate previously published data [2] on Si-Ge interdiffusion Si0.85Ge0.15/Ge SQW structures grown by MBE and annealed at 900°C, 1000°C, and 1100°C for different anneal times in inert and oxidizing ambients. Our implementation of the model takes into account the conservation of lattice site density to relate the vacancy flux to the flux of the two diffusing species. We also account for the dependence of the vacancy equilibrium concentration and the intrinsic diffusivities of Si and Ge on the Ge fraction. Table 1 lists the values of intrinsic self diffusivities of Si and Ge, a function of Ge fraction compared with published values of [3]-[6]. In all cases, values of D0, int and D0, ext, as a function of Ge fraction were chosen to match the diffusion profile of the Si0.85Ge0.15/Ge system. Since these values were fixed, the diffusion behavior under oxidizing conditions was completely accounted for by the model with no additional fitting parameters. At 900°C, the values of D0, int and D0, ext were much higher than reported values. This may suggest that the vacancy exchange mechanism described by vacancy flux model is the dominant mechanism for Si diffusion at a SiGe/Si interface below 1100°C. For high temperatures (1100°C and above) other diffusion mechanisms (e.g., an interstitial mechanism) might play a major role for interdiffusion to occur. References [1] C.-Y. Tai, Ph.D Thesis, Stanford University, CA, 1997. [2] M. D. Griglione, Ph.D thesis, University of Florida, 1999. [3] N. R. Zaenger et al., Phys. Rev. Lett. 87, 125901 (2001). [4] B. L. Sharma, Defect and Diffusion Forum, 70 & 71, 1 (1999). [5] R. J. Borg, and G. J. Dienes, An introduction to solid state diffusion, (Academic Press, Boston, 1998). [6] P. Laithum et al., Phys. Rev. Lett. 86, 8302 (2002).

**E4.30** Trisilane Based Epitaxy of Biaxially Stressed Silicon Films Doped with Carbon and Arsenic for CMOS Applications.

Matthias Bauer 1, Stefan Zollner 2, David Theodore 2, Michael Liu 3, Alex Barr 1, and Alex Baro 1, Physical Analysis Laboratory Arizona, Freescale Semiconductor Inc., Tempe, Arizona; 2 Advanced Process Research and Development Laboratory, Freescale Semiconductor Inc., Austin, Texas; 3Crolles-2, Freescale Semiconductor Inc., Crolles, France; 4Embedded Systems and Science Research Laboratory, Motorola Inc., Tempe, Arizona; 5School of Micro-electronics, Fudan University, Shanghai, China.

Stressed Si channel CMOS is expected to be implemented in the 65nm and later technology nodes to enhance transistor speed and at the same time maintain high drive current. Various approaches to obtain strained Si channel use meta-stable and stressed structures. Thus, stress-related defect generation can great impact device reliability.

In this paper, we present data on the correlation between defect density and leakage current for conventional strained Si CMOS devices on bulk substrates. Various types of defects (thrending dislocation, misfit dislocations, and interface impurities etc) are detected and analyzed by transmission electron microscopy (TEM) and other techniques. Among these defects, misfit dislocations at the Si/Si1Ge interface appear to have the most negative impact on the leakage current. Structural data will also be presented for more advanced strained Si systems such as strained Si on SiGe/SOI. Germanium upper-diffusion has been studied by scanning transmission electron microscopy (STEM). SGOI-devices processed using optimized thermal budget show minimal Ge diffusion and minimal process related defects. These SGOI devices show improved speed and drive current together with good device reliability (e.g. hot-carrier-leakage and negative-bias-temperature-instability).

**E4.31** Device Parametric Shift Mechanism Caused by Boron Halo Redistribution Resulting from Dose Rate Dependence of SDE Implant.

Ukyo Jeong, Jinjing Liu, Bonain Guo, Kyuha Shim and Sandeep Mehta; Varian Semiconductor Equipment Associates, Gloucester, Massachusetts.

Change in sheet resistance was observed for Arsenic source drain extension (SDE) implants when they were performed at various dose rates. The high dose SDE implant amorphizes the surface of the silicon substrate and the thickness of the amorphous layer is strongly influenced by the rate of dopant bombardment. It is well known that the implantation process introduces excess interstitials. While the amorphous region is completely re-grown into single crystal during subsequent anneal without leaving behind extended defects, interstitials that are injected beyond the amorphous layer lead to formation of {311} defects or dislocation loops in the end of range region. During thermal processing, these extended defects dissolve, release interstitials, which in turn lead to subsequent enhanced diffusion of underlying Boron halo dopant. Dopant depth profiles measured by SIMS revealed different amount of Boron pile-up in the near surface region, corresponding to different SDE implant dose rates. In CMOS devices, this surface pile-up would correlate with a Boron pile-up in the channel region that would lead to a shift in transistor characteristics. Through this investigation, we were able to explain the mechanism causing device characteristics shift resulted from SDE implant with the same dose and energy but different dose rates.

**E4.32** Photovoltaic Infrared Detectors based on HgTe/HgCdTe Superlattices.

Charles R. Becker and Volker Latusek; Physics, University of Wurzburg, Wurzburg, Germany.

The HgTe/HgCdTe superlattice (SL) is of fundamental interest as well as potentially a useful material for infrared opto-electronic devices[1]. The initial interest in these SLs was fueled by the possibility of a more accurate production of the desired cut-off wavelength, and the potential of a lower leak current. In the far infrared, it becomes increasingly difficult to reproducibly grow HgCdTe alloys with the desired band gap. For example, a cut-off wave length of $\lambda = 17.0 \pm 1.0$ μm at 40 K as desired for some space applications, requires a Cd concentration given by $x = 0.206 \pm 0.002$. In other words it requires the Cd concentration to be maintained with a precision of
better than 1.0 %, a difficult task. The same wave length criterion can be satisfied with a HgTe/HgCdTe SL with a HgTe well width of 4.8 nm and a barrier width of 7.4 nm. This gives the SL a slight advantage; however, the potential to reduce leak currents and to suppress auger recombinations is much more important. These SL’s can be designed to reduce leak currents perpendicular to the two dimensional layers of HgTe and HgCdTe; the perpendicular electron effective mass, $m_{\perp}$, can be increased by increasing the HgCdTe barrier thickness. However, the desired vertical transport provides a practical limit for $m_{\perp}$. For example, a possible trade-off given by $m_{\perp} = 10 \text{ m}_e$ = 0.16 $m_0$, can be chosen by selecting a HgCdTe barrier width of 5.0 nm. This gives the SL a slight advantage. In very long wavelength photodetectors [2,3], even though more work on p-type doping questions concerning diffusion, etc. is required. [1] J. N. Schulman, and T. C. McGill, Appl. Phys. Lett. 34, 663 (1979). [2] Y. D. Zhou, C. R. Becker, Y. Chang, R. Ashokan, R. T. Boreiko, D. J. Smith, A. L. Bets, S. Sivanathan, J. Electr. Mat. 32, 508 (2003). [3] Y. Selanet, Y. D. Zhou, Y. Zhao, Y. Chang, C. R. Becker, R. Ashokan, C. H. Grein and S. Sivanathan, J. Electr. Mat. 33, 503 (2004).

E4.84 Impact of Small Misceuts of (0001) Sapphire on the Growth of AlGaAsx-xN /AIN Superlattices with a 5 um X 5 um Scan. Thermal dynamics and kinetics during the growth are the key parameters. This has received much attention because of its simple structure and ease in fabrication. A Curie temperature of 285 K [1] has been measured. XRD Williamson-Hall Plot are consistent with the chemical etching method. We found the surface morphologies can be easily controlled by the different substrate miscut angles. The 1-2 monolayers (MLs) step flow morphology for normal- or substrate changed to step bunches of 10 MLs height for 0.5° off. The dislocation densities observed by XRD Williamson-Hall Plot are consistent with the chemical etching method. We found the surface morphologies can be easily controlled by the different substrate miscut angles. The 1-2 monolayers (MLs) step flow morphology for normal- or substrate changed to step bunches of 10 MLs height for 0.5° off. The dislocation densities observed by XRD Williamson-Hall Plot are consistent with the chemical etching method.

E4.85 Magnetic and Transport Properties of Ge: Mn Granular System. Wu Yihong1,2, Li Hongliang1,2, Liu Tie1,2, Wang Shijie1,2 and Guo Zailong1,2. 1Electrical and Computer Engineering, National University of Singapore, Singapore, Singapore; 2Data Storage Institute (DSI), Singapore, Singapore; 3Institute of Materials Research and Engineering (IMRE), Singapore, Singapore.

Among the different types of diluted magnetic semiconductors (DMSs) which are being intensively studied, the Ge-based group IV system has received special attention because of it's simple structure and ease in fabrication. A Curie temperature of 285 K [1] has been reported for epitaxially grown samples. However, it is still not clear if the ferromagnetic properties originate from carrier-mediated ferromagnetism [1] or due to the clusters of GeMn phases. In this work, we fabricated thin films containing GeMn nanocrystallites in an amorphous host matrix, using MBE at a base pressure of 10^{-8} Torr. The typical substrate temperature, growth rate and film thickness are 570 K, 0.08 monolayers/nm, respectively. Using TEM and XRD observations show that the thin film is polycrystalline embedded in an amorphous host matrix. The ZFC and FC measurements showed a Curie temperature of about 285 K, suggesting that the nanocrystallites are either Ge$_2$Mn$_3$ or Ge$_3$Mn$_2$. The M-H curves show characteristic up to 290°, which is a slight difference. However, some scatter has been observed in the temperature-dependent resistivity. The i-V curves measured by a 4 probe technique show a nonlinear behavior in temperature range from 10 K to 300 K, which might be caused by the formation of either Schottky junctions at the nanocrystallite-amorphous interface or tunnel junctions between the nanocrystallites. A zero bias anomaly was also observed in the dI/dV curve when the sample is cooled to below 30 K. We are now fabricating the thin films into nanowires with different dimensions to study the electrical transport properties and correlate them with magnetic contrast.[1] Sunglue Chao et al., Phys. Rev. B 66, 033303 (2002)

E4.36 Radiative Versus Nonradiative Decay Processes in Germanium Nanocrystals Probed by Time-resolved Photoluminescence Spectroscopy. E. B. Gol1, R. Kweon Sanchratty2, B. K. Panigrahi3, and K. G. M. Nair4. 1Department of Physics, Indian Institute of Technology Guwahati, Guwahati, Assam, India; 2Materials Science Division, Indira Gandhi Center for Atomic Research, Kalpakkam, Tamil Nadu, India.

Si and Ge nanocrystals (NCs) have attracted much interest because of their potential application in Si-based optoelectronics, nanophotonics, and electronic/optical memory devices. In contrast to Si NCs, Ge NCs exhibit direct band gap nature and stronger confinement effects and has great potential for optoelectronic and memory device applications. However, the role of defects in the optical properties of the Ge NCs is not clearly understood. In this work, we have investigated the contribution of surface defect states by using time-resolved photoluminescence (PL) from ion-beam synthesized Ge NCs embedded in SiO$_2$ using a 4 probe technique and resolution time PL measurements. Ge nanocrystals of diameter 4-15 nm were grown embedded in thermally grown SiO$_2$ layer by Ge ion implantation and subsequent annealing. X-ray diffraction and Raman (optical and low frequency) measurements were performed to study the evolution of NCs as a function of ion dose and annealing conditions. Steady state PL spectra show a peak at 2.1 eV originating from n-Ge and another peak at 2.3 eV arising from ion-beam induced defects in the SiO$_2$ matrix. Time-resolved PL studies reveal double exponential decay dynamics in the nanosecond time scale. The faster component of the decay with time constant 1.3 ns is attributed to the Si or Ge and slower, and has been identified as having a radiative lifetime, since the time constant reduces with increasing defect density. The slower component with time constant 12 ns is attributed to the radiative recombination at the Ge nanocrystals. Our results are in close agreement with the theoretically predicted radiative lifetime for small Ge NCs. These results suggest that the defects at the surface of the Ge NCs primarily control the light emission and vibrational properties of the Ge NCs.
roughening. Rapid edge diffusion is required to explain the shapes of the observed roughening at low temperatures. This result suggests that the roughening by annealing plays a key role during the ion-induced pattern formation. * Partially supported by the Air Force Office of Scientific Research.

**E4.38**

Elastic Stress Relaxation at Nanoscale: A Comprehensive Theoretical and Experimental Investigation of the Dislocation Loops Associated with As-Sb Nanoclusters in GaAs.

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A comprehensive experimental and theoretical investigation was performed for the system of As-Sb nanoclusters and nanoscale dislocation loops in GaAs/Sb films grown by molecular beam epitaxy at low temperatures. A subsequent ab initio model was developed for the elastic stress relaxation, self-energies and interactions in such cluster-loop nanosystems. The model was based on the experimental investigation of the microstructure of the As-Sb nanoclusters by transmission electron microscopy. The atomic structures of the As-Sb nanoclusters and dislocation loops, as well as their orientation relationships were determined. A strong anisotropic mismatch between the As-Sb nanoclusters and GaAs matrix has been revealed. This mismatch was proved to be a reason for the formation of the prismatic nanoscale dislocation loops nearby the nanoclusters. Our theoretical model explores the elastic properties of an inclusion with uniaxial dilatation. For such inclusions, the elastic stresses and stored energy are determined in a closed analytical form. The theoretical analysis predicts a specific non-linear dependence of the dislocation loop diameter on the cluster diameter, which fits well the experimentally observed one. It is demonstrated that both the change in the inclusion orientation due to diminishing dilatation and the interaction between the dislocation loop and inclusion are important in the relaxation phenomena of stressed nanoscale inclusions in semiconductors.

**E4.39**


Tin dioxide is a wide band gap semiconductor whose technological applications largely depend on the electronic properties of both bulk and surface defects. In this presentation, we discuss the electronic properties of low-density monolithic nanocrystalline SnO2 aerogels synthesized using the epoxide sol-gel method recently developed in our laboratory. Transmission electron microscopy shows that such aerogels are formed by few-nanometer-size particles randomly interconnected into a solid network with a large degree of porosity (> 90%) and high surface area. We study the electronic structure of these nanocrystalline aerogels by synchrotron-based soft x-ray absorption near-edge structure (XANES) spectroscopy at O K as well as Sn M2,3 and M4,5 edges. In such measurements, we study the dependence of the element-specific density of states (PDOS) in the conduction band on (i) porosity (or the undercoordinated surface atom fraction), (ii) the size and crystallinity of ligaments of the nanoflakes, and (iii) the dose of soft x-ray irradiation. Both bulk-sensitive fluorescence and surface-sensitive electron yield detection methods are used. Experimental results are also compared with PDOS calculations. Results show that both soft x-ray irradiation and the presence of undercoordinated surface atoms can induce Sn-related electronic states of f and d symmetry close to the conduction band minimum. These results demonstrate a successful application of XANES spectroscopy to study defect-related electronic states in wide band gap semiconductors. This work was performed under the auspices of the U.S. DOE by the University of California, LNL under Contract No. W-7405-Eng-48.

**E4.40**

Infrared Spectroscopy of Impurities in ZnO Nanoparticles.

W. M. Hsing Oo and M. D. McCluskey; Department of Physics, Washington State University, Pullman, Washington.

Semiconductor nanoparticles have a range of potential applications in electronic, optoelectronic, and spintronic devices. Zinc oxide (ZnO), a wide-bandgap semiconductor, has emerged as an important material for such applications. In this work, impurities in ZnO nanoparticles were investigated with infrared (IR) spectroscopy. Nanoparticles with diameters of 15 nm were synthesized by a reaction of zinc acetate and sodium hydroxide carbonate. IR spectroscopy showed the presence of CO2 impurities in the ZnO nanoparticles. Isotopic substitution was used to verify the frequency assignment. By using different carbon isotope compositions in the precursor materials, peak intensities at 2342 cm\(^{-1}\), 2277 cm\(^{-1}\), and 2250 cm\(^{-1}\) varied according to the 12C\(_2\) and 13C\(_2\) concentrations. These results demonstrate conclusively that the impurities originated from the precursors. Isochronal annealing results revealed that the CO2 molecules are stable at elevated temperatures. The stability of the impurities is markedly different from that of CO2 adsorbed on bulk ZnO surfaces where the molecules are unstable at room temperature. By comparing our observations with studies of CO2 trapped in carbon nanotubes [J. Phys. Chem. B 107, 12030 (2003)], we conclude that the molecules are located inside the ZnO nanoparticles. In addition to unintentional CO2 impurities, experiments were performed to intentionally introduce hydrogen into ZnO nanoparticles. Our results show that post-growth annealing in hydrogen ambient dramatically changes the IR transmission properties of the nanoparticles. This change is presumably due to the increase in free carrier concentration brought about by the introduction of hydrogen donors. A comparison between hydrogen in bulk and nanoscale ZnO will be made. This work was supported by the National Science Foundation and the ACS Petroleum Research Fund.

**SESSION E5: Novel Materials, Synthetic Structures and Nanomanipulation of Defects/Dopants**

Chairs: S.R. Schofield and M. Tabe

Wednesday, March 30, 2005

Room 2006 (Moscone West)

**8:30 AM** E5.1

Electrical Transient Based Defect Spectroscopy in Polymeric and Organic Semiconductors.

Vishal Varshney 1, Vineet Rao 1,2, Samarendra P. Singh 1,3 and Girija S. Samal 2,1, 1Samtel Centre for Display Technology, Indian Institute of Technology Kanpur, Kanpur, U.P., India; 2Materials Science Programme, Indian Institute of Technology Kanpur, Kanpur, U.P., India; 3Department of Physics, Indian Institute of Technology Kanpur, Kanpur, U.P., India.

Organic semiconductors are emerging as attractive material base for many display and electronic applications, specially as light emitting diodes and thin film transistors. Though there has been considerable progress in device structures and materials, there is a lack of studies on relation between electrical defects and degradation, which is necessary to understand trapping and other charge processes in these devices. In this paper, we study defect related charge processes using electrical transients in polymeric and organic diodes. We use popular light emitting diode structures consisting of ITO/PPV/CN-PPV/AI, and similar structures wherein the active layers are based on small molecules. We monitor slow charging and discharge currents as a function of time for both virgin and electrically aged devices. The current and charge transients are analyzed spectroscopically in time domain using a technique called Time Analyzed Transient Spectroscopy, which is similar to DLTS in its implementation. We observe highly stretched exponentials over 4 orders of magnitude in time up to thousands of seconds. We study the existence of large distribution in time constants. In addition we are able to separate out distinctly trap-like sources of charge emission corresponding to localized states. We demonstrate both the need, and our ability to distinguish between trapable and irreducible nature and trap like behavior in organic semiconductors.

**9:00 AM** E5.2

Rare-Earth Doped Silicon Nanoclusters for Microphotonics.

Francesco Priolo 1, Domenico Pacifili 1, Giorgio Franzo 1 and Fabio Iacono 2, 1Dept. Physics & Astronomy, MATIS-INFM & Univ. Catanias, Catanias, Italy; 2IMM, CNR, Catanias, Italy.

Silicon has an indirect band gap electronic structure and for a long time it has been considered a quite poor light emitter. In the last decade, a strong effort has been devoted towards the achievement of efficient light emission from silicon. Among the others, rare earth-doping of Si nanostructures has been shown to be one of the most promising methods. Indeed, light emission two orders of magnitude more efficient than in pure silicon has been obtained from different rare earths, due to the strong sensitization action of rare earth through ion implantation, the Si nanocrystals are able to recrystallize them. Indeed it is demonstrated that as crystalline Si clusters are able to act as efficient sensitizers for the rare earths. Moreover, it is shown that the light emission efficiency of Er can be enhanced by increasing the number of sensitization centers. Aim of this work is to understand the details of the interaction mechanisms occurring between Si nanoclusters and the rare earth ions, with a particular attention to the Er-doped Si nanoclusters system. A model based on an energy level scheme taking
into account the coupling between each Si nanocluster and the neighboring Er ions will be reported. Through a comparison with photoluminescence data, a value of 3(10)-15 cm/s 1 for the diffusion coefficient has been determined. Moreover, an energy transfer time of 1 ms has been estimated, confirming that Si nanoclusters can actually play a crucial role as efficient sensitizers for Er. However, a strong correlation exists between the device efficiency and the diffusion time of the Er ions and characterized by a coefficient of 7x10-17 cm s-1 for Er ions in silica nanocluster, in determining positive gain at 1.54 mm will be investigated in details, and the implications of the diffusion coefficient for the overall efficiency of the energy transfer mechanism will be discussed.

In the present work, due to the finite energy transfer time and the sequential nature of the interaction mechanism, it is shown that pulsed excitation of the Er-doped nanoclusters system with time duration comparable to half of the Er energy transfer time will lead to excited states. On the other hand, under continuous wavelength excitation, as much as 30-40 Er ions can be excited by a single nanocluster, thus making it possible to obtain population inversion. The feasibility of efficient electrical pumping of bound states in nanoclusters and rare earth doped Si nanoclusters embedded in light emitting diodes will be demonstrated. The impact of these findings on the future development of all Si based microphotonic will be discussed.

9:30 AM E5.5 Efficient Spin Injection from NiFe/CoFe into GaAs in Spin-LED Structures. Shin Kim1, Jung Ho Choi1, Donggi Choi1, Jungho Oh1, Hong Chul Hwang2, Kwang Yoo Kim3 and Dong Geun Oh1; 1Department of Physics, Chungnam National University, Daejeon, South Korea; 2Korea Institute of Science and Technology, Seoul, South Korea; 3Korea Basic Science Institute, Daejeon, South Korea.

Ferromagnetic metal (FM) layers of NiFe/CoFe were deposited on top of GaAs-based light (LED) emitting diodes) structures to study electrical spin injection from FM to a semiconductor. The active layers consisted of either undoped or p-doped 30 nm GaAs layers. The samples were mounted in a superconducting magneto-optical cryostat and spin polarizations were measured from the circular polarization of the light emitted from the LED surfaces. In the spectrum of the spin-LEDs, a transition due to bound exciton was dominant at lower temperatures and at higher temperatures free excitonic transition became dominant. The circular polarization of the free excitonic transition was about 15% at 20 K, whereas that of the bound exciton was almost negligible. At relatively high temperatures, the contribution from the light hole became evident, and the contribution from both the heavy and light hole transitions could be separated using a photoelastic modulator together with a monochromator.

For three weeks of operation of the devices, we found that another bound exciton transition appeared and its intensity gradually increased in time, indicating the diffusion of impurities into the active layers.

10:15 AM E5.6 Polyisilicon Memory Switching: The Role of Crystalline Defects. Brad Herren, Carole Jahn and Don Kidwell; Matrix Semiconductor, Santa Clara, California.

Polyisilicon memory switching is demonstrated in vertical n-i-p diodes with TiN contacts using 0.15 μm technology. Polyisilicon memory switching describes the large change in resistance of the material after high voltage biasing. The forward diode current at ±2 V increases by 5 orders of magnitude after a 48 V pulse. A diode rectification ratio of 105 at ±2 V is achieved after high voltage pulse. When TiSi2 is used to contact the p5 cell diode terminal instead of TiN, and the silicon is crystallized after TiSi2 formation, memory switching is eliminated, with equivalent forward current in the diode before and after a 48 V pulse. Transmission electron microscopy reveal a remarkable difference diodes with memory switching (TiN contact) had a high density of silicon grain boundaries and twin defects, while diodes without memory switching (TiSi2 contact) contain few grain boundaries or twin defects. The reduced defect density is consistent with C40 phase TiSi2-seeded crystallization of silicon. These defects are barriers to current flow in the diode, and play a major role in polyisilicon memory switching. The defect-based barriers are reduced by high voltage pulse.

11:15 AM E5.6 Polysilicon Memory Switching: The Role of Crystalline Defects. Brad Herren, Carole Jahn and Don Kidwell; Matrix Semiconductor, Santa Clara, California.

The ability to control the position of dopant atoms in semiconductors with atomic-scale precision has enormous potential for the creation of atomic-scale electronic devices. Here, we demonstrate the positioning of individual P atoms into substitutional Si(001) surface lattice sites with 1 Å accuracy. This result constitutes the first demonstration of the atomic-scale precise positioning of individual atoms in a semiconductor surface and opens an exciting new path to fabricating novel nanoscale atomic-scale devices, e.g., quantum cellular automata, neuromorphic devices such as single electron transistors and the key functional element (qubit) of a solid-state quantum computer. The strategy that we use is as follows. A highly-confined electron beam generated from a scanning tunneling microscope (STM) is used to selectively desorb individual H atoms from a H-terminated Si(001) surface [3]. This patterned H-layer forms a lithographic mask to control the adsorption of phosphine (PH3) molecules, which randomly diffuse to the regions of bare Si exposed by the STM tip [4], as proposed by Tucker et al. [5]. Finally, the individual P atoms from the adsorbed PH3 molecules are incorporated into the top layer of the Si(001) surface using a thermal atomic beam, where P atoms displace a surface Si atom to form a P-Si heterostructure. In order to demonstrate the above process it was necessary first to obtain a detailed understanding of the surface chemistry and chemistry of the interaction of PH3 with Si(001). We studied this system using a variety of techniques over the past two decades, recent observations have revealed that this interaction is much more complex than previously thought [6]. We have combined atomic-resolution STM studies with detailed density functional theory calculations to understand the mechanism of dissociation of PH3 and the substitutional incorporation of P to Si(001). Key results of this mechanism will be presented culminating with the demonstration of the incorporation of single P atoms into Si(001) with 1 Å precision. N. Völkel, S. R. Schofield, E. Stach et al. Phys. Rev. Lett., 91, 136104, 2003. [2] E. Stach, J. L. Macdonald, J. V. Waszczak, J. C. Tsang, D. V. Talapin, S. R. Schofield, E. Stach et al. Phys. Rev. Lett., 91, 136104, 2003. [3] J. R. Tucker and G. C. Schatz, Solid-State Sci., 12, 1061, 1998. [4] J. R. Tucker and T. C. Shen, Solid-State Sci., 12, 1061, 1998. [5] H. F. Wilson, O. Warschkow, N. A. Marks, S. R. Schofield, et al. Accepted for publication in Phys. Rev. Lett. (2004).

10:45 AM E5.5 Imaging Electrically Deactivating Defects in Si One Impurity at a Time. Paul Voyles1, David Muller2 and John Graual2; 1Materials Science and Engineering, University of Wisconsin, Madison, Wisconsin; 2School of Applied and Engineering Physics, Cornell University, Ithaca, New York.

We have demonstrated the first images showing statistically significant contrast from single impurity atoms inside a host crystal using annular dark-field (ADF) “Z-contrast” STEM on heavily sulfur-doped Si [1]. These images showed that the electrically deactivating defect in low-temperature MBE grown Si-doped Si must contain only two Sb atoms. For a given layer, the strain sensitive ADF and high-angle Z-contrast images measured the off-site displacement of the Sb atoms due to the deactivating defects. These images lead to the proposal of a new deactivating defect, the donor-pair vacancy-interstitial complex [2]. Expected new aberration-corrected STEMs, these techniques are generally applicable to image high-z impurities in low-zenith hosts, one impurity at a time. [1] P. M. Voyles, D. A. Muller, J. Graual, P. H. Citrin, and H.-L. Gossmann, Nature 416, 826 (2002). [2] P. M. Voyles, D. J. Chadi, P. H. Citrin, D. A. Muller, J. L. Graual, P. A. Northrup, and H.-L. Gossmann, Phys. Rev. Lett. 91, 125505 (2003).
deformation mechanisms. The loads required to produce sub-150 nm width indentations in GaAs are in a lower regime of ∼0.2 mN. These loads approach incipient plasticity behavior of GaAs. At such low loads and small scale, the preparation of the sample for TEM becomes difficult and extremely so for cross-sectional TEM, as the indent is difficult to locate and image, and sample manipulation must be performed delicately to maintain damage to the indenter. Indents of less than 200 nm in size were generated using loads below 450 uN with a sharp cube corner indenter. The subsurface deformation of the nanoindentors was studied by cross-sectional transmission electron microscopy. A focused ion beam system was used to prepare the electron transparent areas through the indents. The deformation mechanisms and plastic zone were analyzed as a function of load. The crystal was observed to deform solely by dislocation activity with no evidence of amorphization, twinning, or nanoindentation transformation. Comparison of plastic zone size with the residual indent impressions indicate that the plastic zone extends approximately 1.5 times the indentation depth and 1.5 times the width. These findings are being correlated to the growth of quantum dots on the indentation sites. The success of this work could lead to a relatively simple and inexpensive process for the development of various kinds of electronic-photonic devices, for example, on-chip optical communication using quantum dots.

11:45 AM E6.1
Hydrogen in GaMnAs: Engineering of Magnetism by Defects.
Martin S. Brandt1, Christoph Bihler1, Hans Huebl1, Sebastian T. B. Goennenwein2, and Wladimir Schoch3
1Department of Engineering, Australian National University (ANU), Canberra, Australian Capital Territory, Australia; 2National Renewable Energy Laboratory, Golden, Colorado; 3BP Solar, Fredrick, Maryland.

Hydrogen in GaMnAs: Engineering of Magnetism by Defects.

Manganese acceptors in GaPAs provide both the localized magnetic moments as well as the itinerant holes necessary to obtain a ferromagnetic semiconductor. Recently, Bouamani-Rabhi, Lemaitre and coworkers as well as our group have shown that the hole concentration in this material can be adjusted independently from the concentration of Mn by post-growth incorporation of hydrogen. When hydrogen is introduced in concentrations similar to the Mn concentration, thin films of GaMnAs, which are ferromagnetic and metallic in their as-grown state, become semiconducting and paramagnetic in the hydrogenated state. FTIR experiments indicate that Mn-As-H complexes are formed, which lead to the observed passivation of the Mn acceptors. In this contribution, we address two important issues concerning H in GaMnAs: the lattice expansion upon hydrogen incorporation and the diffusion of hydrogen through GaMnAs. GaMnAs thin films grown at low-temperature molecular beam epitaxy were hydrogenated or deuterated at 170°C with the help of a DC plasma operating at 0.3 mbar. X-ray diffraction shows that both the as-grown and hydrogenated GaMnAs are pseudomorphically strained. Upon hydrogenation, the unstrained lattice constant of the GaMnAs epilayer increases by Δa/na=0.6x10^{-2} cm^2/H. This increase is markedly lower than the corresponding increase in hydrogenated Si:B of 2.4x10^{-2} cm^2/H, where B is incorporated as a donor to form a donor-center. This difference can be attributed to the fact that H is built into GaMnAs on a lattice site which leads to a small lattice dilatation only such as the antibonding site. The effective contrast of hydrogen in GaMnAs is determined via measurements of the fcc-morphotropic phase boundary to the tetragonal phase and the hysteresis loop of the hole concentration, the spin wave resonances observed are localized at the surface and therefore are very sensitive to short hydrogenation treatments. The temperature- and time-dependence of the shift of the collective spin-wave mode upon hydrogenation and anneal and the comparison of these shifts to those found upon wet-chemical etching of the films show a critical balance between in-and out-diffusion at the temperatures used. Such brief hydrogenation treatments can be used to change the magnetic properties of the ferromagnetic thin films such as the magnetic anisotropy and therefore allow a magnetic device engineering via defects.

SESSION E6: Defects in Devices
Chairs: Peter Kiesel and W.C. McColgin
Wednesday Afternoon, March 30, 2005
Room 2006 (Moscone West)

1:30 PM *E6.1
Electronically Stimulated Degradation of Crystalline Silicon Solar Cells.
Erik Kortenbaas1, Daniel Macdonald3, James Adey3, Robert Jones3, and Derek Palmer3; 1Institute of Solar Energy Research Hämeln/Emmerthal (ISFH), Emmerthal, Germany; 2Department of Engineering, Australian National University (ANU), Canberra, Australian Capital Territory, Australia; 3School of Physics, University of Exeter, Exeter, UK and King’s College, London, UK.

Carrier lifetime degradation in crystalline silicon solar cells under illumination with white light is a frequently observed phenomenon. The two main causes of such degradation effects have been identified in the past, both of them being electronically driven and both are related to the most common dopant element, boron: (i) the dissociation of interstitial iron-substitutional boron (Fe,B,) pairs and (ii) the formation of recombination-active boron-oxygen complexes. In solar-grade multicrystalline silicon (mc-Si), the first mechanism is most relevant. This well-known process, which is linked to the degree of iron contamination in the material, can also be observed in single-crystalline iron-contaminated B-doped float-zone (FZ) and Czochralski (Cz) silicon and is not restricted to mc-Si. The second carrier lifetime degradation effect can be observed in metal-impurity-free B-doped Cz-Si rich in oxygen. This effect is attributed to the simultaneous presence of B, and interstitial oxygen (O). Interestingly, as for the Fe,B, dissociation, this degradation effect also occurs in the dark when minority-carriers are injected (e.g., by a forward-biased pn junction), leading to the conclusion that the degradation is caused by the presence of minority-carriers and that photons are not directly involved. However, in contrast to the Fe-B-,related lifetime degradation, which also occurs during annealing above 100°C, the latter degradation effect is fully reversible by annealing above 200°C, i.e., the degraded lifetime recovers during low-temperature annealing, making it relatively easy to distinguish between the two effects. Much research has been devoted to the boron-oxygen-related degradation problem, which is presently the main obstacle for making single-crystalline Cz-Si an ideal cost-saving material for high efficiency solar cells. Only about 1% efficiency, indicating presence of other performance limiting mechanisms. Our analyses have identified this mechanism to be related to a new type of defect, now called a defect cluster. Defect clusters occur during crystal growth and form filament-like structures. This effect is attributed to the simultaneous presence of B, and O, complex, acting as a highly effective recombination center. Results of theoretical calculations using density functional theory show that B,O, is a bistable defect with a donor level in the upper half of the silicon band gap, in good agreement with the results of temperature- and injection-dependent lifetime measurements. Calculated activation energies for the dissociation and association of the B,O, complex are also in excellent agreement with the barrier energies determined experimentally on lifetime samples and solar cells.

2:00 PM E6.2
Efficiency Limitations of Multicrystalline Silicon Solar Cells Due to Defect Clusters.
Bhushan Sopori1, Chuan Li1, S. Narayan2 and Dave Carlson3; 1National Renewable Energy Laboratory, Golden, Colorado; 2National Renewable Energy Laboratory, Golden, Colorado; 3BP Solar, Fredrick, Maryland.

The current methods of impurity gettering and defect passivation yield commercial solar cells reaching, in most cases, only about 15% efficiency, indicating presence of other performance limiting mechanisms. Our analyses have identified this mechanism to be related to a new type of defect, now called a defect cluster. Defect clusters occur during crystal growth and form filament-like structures. This effect is attributed to the simultaneous presence of B, and O, complex, acting as a highly effective recombination center. Results of theoretical calculations using density functional theory show that B,O, is a bistable defect with a donor level in the upper half of the silicon band gap, in good agreement with the results of temperature- and injection-dependent lifetime measurements. Calculated activation energies for the dissociation and association of the B,O, complex are also in excellent agreement with the barrier energies determined experimentally on lifetime samples and solar cells.

The input data to the model comes from LBIC measurements, defect maps, and a data bank that relates dark current components on the model of the total cell and spatial distribution of cell voltages as a function of load. The model takes into account the cell area, quality of the base material (the regions with no defects), and the depletion region, and the cell performance is limited by the dissolution of impurities only, and cell processing technology. (vi) Defect clusters
produce an efficiency loss of 3 to 4 absolute points in efficiency. To overcome this, several techniques have been developed to suppress or manage these defects, such as optimizing the post-implant anneal conditions, using different wafer vendors, and employing gettering processes to reduce impurities.


3:15 PM E6.5


depending on fabrication parameters and annealing conditions such as the ion species, energy, dosage, and annealing temperature and time, the defects may be interstitial clusters. \{11\} perfect Frank dislocation loops along c<110>, Si, \{111\} perfect prismatic dislocation loops with a Burgers vector of a/2<110>, and \{111\} faulted Frank dislocation loops with a Burgers vector of a/2<11\\rangle. Here, a is the lattice constant of silicon. We studied the electron-beam-induced current (EL) and photoluminescence (PL) of boron-implanted p+ junction silicon light-emitting diodes in correlation with the implant-induced defects of different types and their combined effects. We found that the extended defects of different types and by using plan-view transmission electron microscopy (PTEM) to identify them, we found that \{113\} defects along \{110\} are the ones that result in strong silicon light emission. The \{113\} defects are related to silicon band-edge recombination. The high light emissions resulting from the \{113\} defects are attributed to their highly localized strain fields, which create effective potential wells for both electrons and holes and hence enhance the radiative decay of carriers localizing them in the radiation-damaged regions.

We have observed similar effects in Si nanophotonics. Measurements of both EL and PL at low temperatures indicated that the emissions from extended defects are related to silicon band-edge recombination. The high light emissions resulting from the \{113\} defects are attributed to their highly localized strain fields, which create effective potential wells for both electrons and holes and hence enhance the radiative decay of carriers localizing them in the radiation-damaged regions.

We have observed such rings in n epilayers on n wafers and p epilayers on p+ wafers, including silicon from different wafer vendors. Striations in images have been previously reported, but the explanations do not seem to apply. We will show that the defects that give rise to these dark-current rings can be correlated with substrate properties. L. Jastrzebski, P.A. Levine, A.D. Cope, W.N. Henry, and D.F. Battson, "Material Limitations Which Cause Striations in CCD Imagers," IEEE J. of Solid-State Circuits SC - 15, 739 (1980).

3:30 PM E6.5

Silicon Light Emissions from Boron Implant-Induced Extended Defects. Grant Z. Pan 1, Ronald P. Ostrounlova 2, Yaguang Lian 1, Liping P. Ren 2, and Kang L. Wang 2; 1Microfabrication Laboratory, University of California at Los Angeles, Los Angeles, California; 2Device Research Laboratory, and MARCO Focus Center on Functional Engineered Nano Architectonics-FENA, University of California at Los Angeles, Los Angeles, California; 3Nanoarchitectonics and Nanophotonics Laboratory, Global Nanosystems, Inc., Los Angeles, California.

Efficient silicon light-emitting diodes (Si LEDs) can allow integration of optics with electronics in high-density Si nanoelectronic integrated circuits [1]. It was reported that a planar p-n junction Si LED integrated with boron implant-induced extended dislocation defects could have quantum efficiency as high as 10^{-3} [2]. There are types of extended defects that develop during the post implant anneal [3]. Depending on implant parameters and annealing conditions such as the ion species, energy, dosage, and annealing temperature and time, the defects may be interstitial clusters. \{11\} perfect Frank dislocation loops along c<110>, Si, \{111\} perfect prismatic dislocation loops with a Burgers vector of a/2<110>, and \{111\} faulted Frank dislocation loops with a Burgers vector of a/2<11\\rangle. Here, a is the lattice constant of silicon. We studied the electron-beam-induced current (EL) and photoluminescence (PL) of boron-implanted p+ junction silicon light-emitting diodes in correlation with the implant-induced defects of different types and their combined effects.

We first show that the hole-enhanced direct dissociation of a passivated dangling bond, a mechanism that is commonly invoked as the first step during NBTI degradation, is actually not activated under standard NBTI stress conditions. Instead, we find that the most likely mechanism is the release of hydrogen atoms bound in the substrate, particularly at dopants, which then de-passivate dangling bonds. Hydrogen release from dopants is greatly enhanced in the depletion region, where the substrate is driven into inversion, as happens under typical NBTI stress conditions. Thereupon, they are swept to the interface of the applied negative bias. Once at the interface, these protons can either de-passivate Si-H bonds to create interface traps, or enter the oxide to contribute to oxide trapped charge. The combined effects of the drift of protons and the reaction of the oxide and the passivation reaction act as a sink for hydrogen motion that drives the NBTI degradation process. We show that this scenario is consistent with a number of key experimental NBTI features. First of all, we explain the observed pinning point of the threshold voltage degradation, which is concentration and field-dependent, by the reaction-limited and diffusion-limited, possible depending on the stress time and temperature. We also show that the obtained activation energy in each case is in agreement with measured values. We then discuss the role of the polarity of the substrate (n-type or p-type), the polarity of the applied bias, and the possible role of water...
or hydrogen molecules, on the overall degradation.

The single-electron-tunneling device (SED), which has quantum dots (QDs) in its channel to control the charge state level of an elementary charge. The single-electron-pump and tunneling are members of the SED family and enable single-electron transfer synchronized with the gate clock. They have the potential for extremely low power consumption. Therefore, studies are thus expected to be building-block devices for future information processing. We have been pursuing the fabrication of silicon-based SEDs using CMOS technology with the help of electron-beam lithography and have recently demonstrated a silicon single-electron-pump [1] and tunneling [2]. They are composed of one silicon quantum dot and two tiny MOS gates and have achieved 30-k operation, which is the highest-temperature operation ever reported. This opens up the possibility of the practical use of the pump and tunnel. Another path to realizing single-electron transfer, which we will here propose, might be to use a localized state in the silicon bandgap instead of quantum dots. The localized states could be donor/acceptor levels or any other states created by crystal-line imperfections. They are free from the problem of critical size control in quantum-dots fabrication, which might lead to a new era of single-electronics in combination with the rapidly developing research field of defect engineering. In the talk, after introducing our pump and tunnel, we will point out the similarity between their operation procedure and the technique known as charging pump. We will then discuss the possibility of single-electron manipulation by single dopant levels in silicon. We will also discuss the possibility of charge pumping. We will then discuss the possibility of single-electron manipulation by single dopant levels in silicon. We will also discuss the possibility of charge pumping. We will then discuss the possibility of single-electron manipulation by single dopant levels in silicon.

Random Telegraph Signals in Carbon Nanotube Field Effect Transistors. Fei Liu1, Mingqiang Bao2, Kang L. Wang1, XiaoLei Liu2, Chao Li2 and Chongwen Zhou1; 1UCLA, LA, California; 2EE, USC, LA, California.

Self-assembled carbon nanotube (CNT) and nanowire field effect transistors (FETs) have been fabricated. However, atomic level interface imperfection and single defect can dramatically affect device performance in these nanoscale devices. In this work, giant random telegraph signals (RTSs) are studied in p-type semiconducting single wall carbon nanotube field effect transistors at various temperatures as a sensitive probe for characterizing the defects. CNT FETs were fabricated on silicon substrate covered with a 500 nm thermal oxide as the gate oxide and single wall carbon nanotubes (SWNTs) were synthesized using a standard chemical vapor deposition (CVD) method. The processes produced nanotubes with a diameter of 1.3 nm. The length of the SWNT is on the order of several nm. After the synthesis, photolithography was applied to define the source and drain electrodes on top of the nanotube, followed by Ti/Au deposition as the contacts. The following measurements were carried without electrically stressing on the gate of the device. Giant random telegraph signals are observed in p-type semiconducting SWNT field effect transistors. The characteristics of the RTSS are further analyzed under different gate (Vg) and source-drain (Vds) biases. The amplitude of the RTSS is up to 60% of the total current at 2 K. The giant switching amplitude of RTSS is believed as the result of the strong mobility modulation caused by charging of defects to affect in part the ultra-small CNT transport (two channels with a CNT diameter on the order of 1 nm). At certain gate biases, the observed RTSS show 4-leveled switching. This effect is attributed to trapping and de-trapping of the two defects inside SiO2 or at the interface between the CNT and SiO2. The switching magnitude of RTSSs is shown to scale to large low level (0.1 V) noise power for this kind of devices. It seems to suggest that in order to improve the noise performance, defects in the dielectric layer and at the interface must be reduced. On the other hand, the giant RTSSs in the CNTs may be used for single defects detection. Random telegraph signal-to-noise ratio. The RTSSs in nanoscale devices are thus proposed as a sensitive nano-metrology tool to study defects or interface states of nanodevices and novel dielectric material properties. The work is in part supported by MARCO Focus Center on Functional Engineered Nano Architectonics (FENA).

A Novel Method to Synthesize Blue Luminescent Doped GaN Powders. Rafael Garcia1, Abigail Bell1, Fernando A. Ponce1 and Alan C. Thomas2; 1Physics & Astronomy, Arizona State University, Tempe, Arizona; 2Roger Corporation, Durel Division, Chandler, Arizona.

Gallium nitride is an important material in optoelectronic devices because of its direct band gap at 3.45 eV. Until now, most research has focused on GaN thin films for the production of blue/UV LEDs and laser diodes. GaN powders have been largely overlooked despite having high potential impact in the electroluminescent lighting industry. Currently electroluminescent (EL) powders are based on ZnS:Cu,Cl and can be found in many applications including keypad lighting in cellular phones, automobile instrument cluster lighting, and as LCD backlights in small electronic devices. Current ZnS EL device efficiencies are not improving as fast as technology requires and so it is necessary to look at other semiconductors as possible alternatives. GaN is a very robust material with similar structural and electronic properties to ZnS. We have recently produced high quality undoped GaN powders with exceptional luminescent properties and also we have achieved Mg and Si doped GaN powders. The highly luminescent GaN powders have been grown by direct reaction between Ga and ammonium in a horizontal quartz tube reactor at 1100 °C. Si doped powders were prepared by reaction between a homogeneous Ga-8 1 alloy and ammonium in a horizontal quartz tube reactor at 1200 °C and the Mg doped GaN powders were prepared by reacting a high purity Ga-Mg alloy with ammonium in a horizontal quartz tube reactor at temperatures between 1100 and 1200 °C for several hours. Electron microscopy indicates that the light-gray powders produced by these methods consist of at least two different shaped crystallites; large columnar crystals sized more than 10 µm and small platelets crystals between 1 and 2 µm. X-ray diffraction showed that these crystallites have well defined wurtzite structure. Cathodoluminescence spectra taken at helium temperatures show absence of yellow luminescence in the undoped materials, strong donor-bound excitons in the Si-doped materials, and, in the Mg doped powders the Mg-related donor-acceptor pair band. At 25 °C the peak on AAS of the powders exhibit bright blue cathodoluminescence and photoluminescence emission around 2.94 eV (422 nm). These results indicate that these powders have excellent optical properties for applications in electroluminescent displays.
Vacancy Engineering in Bulk and SOI Substrates for Ultra-Shallow Boron Junctions.

Andy James Smith, Benjamin Desvioues, Rachid El Bouayadi, Maryse Laurenç, Esidor Ntsoenzok, and Bernard Pichaud.

Laboratoire TECSEN, Marseille, France: 2 LPM, INSA, Lyon, France.

The knowledge and control of dopants diffusion and electrical activation are crucial issues for the aggressive scaling down required by the future Si-based microelectronic devices. A key role is played by the interaction of dopants with point defects and impurities, as all the dopants diffuse in Si via a native defect mediated mechanism. In particular, the ion implantation process in crystalline silicon (c-Si) (which is widely used for several device production processes such as the doping itself) and post implantation annealing induce a huge injection of Si self-interstitial defects (I's). This promotes the well known Transient Enhanced Diffusion (TED) and clustering of boron, which are the main process responsible for shallow junctions (and therefore also the most studied ones). Here we report on our recent experimental investigations on the formation and dissolution of B clusters generated by ion implantation in c-Si [1]. The I's are injected by Si ion implantation and annealing on B-doped boron superlattices, grown by molecular beam epitaxy. We have investigated in detail the migration of the I’s and their interaction with B. I’s are shown to diffuse, to interact with intrinsic traps (such as C), and to promote ionization and/or clustering depending on ion implantation energy (and therefore also the most studied ones). Here we report on our recent experimental investigations on the formation and dissolution of B clusters generated by ion implantation in c-Si [1].

1. The I’s are injected by Si ion implantation and annealing on B-doped boron superlattices, grown by molecular beam epitaxy. We have investigated in detail the migration of the I’s and their interaction with B: I’s are shown to diffuse, to interact with intrinsic traps (such as C) and to promote ionization and/or clustering depending on ion implantation energy (and therefore also the most studied ones). Here we report on our recent experimental investigations on the formation and dissolution of B clusters generated by ion implantation in c-Si [1].

2. The I’s are injected by Si ion implantation and annealing on B-doped boron superlattices, grown by molecular beam epitaxy. We have investigated in detail the migration of the I’s and their interaction with B: I’s are shown to diffuse, to interact with intrinsic traps (such as C) and to promote ionization and/or clustering depending on ion implantation energy (and therefore also the most studied ones). Here we report on our recent experimental investigations on the formation and dissolution of B clusters generated by ion implantation in c-Si [1].
Either spherical or facetted-cube-octahedral cavities can be introduced in silicon by implantation of He+ followed by a thermal treatment. These cavities are being intensively studied for decades since they can gather metallic impurities and, thus, improve the electrical properties of microelectronic devices. Nevertheless, no one is actually able to predict the final cavity shape after a given experimental treatment. Our goal is to determine the eventual impact of both the surface properties and the lattice structure on the cavity morphology. For such a purpose, we implanted both as-grown and metal-diffused (Pt, Au, Ni) silicon with He+. The He+ projection range (Rp), derived by transport range of ions in matter (TRIM) simulations, was varied from 90 nm to 5.5 μm, and the implantation energies ranging from 10 keV to 1.6 MeV. The dose of each implantation was chosen thanks to TRIM He+ profiles to keep each cavity formation at the concentration of He, cavity nucleation and growth parameters are assumed to be the same but the distance of cavities from the surface silicon. Indeed, the closer the Hp the higher the probability to recombine vacancies with self interstitials or to annihilate them at the surface. The thermal annealing was performed at temperature ranging from 673K to 1323K. Cross section transmission electron microscopy (XTEM) observations show that implantations in as grown silicon at Rp beyond 350 nm give facetted cavities, whatever the annealing temperature. On the contrary, cavities created at 90 nm close to the silicon surface exhibit rounded-shape for all He+ doses and annealing temperature studied. Besides, in metal-diffused silicon, the shape of the cavities is found to drastically depend on both the nature and the amount of the contaminant trapped at cavities. The latter was measured by secondary ion mass spectroscopy (SIMS). A simple model based on the surface energy associated to a cavity [1,2] and a finite element method simulation [3] was found to be consistent with the experimental data. This model allows both the cavity equilibrium shape to be understood, and the chemisorption hypothesis [4] to be experimentally demonstrated and improved. Nevertheless, the origin of the spherical shape of cavities grown at 90 nm under the surface in as grown silicon is still unclear. Experiments are on progress to check the impact of He desorption during annealing on the equilibrium shape of cavities. [1] D. J. Eaglesham, A. E. White, L. C. Feldman, N. Moriya, D. C. Jacobson, Phys. Rev. Lett. 83, 3530 (1999). [2] L. C. Feldman, A. E. White, J. Cryst. Growth, 146, 193 (1995) [3] G. A. Petersen, S. M. Myers, D. M. Follette, Jr., Nucl. Inst. and Meth. B 127/128, 301 (1997). 10:30 AM E7.6 Theory of Fluorine-Induced Suppression of Transient Impurity Diffusion in Silicon. Vincenzo Fiorentini1, 2, Giorgia Lopez1, 2, Giuliana Inferzeller1, Salvatore Mirabella1 and Enrico Napolitani1, 2; 1Dept. of Physics, University of Cagliari, Monserrato, Italy; 2INFN-Matix, Cagliari, Italy. The transient enhanced diffusion of acceptor impurities affects severely the realization of ultra-high doping regions in miniaturized Si-based devices. Fluorine co-implantation has been found to suppress this transient diffusion, but the mechanism underlying this effect is not understood. It has been proposed that fluorine-impurity, or fluorine-native-defect interactions may be responsible. Here we clarify this mechanism by first-principles theoretical studies of fluorine in Si in connection with purposely-designed experiments on boron- and fluorine-containing Si structures. The central interaction mechanism is the preferential binding of fluorine to vacancy- or fluorine dangling bonds, which determine the subsequent formation of vacancy-fluorine complexes. The latter effectively act as traps for the excess self-interstitials which would normally cause boron transient enhanced diffusion. Fluorine-boron interactions are considered marginal and do not play any significant role. Our results are also consistent with other observations such as native-defect trapping and bubble formation. In the case of the boron acceptor, fluorine suppresses interstitial-assisted transient diffusion; however, in view of the efficient fluorine trapping, we suggest that fluorine will also suppress vacancy-assisted diffusion, which is most relevant for donors. 10:45 AM E7.7 Fluorine Behavior in Preamorphized Si: Segregation and Point Defect Interaction. Giuliana Inferzeller1, Salvatore Mirabella1, Lucia Romano1, Maria Grazia Grimaldi1, Francesco Priolo1, Enrico Napolitani2, and Alberto Carni; 1MATTIS-INFN-University of Catania Department of Physics and Astronomy, Catania, Italy; 2MATIS-INFN-University of Padova, Department of Physics, Padova, Italy. In recent years, there has been considerable interest in the effect of F on B diffusion in Si. In particular, F implanted in preamorphized Si is able to suppress the B transient enhanced diffusion (TED) [1,2] and to improve the thermal stability of activated junctions [3]. The origin of these effects is a matter of current debate. To shed light upon these phenomena we undertook a detailed study about the F incorporation and diffusion in preamorphized Si. We investigated the F incorporation during the regrowth process by solid phase epitaxy (SPE) at different temperatures (580, 700 or 800 °C) and for several implanted F energies (65-150 keV) and fluxes (0.07-5x10^14 F/cm^2). We always observed a strong F segregation towards the surface, promoted by the relatively high F diffusivity in amorphous Si compared to the SPE rate. We measured a diffusion coefficient of (0.9±0.1)×10^{-14} cm^2/s at 580 °C. The above phenomenon is accompanied by a SPE rate retardation and to a consistent F loss through the surface. Most of the F concentration measured in our samples increased by increasing the SPE temperature. In samples doped with B atoms (1x10^{14} B/cm^2, 10 keV), we observed also an anomalous F accumulation at the B implantation peak during the SPE process. As we demonstrated in a previous paper, the absence of any B-F chemical bonding during SPE and post-SPE annealings [4], we believe that the above increased F incorporation is due to the increased F diffusion rate promoted by B. We investigated also the diffusion of F during a post-SPE thermal treatment. As already known, the amorphizing implant induces at the end of the implant range a defect-rich region, called end-of-range region (EOR), which acts as a source of fluorine. Theory of Fluorine-Induced Suppression of Transient Impurity Diffusion in Silicon. Vincenzo Fiorentini, 1 Giorgia Lopez, 1 Giuliana Inferzeller 1, Salvatore Mirabella 3, Enrico Napolitani 2 and Alberto Carnera 2. The EOR region is not affected by the F implanted in the amorphous layer. Fluorine is able also to suppress the B thermal diffusion (TD). In conclusion, our data support the idea of an interaction between F and B, leading to a non Fickian diffusion and to a SPE rate and TD reduction. This F-B interaction causes a very strong lowering of the Is population. [1] D. F. Downey, J. W. Chow, E. Ishida and K. S. Jones, Appl. Phys. Lett. 73, 1283 (1998). [2] A. Mokhberi, R. Khazaei, P. B. Grün and J. D. Plummer, Appl. Phys. Lett. 81, 5530 (2002). [3] L. C. Feldman, A. E. White, J. Cryst. Growth, 146, 193 (1995). [4] G. A. Petersen, S. M. Myers, D. M. Follette, Jr., Nucl. Inst. and Meth. B 127/128, 301 (1997).
band (VB) electronic structure of InN containing these very high concentrations of free electrons and defects. XAS, a probe of unoccupied CB state, shows a depletion of states near threshold absorption corresponding to free-carrier filling of the CB, and the creation of two new peaks for irradiated InN that correspond to (i) the N-vacancy defect level, and (ii) the formation of N-pairs. XES, a probe of occupied states, shows additional emission above the CB maximum, not present in non-irradiated InN, resulting from filled CB states and from elastic scattering. The elastic scattering intensity shows an enhancement for photon excitation at the localized defect level and the CB emission consists with a band gap narrowing of ≈0.4 eV arising from free-carrier electron-electron and electron-ionized defect interactions. The results provide additional support for previously reported low energy gap and large Burstein-Moss shift in heavily doped InN [1] [1] J. Wu et al., Phys. Rev. B 66, 204103 (2002).

11:30 AM E7.10 Electronic and Optical Properties of High Energy Particle-Irradiated In-rich InGaN Alloys. Sonny X. Li1,2, Kim Man Yu1, Rebecca E. Jones1, Junqiao Wu1, Wladek Wulakiewicz1, Joel W. Ager1, Wei Shan1, Eugene E. Haller1, Hai Lu1, William J. Schaak2 and William Kemp1; 1Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California; 2Department of Materials Science and Engineering, University of California, Berkeley, Berkeley, California; Department of Electrical and Computer Engineering, Cornell University, Ithaca, New York; 4Air Force Research Laboratory, Kirtland Air Force Base, Kirtland AFB, New Mexico.

InGaN alloys, whose fundamental bandgaps span almost perfectly the solar spectrum, are potential materials for high-efficiency tandem solar cells [1]. An important consideration for high-efficiency solar cell in space applications is the radiation resistance of the materials. We have carried out a detailed study of the effect of irradiation on the electronic and optical properties of InGaN alloys over the entire composition range. Three different types of energetic particles (1 MeV electrons, 2 MeV protons, and 2 MeV alpha particle) were used to produce displacement damage states (D2) spanning over five orders of magnitude. The electron concentrations in InN and In-rich InGaN increase with D2 and finally saturate after a sufficiently high dose of irradiation (typically over 1015 MeV/m2). The saturation of carrier density is attributed to the Fermi level pinning at the Fermi Stabilization Energy (EF,F), as predicted by the amphoteric native defect model [2]. Electrochemical capacitance-voltage (ECV) measurements reveal a surface electron accumulation whose concentration is determined by pinning at EF,F. Using the room temperature photoluminescence intensity as an indirect measure of minority carrier lifetime, it is shown that Inx−yGaxN retains its optoelectronic properties at radiation damage doses at least 2 orders of magnitude higher than the damage thresholds of the materials currently used tandem solar cells (GaAs and GaInP). [1] J. Wu et al., J. Appl. Phys. 94, 6477 (2003). [2] W. Wulakiewicz, Physica B 302 – 303, 123 (2001).

12:45 AM E7.11 Intrinsic and N-related Defects in Hydrogen-Free ZnO Films Fabricated by Plasma Immersion Ion Implantation. Y. F. Mei1,2, G. G. Siu1, Paul K. Chu1,2, and W. K. Ge3; 1Physics & Materials Science, City University of Hong Kong, Kowloon, Hong Kong; 2Physics, Hong Kong University of Science & Technology, Clear Water Bay, Kowloon, Hong Kong.

Zinc oxide, which is a wide band gap (3.37 eV at room temperature) semiconductor material, is considered a potential material in short wavelength optoelectronic devices such as light-emitting diodes and lasers in the ultraviolet and blue regions. Undoped and doped ZnO films that can be fabricated by thermal evaporation, metal organic chemical vapor deposition (MOCVD), pulse laser deposition (PLD), and molecular beam epitaxy (MBE) have been studied for their intrinsic properties and p-type doping mechanism. However, p-type doping of ZnO is not easy and the feasibility has been studied extensively. Nitrogen is regarded to be the more soluble group-V impurity also having the shallowest acceptor level relative to P and As. Cluster-doping has been investigated because of the stable bonds and low doping enthalpy. The doping bottleneck is generally due to intrinsic defects, unintentional hydrogen impurity, and low N solubility. In this work, a dual plasma technique comprising zinc arc plasma and mixture gas (oxygen, and nitrogen) plasma is used to fabricate undoped and N-doped ZnO thin films in which no hydrogen exists. Intrinsic and N-related defects such as shallow donors, deep centers, and N acceptors, are identified by photoluminescence (PL) and Hall-effect measurements at room temperature and low temperature are compared to those of single crystal ZnO. The N-related behavior revealed by cathodoluminescence (CL) and Raman scattering are discussed with respect to its bonding type and stability. Our work is helpful to understand the nitrogen-doping mechanism in ZnO.

SESSION E8: Defect Properties, Activation, Passivation and Reaction

Chairs: N. M. Johnson, and P. G. Voyles

Thursday Afternoon, March 31, 2005

Room 2006 (Moscone West)

1:30 PM E8.1 Mutual Passivation in Dilute GaN, Asx 1−y, Alloys. Kim Man Yu1, Wladek Wulakiewicz1, Junqiao Wu1, D. E. Marx1, Michael A. Scarpulla1 and Oscar D. Dubon1; 1Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California; 2Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts; 3Aglent Laboratories, Palo Alto, California; 4Department of Materials Science and Engineering, University of California, Berkeley, California.

The dilute GaN, Asx 1−y, alloys exhibit many unusual properties as compared to the conventional binary and ternary group III-V semiconductor alloys. We report on a new effect in the GaN, Asx 1−y, alloy system in which electrically active substitutional group IV donors and isoelectronic N atoms passivate each other’s activity. Absence of any passivation of electrical activity of group VI donors indicates that the mutual passivation occurs through the formation of nearest neighbor VAs −N pairs. The passivation of the shallow donors and the NAs atoms is manifested in a drastic reduction of the free electron concentration and, simultaneously, an increase in the fundamental bandgap. For example, the electron concentration of a highly Si-doped GaN 0.82:As 0.18 (with Si concentration of 9×1010 cm−2) starts to decrease rapidly at an annealing temperature of 700°C from 3×1010 cm−2 in the as-grown state to n<1018 cm−2 after an annealing schedule of 900°C for 10 sec. At the same time an annealing of this sample at 950°C increases the gap by about 35 meV. This increase in band gap corresponds to a reduction of the concentration of the active N atoms by 8×1018 cm−3, very close to the total Si concentration. Calculations show that the passivation process can be well quantitatively explained by Ga vacancies mediated diffusion of randomly distributed donor species to the nearest N sites. The general nature of this mutual passivation effect is confirmed by our study of Ge doped GaN, Asx 1−y, layers formed by N and Ge co-implantation in GaN layers followed by pulsed laser melting. Consequently, GaN, Asx 1−y, alloys doped with group IV donors result in a highly resistant GaN, Asx 1−y, layer with fundamental band gap governed by a net “active” N equal to the total N content minus the donor concentration. The mutual passivation effect described here may therefore be exploited for electrical isolation, band engineering, and quantum confinement.

2:00 PM E8.2 Quantitative Modeling of Self-Interstial Diffusion in Silicon. N. A. Modine1, 1112, Sandia National Labs, Albuquerque, New Mexico.

Predictive modeling of the early-time transient annealing of radiation damage in electronic devices requires a detailed, quantitative understanding of the behavior of the fundamental defects in the device material. The isolated self-interstitial in silicon is extremely difficult to observe experimentally, and therefore accurate theoretical results should be very valuable. We apply electronic structure calculations based on the Kohn-Sham Density Functional Theory (DFT) in concert with Kinetic Monte-Carlo (KMC) techniques to study diffusion of the silicon self-interstitial as a function of the majority and minority carrier populations. Using the DFT, the structures that are locally stable (stable or metastable) for each charge state are identified by relaxing the system starting from numerous different low symmetry configurations. We then apply the nudged elastic band method to obtain transition barriers and transition states for transformation between these configurations. The resulting transition barriers are incorporated into a KMC model to determine the diffusion rates as a function of temperature and Fermi level and to evaluate the importance of enhanced diffusion due to charge state fluctuations resulting from the capture of carriers. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

2:15 PM E8.3 Dopant Deactivating Mechanisms and Co-Doping Strategies in Heavily Doped Silicon. Dominik Christoph Mueller and Wolfgang Fichtner; Integrated Systems Laboratory, Swiss Federal Institute of Technology, Zurich, Zurich, Switzerland.

Deactivation of donors in heavily doped silicon is one of the predominant problems that CMOS technology has to deal with in
connection with the down-scaling of semiconductor devices. In the near future, source, drain, and channel regions of transistors need to feature doping spikes in an atomic level. The dopant solubility limits. At the same time, every donor atom should release one of its electrons to the bulk, thereby contributing to a raise in electrical conductivity in the corresponding region. Unfortunately, a large percentage of up to 90% of the donors introduced are compensated during the wafer manufacturing process. Co-doping is considered to be one method that could potentially forestall donor deactivation. Prerequisite for its investigation is a deep understanding of the defect structures in Si on an atomic level. Both experimental data as well as our extensive ab initio calculations have led us to suggest a model involving 3 steps: 1. donor deactivating distortions (dD for short), 2. donor-vacancy clustering, and 3. ultimate precipitation of isolated As. The objective of this work is to evaluate the effectiveness of various Group I, II, and IV elements as possible co-dopants in highly n-type Si. A possible co-dopant should exhibit a high binding energy with both vacancies and donor-vacancy complexes. At the same time, the co-dopant should have the capability to annul the acceptor states of such a complex. Moreover, the co-dopant should be rather small in order not to increase the strain in the silicon lattice and to reduce the diffusion resistance of the atoms. We have found that the isovalent impurities C and Ge are unsuited for the intended purpose of clustering inhibition. Lithium and Magnesium, on the other hand, both bind strongly to vacancies while reducing the number of deep acceptor levels of compensating complexes in the band gap. Our ab initio results clearly favor the double donor Magnesium as a co-dopant of both P and As, possibly also for Sb.

3:00 PM E8a.4 Determination of Diffusivities of Si Self-Diffusion and Si Self-Interstitials using Isotopically Enriched Single- or Multi-30Si Epitaxial Layers. Satoshi Matsumoto1, S. Seto1, S. Aida, T. Sologubchik1, Y. Nakabayashi1, K. Togoyama1, Y. Shimamura1, T. Murata1, K. Wada2 and T. Abe1; 1Electrical Engineering, Keio University, Yokohama, Japan; 2Tohoku University, Sendai, Japan.

In order to understand the properties of point defects (vacancy, Si self-interstitial) in Si, it is important to clarify diffusivity of Si self-diffusion over a wide temperature range. We used highly isotope-enriched 30Si epitaxial layers on Si substrate to study the diffusion behavior. 30Si epitaxial layers were grown on CZ-Si substrates by gas-source MBE or low-pressure chemical vapor deposition (LCVD) systems, using 30SiH4 source purchased from Kurchakov Laboratory. Diffusion was performed under various temperature (970-1200)C) atmosphere at 867-1300C. The concentrations of the respective Si isotopes were obtained with SIMS analysis. Diffusivity of 30Si (called Si self-diffusivity, Dsd) was determined using numerical fitting process with SIMS profiles. In this process, the as-grown profile of 30Si was used as an initial condition. The best fit was determined by minimizing the root-mean-square error. Dsd can be described by an Arrhenius equation with one single thermal activation enthalpy, Dsd=14exo(-4.37eV jkT). The present result is in agreement with recent experimental observations that suggest the importance of interstitials in arsenic-vacancy complexes.

3:30 PM E8a.5 Diffusion of Arsenic-Silicon Interstitial Complexes. Scott A. Harrison, Thomas F. Edgar and Gyeong S. Hwang; Chemical Engineering, University of Texas at Austin, Austin, Texas.

Arsenic doping is an essential ingredient in the fabrication of silicon devices. As device dimensions scale down in nanometer structures, atomic-level control of doping profiles becomes necessary. Low-energy ion beams are currently most widely used to introduce dopants into the Si lattice. As a result of high-temperature anneal, substrate damage may occur and may be mitigated by energetic ion bombardment and to electrically activate the injected dopants. During the annealing, the arsenic atoms exhibit transient enhanced diffusion (TED). While the underlying TED mechanism is still unclear, recent theoretical studies have suggested that arsenic-vacancy complexes, such as AsV and As2V, may be primarily responsible for the TED. However, recent experimental observations have suggested interstitials promote As TED. In addition, recent studies of di-vacancy arsenic complexes appear to easily be annihilated in the presence of interstitials. In this talk, we will present the interaction of interstitials with arsenic and arsenic-vacancy complexes based on density functional theory calculations with the generalized gradient approximation. We have identified the structure and diffusion of arsenic-interstitial and di-arsenic pairs. For arsenic-interstitial pair diffusion, our DFT calculations predict two pathways, with overall barriers of 0.28 (0.40) eV in neutral (+1 charge) state, respectively. The arsenic-interstitial binding energy with respect to substitutional arsenic and interstitial is calculated to be approximately 0.45-0.6 eV, depending on their charge states. Di-arsenic pair diffusion is predicted to occur by overcoming an overall barrier of 1.35 eV. The di-arsenic binding energy with respect to substitutional arsenic and arsenic-interstitial pair is estimated to be 1.04 eV in the neutral state. The large binding energy of the di-arsenic pair suggests that it can also play an important role in arsenic TED when the arsenic concentration and the annealing temperature are high. We will also discuss the interaction of single interstitials with arsenic-vacancy complexes. Our calculation results are consistent with recent experimental observations that suggest the importance of interstitials in arsenic TED. The increased understanding our study will provide greatly assist in improving current models for arsenic junction formation.

3:45 PM E8b.6 Effects of Silicon Nitride Passivation Layer on Mean Dark Current and Quantum Efficiency of CMOS Active Pixel Sensors. D. Benoist1, P. Morin2, M. Cohen3 and J. L. Regolini1; 1STMicroelectronics Cr0leksi, Crolles, France; 2STMicroelectronics Crolles2 Alliance, Crolles, France.

Dark current reduction and quantum efficiency (QE) improvement in CMOS Active Pixel Sensor (CMOS APS) are fundamental in image sensors performance. In the present study, we have analyzed the influence of the silicon nitride (SiN) passivation layer properties on the mean dark current and the quantum efficiency of CMOS APS through electrical characterization of lot wafer processed with three different SiN passivation films. The SiN layers were characterized by Spectroscopic Ellipsometry (SE) and Fourier Transform Infra Red (FTIR) spectroscopy to determine the optical indices and the hydrogen content of the films, respectively. For the films light absorption, the [Si-Si] bond concentration has been determined assuming a linear dependence with the extinction coefficient value at 300 nm. This relationship was justified by simulation results according to the Si-centered tetrahedral model. Thanks to these data and the graviometric density results, we have also determined the [Si-N] bond concentrations and therewith the Si/N ratio of the thin film. In the temperature range close to those of the passivation anneal was also studied by Thermal Desorption Spectrometry (TDS) experiments. The different bond concentrations enable to explain the device performances. As previously observed and confirmed by the TDS results, high [Si-H] and low [Si-N] bonds concentrations lead to high hydrogen desorption from the SiN films. Thus, the lowest mean dark current values have also been obtained with such silicon nitride passivation layers. Consequently, results are in agreement with the hydrogen passivation of defects being responsible of thermally generated electrons. Concerning the quantum efficiency, it is highly influenced by the optical indices of the SiN passivation layer. Actually, the refractive index of the SiN layer, which is the highest of the whole dielectric stack over the photodiode, drives the light reflection, while the light absorption in the visible range is controlled by the [Si-Si] bond concentration. A model describing the effect of the two indices on the quantum efficiency of SiN layers is proposed. Requirements to minimize the mean dark current and to maximize quantum efficiency are somewhat in opposition. Actually, high [Si-H] and low [Si-N] bonds concentrations (for good performance) are generally observed in silicon-rich SiN films, which contain high amount of [Si-Si] bonds (inducing high absorption, thus low QE). Increase simultaneously the [Si-H] and [N-H] bonds concentrations in the passivation layer can be a way to have high hydrogen desorption during passivation anneal just preserving a transparent layer. [1] D. Aspnes and J. B. Theeten, J. Appl. Phys. 50 (1979) 4928 [2] Z. Yin and F. W. Smith, Physical review B 42 (1990) 3658 [3] A. W. Weeber, H. C. Rieffe, W. C. Shinke and W. J. Soppe, 10th European Photovoltaic Solar Energy Conference and Exhibition (2004)
Origin of Vacancy and Interstitial Stabilization at the Amorpha- 
Crystalline Silicon Interface. Scott A. Harrison1, 
Taras A. Kirichenko2, Decai Yu*, Thomas F. Edgar1, Sanjay K. 
Banerjee2 and Gyeong S. Hwang1; 1Chemical Engineering, University 
of Texas at Austin, Austin, Texas; 2Electrical Engineering, University 
of Texas at Austin, Austin, Texas.

Fabrication of forthcoming nanometer scale electronic devices faces 
many difficulties including the formation of extremely shallow and 
highly doped regions, highly mobile and inherently disordered 
implanted silicon, along with dislocations, other extended and point-like 
defects. The importance of the implanted section is that the 
mutual behavior of native defects in the amorphous regions would be 
different from that in the crystalline regions. This can in turn affect 
the density of spatial distribution of defects. For instance, if there is 
a difference in formation energy between the amorphous and 
relative density of interstitials and vacancies will vary with the phase. 
Since single vacancies and interstitials are highly mobile even at room 
temperature, their clustering and annihilation behaviors can be 
greatly affected by substrate amorphization during implantation and 
earby stage of thermal annealing where the amorphous region is not 
fully recrystallized. Despite its technological importance, there is still, 
to our best knowledge, no clear description available of defect dynamics 
in the vicinity of the amorphous-crystalline (a-c) Si interface. In this 
paper, we will present the results of our recent density functional 
theory study on the structure and dynamics of vacancies and 
interstitials in the vicinity of the a-c Si interface. We find that both 
vacancies and interstitials prefer to reside on the amorphous side of 
the interface. In both cases, the most stable defects occur 3-4 Å from 
the a-c interface. Vacancy stabilization is found to be due to strain 
relief provided to the substrate lattice while interstitial stabilization is 
due largely to bond rearrangement arising from interstitial integration 
into the substrate lattice. We also discuss the effect of the 'sponge-like' behavior of the amorphous phase toward native defects 
on ultrashallow junction formation in the fabrication of electronic 
devices. The fundamental understanding and data provided by this 
study will be very useful in developing a comprehensive kinetic model 
for ultrashallow pn junction formation. 

A New Post Annealing Method for AlGaN/GaN 
Heterostructure Field-Effect Transistors Employing XeCl 
Excimer Laser Pulses. Min-Woo Ha, Seung-Chul Lee, Jong-Hyun 
Park, Yeong-Joon Hong and Min-Koo Hong; School of 
Electrical Engineering #50, Seoul National University, Seoul, South 
Korea.

The wide-band gap material of GaN has attracted for the high power 
and the high temperature applications due to a high two-dimensional 
electron gas (2DEG) concentration and a high critical electric field. 
The high voltage switching AlGaN/GaN heterostructure field-effect 
transistors (HFET) are reported to decrease a leakage current. But, 
the drain current of a thermal annealed AlGaN/GaN HFET decreases and the 
threshold voltage of that shifts positively due to the decrease of the 
two-dimensional electron gas concentration and the Schottky gate 
metal diffusion into a GaN layer. The purpose of our work is to 
propose a new post annealing method employing the excimer laser 
pulses, which increases a drain current and suppresses a leakage 
current without degrading the Schottky gate metal and a threshold 
voltaget. Thermal annealed AlGaN/GaN HFET is post annealed by 
XeCl excimer laser pulses operating at 308 nm. The 3 µm 
unintentionally doped GaN layer can only absorb the excimer laser 
due to its lower energy band gap (3.4 eV) than excimer laser photon 
energy (4.025 eV) and the absorption coefficient of GaN (α=1.3x106 
cm^-1). During post annealing, in the unintentionally doped GaN 
can diffuse the region between the Schottky gate and the 
GaN layer. The interface defects under the Schottky gate decreases. In 
the proposed method, the Schottky gate metal does not diffuse into a 
GaN layer due to the Schottky gate metal reflection to the laser and 
the instant heat diffusion. After a single laser pulse with the energy of 
100 mJ/cm², the drain current increases by 250 mJ/cm² and a 
threshold voltage increase of 98.9 mS/mm to 98.9 mS/mm. Those of the 
virgin device are 363.7 mS/mm and 89.9 mS/mm. When a single laser pulse with the energy of 
50 mJ/cm², the gm is increased from 88.9 mS/mm to 88.9 mS/mm. The laser pulse energy determines the surface temperature of the device 
and the laser pulse with the energy of 250 mJ/cm² damages the 
Schottky gate. The proposed post annealing method decreases the 
leakage current from 1.05 mA/mm to 1.55 mA/mm.

Fabrication of Silicon Carbide PIN Diodes by Laser Doping 
and Planar Edge Termination by Laser Metallization. Z. 
Tian1, N. R. Quick2 and A. Kari1; 1College of Optics and 
Photonics/CREOL, Mechanical, Materials, and Aerospace 
Engineering Department, University of Central Florida, Orlando, 
Florida; 2Applicate Associates, LLC, Orlando, Florida.

Silicon carbide PIN diodes with planar edge termination have been 
fabricated using a direct write laser doping and a laser annealing 
technique. Trimethylaluminum (TMA) and nitrogen are precursors 
used to laser dope p-type and n-type regions respectively and a 2.8 
mm p-type doped junction and 4 mm n-type doped junction are 
fabricated in semi-insulating 6H-SiC wafers. Rutherford 
backscattering studies show that no amorphization occurred during 
laser doping process. A planar edge termination is created by laser 
metallization of vanadium to form a high resistivity layer. With this 
termination, the breakdown voltage of the PIN diodes can be 
improved dramatically compared to that of diodes without edge 
termination. An annealing technique is also used to tailor the 
performance of the diodes.

Nanoinindentation as a Tool for Formation of Thin Film-Based 
Barrier Structures. Halyna M. Khlyap1 and Petro G. Sydorchuk2; 
1Physics, University of Technology, Kaiserslautern, Germany; 
2Physics, State Pedagogical University, Drohobych, Ukraine.

AZnCdHgTe semiconductors and their solid solutions (ZnSe, 
ZnTe, CdTe, 
ZnCdHgTe) are matter of choice for near- and far-infrared 
optronics. The importance of nanoindentation on the 
substrate is not always successful due to lattice paranleters 
compatibility and a good selection of a proper buffer layer may also pose 
some unavoidable problems. From this point of view the 
nanoindentation as a tool of defect engineering can be effective for 
fabrication of surface barrier structures. The abstract presents first 
theoretical results and numerical simulation of experimental data 
without investigation of nanoindentation effect on electric 
characteristics (in particular, current-voltage and capacitance-voltage) 
of ZnCdHgTe thin films and ZnCdHgTe/CdTe heterostructures at 
the room temperature. It is shown that nanoindentation leads to 
appearance of double-barrier structures. Experimental data reported 
in the work show sufficient effect of mechanical impact on 
room-temperature current-voltage and low-frequency (f = 1 kHz) 
capacitance-voltage characteristics of heterostructure 
p-ZnCdHgTe/p-CdTe grown by modified LP technology. 
Experiments demonstrated dramatically changes in the capacitance 
properties of the heterostructure as well as drastically changed energy 
band diagram. Appearance of quasi-triplet barriers seems to be 
development on the composition of the epilayer ZnCdHgTe and may be 
governed technologically (variations of the growth conditions, 
doping levels, etc.). At the same time, influence of indentation on 
the current-voltage characteristics of the substrate (p-CdTe) is also 
significant. Changes of the carrier transport nodes at room 
temperature can be used for previous barrier construction before 
growth of the film.

Archiving of the Defomation-Induced Damage in Silicon 
Detected by Oxygen Agglomeration. NikolaI Yarykin1 and Ellen 
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University of Technology, Dresden, Germany.

The plastic deformation at moderate temperatures introduces in 
silicon, along with dislocations, other extended and point-like defects. 
Structure of the defects is not established yet, that supports the 
academic interest to the field. In some aspects the 
deformation-induced defects are similar to those formed in silicon 
during post-implantation annealing [1]. This is why the investigations 
of plastically defomned silicon may be of a technological importance. 
In this work the IR absorption spectroscopy is used to study the
decay of oxygen supersaturated solution in plastically deformed silicon is shown that the decay is

Free-standing silicon layer is possible in the absence of any handle wafer (usually oxidized Si). The goal of this study is to determine the threshold thickness above which lift-off of a free-standing silicon layer is possible in the absence of any handle wafer. In other words, the layer thickness required to obtain free-standing films lifted off Si by the hydrogen-implantation-induced defect layer. We implanted H into Si over the energy range 50 to 1150 eV. The dose required for layer lift-off has been found to depend upon the implanted depth of hydrogen.

E9.6 Comparison of the Deep-Level Spectra Produced by Particles of Different Mass in p-Type Silicon Crystals. Nikolai Varyakin and George A. Rozgorz; 2 Institute of Microelectronics Technology RAS, Chernogolovka, Moscow Region, Russian Federation; 3 Department of Science & Engineering, North Carolina State University, Raleigh, North Carolina.

The spectrum of defects produced in silicon due to bombardment with energetic particles - and consequently the deep-level spectrum - are known to depend on the mass of incident particles. For instance, the second acceptor level of divacancy is suppressed in silicon implanted with heavier ions [1]. In p-type silicon the K2 center was recently observed [2]. Although the center is dominant in silicon implanted with Si and Ge ions, its nature is still unknown. The K2 center introduction rate decreases essentially for lighter ions, and the center was not unambiguously reported in electron-irradiated samples until now. At the same time, such observations cannot be reconciled with its nature. In this work we compare the deep-level spectra of ion-implanted and electron-irradiated silicon crystals using the capacitance spectroscopy (DLTS). Since the defect spectra are strongly influenced by the impurity profile, the comparison is done on the same set of crystals of different purity. It is observed that the K2 center can be created by irradiation with 5 MeV electrons. Its introduction rate in electron-irradiated samples is found to be more sensitive to the crystal purity than in case of ion implantation. A notable concentration of the K2 centers is detected after electron irradiation only in epitaxial wafers. A possible nature of the K2 center and details of its near-surface distribution are discussed. [1] B. G. Svensson et al., J. de Phys. 14, 43, 4292 (1991). [2] R. C. Cho et al., Appl. Phys. Lett. 74, 1263 (1999).

E9.7 He Implant Energy Dependence of Thermal Growth of Nanocavities in Si. Eizidor Nsengzoi, Rachid El Bouayadi, Gabrielle Regula, Bernard Pichaud and S. Ashok; 1 CNRS-CERI, Orleans, France; 2 ETECSE, Case 151, Faculte des Sciences St-Jerome, Marseille, France; 3 Department of Engineering Science and Mechanics, the Pennsylvania State University, University Park, Pennsylvania.

Although bubbles/cavities induced by helium in silicon have been studied for decades, it is still a big controversy concerning the thermal growth of these nano-objects. The goal of this work is the study of bubbles/cavities thermal growth by a new approach. Float Zone (FZ) silicon samples have been implanted with helium ions at energies ranging from 0.8 MeV to 1.0 MeV in increments of 0.1 MeV, with the ion flux maintained between 5 x 1012 and 1 x 1013 He cm2·s-1. Cavities might then be created at depths varying from 2.8 to 9.1 microns according to TRIM simulations. The dose was kept at 5 x 1016 He cm-2 for all the energies except 0.8 MeV. The annealing results in a clean lift-off of a silicon layer with thickness equal to the hydrogen implant depth. Blistering and transfer/lift-off of thin silicon layer are the consequences of thermal growth of platelets by the Ostwald ripening mechanism that involves exchange of He and silicon atoms. The results are analysed in conjunction with the literature data on the annealing of the implantation-induced damage. [1] N. Varykin and E. A. Steinman, Physica B 340-342, 756 (2003).

E9.9 Variation of Surface Sink Possibility for Point Defects Removing in Annealing. Min Yu1, Xiao Zhang1, Kai Zhan1, Ru Huang2, Xing Zhang1, Yangyuan Wang1, Jinyu Zhang2 and Hideki Oka3; 1 Institute of Microelectronics, Peking University, Beijing, China; 2 Fujitsu R&D Center Co., Ltd., Beijing, China; 3 Fujitsu Laboratories Ltd., Atsugi, Japan.

Bubbles of point defects in annealing is focused in order to suppress the Transient Enhanced Diffusion (TED) of boron urged by the development of integrated circuits. Silicon surface sink possibility for point defects is important in the case of ultra-shallow doping, however it is still ambiguous considering the inconsistent results. In this paper the variation of surface sink is studied. By using experimental results with Kinetic Monte Carlo simulation, we proposed that surface sink possibility varies in different cases. Specially, the comparison results of different treatment on surface are reproduced by simulation with variation of surface sink. This will not only improve the understanding of surface sink but also indicate the new way to improve shallow junction technology. Kinetic Monte Carlo model is applied to simulate diffusion in high temperature annealing. The annealing on low energy implantation into silicon can be simulated and verified by SIMS data. TED of boron is reproduced by simulation and agreement to SIMS data is achieved. The simulation studies show that with complete sink surface model, TED for very low energy implantation, is obviously underestimated and only with very small surface sink possibility can it be well described. Similar conclusion is also achieved by Edmund G. Seebauer (IEEE ICSICT 2004). Second, the annealing on self-ion implantation into silicon is also simulated. The evolution of extended defects is studied and simulation results on face density of extended defects agree with data extracted from TEM experiments. In this case, complete sink surface model can well describe the phenomenon. And it is concluded that enhanced surface sink possibility to show that amount of diffusion decreases with the increase of surface sink possibility. It is concluded that enhanced diffusion is obviously impacted by surface sink possibility. To understand and suppress enhanced diffusion, surface sink possibility must be considered.

E9.10 Abstract Withdrawn

E9.11 Optical Properties of Hydrogen Implanted ZnO. Jung-Kun Lee1, Michael Nastasi2, Don Lucca2; 1 Materials Science and Technology, Los Alamos National Laboratory, Los Alamos, New Mexico; 2 School of Mechanical and Aerospace Engineering, Oklahoma State University, Stillwater, Oklahoma.

The optical and structural properties of ZnO are investigated using low temperature photoluminescence (PL), Rutherford backscattering spectroscopy (RBS), and infra-red spectroscopy (IR). H implantation changed the relative ratio of the luminescence from the donor bound exciton and the overall intensity of the PL spectrum. The PL spectrum for the H implanted ZnO and the RBS spectra for H implanted ZnO demonstrated that the implantation damage was partially responsible for these variations. IR spectra of H implanted ZnO showed that the luminescence from the donor bound exciton is the origin of the 3.9 eV peak coincides with an appearance of the H vibration mode in the ZnO lattice. These results of present study suggest that the H in the ZnO provides the shallow donors for the collapse of excitons as well passivates ZnO grown defects.
Zinc oxide is one of the candidate materials for future opto-electronic devices. A lot of studies were carried out but still we have several open problems. For example, origin of deep levels are still unclear. In the present study, we investigated defect structures in doped ZnO to clarify the charge compensation mechanism. We used CASTEP code for calculation of defect structures. Local structure around the defects was evaluated by using super-lattice model and the formation energy of defects was calculated. For the calculation of charge compensation, complex defects, such as aluminum at zinc site with vacancy in zinc site, were calculated. Moreover, impurity at the surface was also studied. As a result, it was predicted that the magnitude of the structural relaxation at the surface varies with impurity element. For example, local structure around Al impurity shown different from that of Ge on surface. We discuss about the structural relaxation and charge compensation phenomena in relation with our previously reported experimental results.

**E9.12**
*Defect Structure in ZnO Studied by ab-initio Calculation.*
Naoki Ohishi and Hajime Haneda; Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Ibaraki, Japan.

In this study, we investigated defect structures in doped ZnO to clarify the charge compensation mechanism. We used CASTEP code for calculating defect structures. Local structure around the defects was evaluated by using super-lattice model and the formation energy of defects was calculated. For the calculation of charge compensation, complex defects, such as aluminum at zinc site with vacancy in zinc site, were calculated. Moreover, impurity at the surface was also studied. As a result, it was predicted that the magnitude of the structural relaxation at the surface varies with impurity element. For example, local structure around Al impurity shown different from that of Ge on surface. We discuss about the structural relaxation and charge compensation phenomena in relation with our previously reported experimental results.

**E9.13**
*Fabrication of n+p Junction Diode using Plasma Doping Formulation by Low Temperature Annealing.*
Kiju Im1; Yu Cho1, Chang-Geun Ahn1, Jong-Heon Yang1, In-Bok Baek1, Seoonje Lee1, Sungkweon Baek1 and Hyunsang Hwang1; 1Nano Electronics Devices Team, ETRI, Daejeon, South Korea; 2Material Science, GIST, Kwangju, South Korea.

High performance devices require the scaling of size and highly conductive material such as metal gate or metal substrate. The scaling of device size requires shallow S/D junction to suppress short channel effects. This is required for improving process window of the junction formation must be decreased. In addition, the thermal budget of post-implantation annealing must be reduced to minimize implanted dopant diffusion. However, lowering the beam energy in conventional ion implantation equipment inherently decreases the beam current, prolonging the implantation time which results in low throughput. Accordingly, plasma doping is receiving more and more attention for its very high ion current and dose rate capability at very low ion energy. In this paper, we report the low-temperature annealing of the ion-implanted matrix formed by plasma doping. The electrical characteristics, such as activation annealing methods such as spike anneal, laser anneal are being studied. However, in their inherent exposure to high temperature annealing, these methods induce negative effect on the low thermal budget materials such as low resistivity metal with low melting point and hi-k gate dielectric. As an alternative to high temperature activation process, we developed a noble shallow junction formation technique with low defect density and sheet resistance of 30 Ohm/sq using elevated temperature plasma doping followed by low temperature annealing. The proposed process makes it possible for low thermal budget material to be compatible with the CMOS process.

**E9.14**
Sungkweon Baek1, Dongkyu Lee1, Hyunsang Hwang1, Yu Cho1, Chang-Geun Ahn1, Jong-Heon Yang1; 1Nano Electronics Devices Team, ETRI, Daejeon, South Korea; 2Material Science, GIST, Kwangju, South Korea.

Silicon substrate has low hall electron mobility due to the intrinsic material property, which is enhanced in case of high-k oxide deposition due to the high defect density. To overcome this problem, germanium(Ge) substrate has regained considerable attention. Recently, due to the small band gap, the junction formed on Ge showed high leakage current. Therefore, most of research used high energy ion implantation with furnace annealing and rapid thermal annealing. For the fabrication of Ge wafer on the semiconductor device technology, the junction characteristics such as junction depth and activation level, should be improved. In this study, for the formation of n+/p junction, the low energy plasma doping and excimer laser annealing were applied. In addition, the electrical characteristics such as activation level and junction diode leakage current, of n+/p ultra-shallow junction were presented. The (100)-type Germanium wafer with resistivity of 15-23 Ohm cm was used as a substrate. Prior to plasma doping, oxide mask was formed by the plasma oxidation. The plasma doping system was performed using PIII(13%) gas diluted with H2 balance gas. The plasma doping was performed in the energy of 1kV. The activation was performed by rapid thermal annealing and laser annealing. The laser annealing was performed in a vacuum ambient at temperature of 500°C for 10min. The laser annealing was conducted by a KrF excimer laser with 248nm wavelength in the energy 300 500mJ/cm2 at 1 pulse. The fabricated samples were analyzed by hall measurement, SIMS analysis and diode leakage current evaluation. Hall measurement was conducted in the liquid nitrogen atmosphere at 77K due to the small Ge band gap, which was resulted to the leaky characteristics. The laser-annealed sample in the energy of 300mJ/cm2 at 1 pulse showed the sheet resistance of 2800ohm/sq, and the activated carrier concentration of 2.3E14/cm2 at 77K. Based on SIMS analysis, the junction depth was less than 30nm due to the low plasma doping and laser annealing energy. The laser-annealed junction diode on Ge in the energy 300mJ/cm2 at 1 pulse showed the leakage current level of 2 orders of magnitude than annealed by RTA at 500°C for 10min. The n+/p junction on Ge formed by rapid thermal annealing showed the superior electrical characteristics, and could be applied to the fabrication of the next generation device.

**E9.15**
*The Electrical Phenomena of Non-Planar Structures and Devices with Novel Plasma Doping.*
Jong-Heon Yang, In-Bok Baek, Kiju Im, Chang-Geun Ahn, Sungkweon Baek, Won-Ju Cho and Seoonje Lee; Future Technology Research Division, Electronics and Telecommunications Research Institute, Daejeon, South Korea.

Near future a semiconductor technology will be faced to another red brick wall of quantum mechanical phenomena and a device-level scaling will be too difficult to carry on Moore’s law. Therefore present integration technology using two-dimensional design with planar devices should be replaced by three-dimensional integration scheme with novel structure devices and together with new doping process for these devices. The non-planar SOI-MOSFET devices like FinFET, Tri-Gate, p-Gate structures are promising candidates for sub-10 nm MOSFET applications due to their ability to relax the short-channel effects. A plasma doping process, one of ultra-shallow junction technology solutions, has many advantages of high dose, low acceleration voltage and multi-directional dopant implantation because wafers are exposed to high density plasma directly. Novel plasma dopant doping efficiency for high-k dielectric and metal gate. We fabricated several tens-nm wide fins and 60 nm gate length FinFETs, and measured their I-V characteristics. Fins and FinFETs using novel plasma doping show good current drivability and low sub-threshold slope. However, without plasma thermal annealing, this process produces defects and traps as well as hydrogen ions on the interface and inside silicon, and these degrade device reliability. On the other hand, results of our ultra-small MOSFET research show possibility of new memory devices with these traps and ions in devices.

**E9.16**
*Theoretical Investigation of Formation of (n-n+)-Junction in the Ion-implanted Crystalline Matrix.*
Halya M. Khlyap1 and Roman M. Peleshchak2; 1Physics, University of Technology, Kaiserslautern, Germany; 2Physics, State Pedagogical University, Drohobyx, Ukraine.

There is no need to talk about importance of high-quality structures for designing different devices for nano- and spin electronics. Ion implantation is not only a famous tool for successful doping of semiconductor wafers, but also a good instrument for defect engineering in order to form isotope or anisotype junctions in the subsurface region of the substrate (the depth of this region depends on the energy and the mass of the ions in the beam). For obtaining materials with in-advanced defined properties it is very important to predict the profile of implanted ions distribution in the crystalline matrix as well as to get information about the self-consistent distribution of charge carriers and electrostatic potential in the implanted lattice. The abstract reports results of theoretical calculations performed for clarifying redistribution of electrons and electrostatic potential in the implanted crystalline matrix (100)-GaAs+Sb[Al] due to electron-deformation effects. The model requires self-consistent solution of the following set of equations: 1) time-independent Schroedinger equation; 2) equation of mechanical equilibrium; 3) Poisson equation to determine the distribution of electrostatic potential; 4) equation for determining carriers concentration and 5) equation for calculation of chemical potential in the implanted system. The most important result is as follows: it is shown that in the elastic region of the implanted matrix forms (n-n+)-junction. Current-voltage characteristics of the junction are numerically simulated.

**E9.17**
*First-Principles Study of Silicon Point Defects.*
Jinyu Zhang1, Roman M. Peleshchak2; 1Physics, University of Technology, Kaiserslautern, Germany; 2Physics, State Pedagogical University, Drohobyx, Ukraine.

Using density functional theory (DFT) calculations within the...
generalized gradient approximation (GGA), we have investigated the structure, energies and diffusion behavior of Si defects including interstitial, vacancy, FFCD and divacancy in various charge states. All atomic and electronic structures and total energies were calculated within the CATSP using the GGA functional and ultra-soft pseudo-potentials. All the calculations were performed in a 64-atom supercell with periodic boundary conditions [2p2p2p]. In Monkhorst-Pack k-point sampling with an energy cut-off 160 eV. We have calculated pathways and barriers using Linear Synchronous Transit (LST) method. For the structure and formation energy of interstitials, C, three different interstitial configurations, (110)-split, Hexagonal (H), and Tetrahedral (T), were examined. In neutral charge state, the (110)-split and H site are energetically equivalent, 0.15eV lower than T site. This is in good agreement with previous DFT studies. In -1 charge state, the (110)-split configuration is 1.8eV lower in energy than the neutral configuration. In positive charge states, the H site becomes unstable. It spontaneously changes its form to T site. (110)-split is stable in +1 charge state but also changes to T site in +2 charge state. The T site becomes the most stable in positive charge state. We found +2 charge state of T site to be most stable at midgap. Different diffusion paths in 0, +1 and +2 charge state are investigated. The migration barriers in 0, +1 and +2 charge states are 0.23 eV, 0.44 eV and 1.26 eV respectively. Next the structure and formation energy of vacancy in different charge state are studied. The ionization levels for vacancy are in agreement with experimental results and previous studies. The migration barriers are 0.16 eV, 0.36 eV, 0.30 eV and 0.75 eV for -1, 0, +1 and +2 charge state respectively. It was found that the migration barrier increases as the positive charge increases. The same tendency also exists in interstitial migration. We also studied the fourfold coordinated (FFCD) point defect which is recently considered. The formation energy of FFCD is 0.5 eV and 0.86 eV lower than that of the neutral split-(110) interstitial and vacancy. This is in agreement with previous DFT studies. The migration barrier between FFCD and perfect silicon lattice is 0.37 eV much smaller than the migration barrier given by previous tight-binding calculation. Our calculation shows that FFCD is the L-v complex proposed by previous tight-binding calculation. Its migration barrier can be considered as I-V recombination barrier in agreement with the values used in many analytical models of I-V recombination. For the activation energy of Pandey’s concerted exchange mechanism of 4.54 eV is in good agreement with earlier calculations. The diffusion behavior of divacancy is studied. The formation energy of the neutral divacancy goes from 3.06 eV to 0.71 eV depending on the charge carrier density. We found that the migration barriers of divacancy in -1, 0 and +1 state are about 1.46 eV in good agreement with experimental results.


The precipitation and diffusion of oxygen in heavily arsenic doped Czochralski (CZ) silicon wafers (with starting oxygen concentration of 7x10^{17} / cm^3) have been studied for different thermal budgets and different back surface treatments. After annealed at 1200 °C for 45 minutes and 900 °C for 13hrs sequentially, the wafers with damaged back surface show rapid oxidation and plate like SiO_2 precipitates. These defects extended about 1 μm into silicon back from the back surface. They all have a habit plane of {111}. This morphology has only been observed at low temperature (~<300°C) in lightly doped CZ silicon wafers. For the same annealing condition, the wafers sealed with polycrystalline film of 1.3μm (polysilicon) show no oxygen precipitates in the silicon substrates. Only polyhedral oxygen precipitates were observed at the interfaces between the polysilicon film and the silicon substrate. They have a habit plane of {100}. These results differ significantly from the previous observations in heavily boron and antimony doped silicon wafers which show drastically enhanced oxygen precipitation when the back surface is sealed with polysilicon. The kinetics of this oxygen precipitation behavior is discussed in detail. The SIMS and EDS analysis indicate that the diffusion of oxygen from the substrate to the epitaxial layer has been significantly reduced in the wafers with damaged back surface, compared with those with polysilicon sealed back surface. This diffusion difference shows significant impact to the performance of the devices built on these substrates.

E9.19 Influence of Oxygen Vacancies and Strain on Electronic Reliability of SiO_2 Films. Ken Saga1, Hideo Miura and Tetsuo Sioji1, Fracture and Reliability Research Institute, Tohoku University, Sendai, Miyagi, Japan.

Local defects in thin gate oxide films used for sub-100 nm devices play a very important role in both the electronic performance and reliability of the devices. One of the most important local defects in the gate oxide is the compositional fluctuation caused by oxygen or Si vacancies. They are mainly introduced near the interface between the thermally oxidized Si-dioxide and the removed Si. In addition, mechanical stress or strain has been increasing in the gate oxide film and high tensile strain decreases the band gap of the film and thus, increases the leaking current through the film. In order to make clear the effect of the strain on both electronic and structural characteristics of SiO_2, we performed a quantum chemical molecular dynamics analysis for SiO_2−x structure under strain using the colors code [1]. The formalization of this program is based on an extended Hückel approximation, resulting in much faster simulations than those based on regular first principle calculations. Three dimensional periodic unit cell of α-crystallite with oxygen vacancies was used for the simulations. The simulation allowed us to predict the strain effect in the structure and electronic properties of SiO_2 with oxygen vacancies on the atomic level. We found that oxygen vacancies in SiO_2 make silicon monoxide molecules and that the plural monoxide molecules start to cluster in the crystal. These structural changes seriously decrease the band gap of SiO_2. The calculated band gap of SiO_2 determined from energy difference between HOMO and LUMO was 8.5 eV. On the other hand, the band gap value was 7.2 eV on average in SiO_2 with an oxygen vacancy. It was found that the insulating property decreases in the SiO_2 film with oxygen vacancies. In addition, the band gap decreases further under high tensile strain. We found that the serious decrease of the band gap occurs when both the number of oxygen vacancies and tensile strain increase in the SiO_2 film. [1] K. Suzuki, Y. Kuroiwa, S. Takami, M. Kudo, A. Miyamoto and A. Imamura, Solid State Ionics, 152-153 (2002) 273-277.


A theoretical modeling of the oxygen diffusion in silicon and germanium crystals both at normal and high hydrostatic pressure has been carried out using mechanics, semiempirical and ab initio methods. It was established that the diffusion process of an interstitial oxygen atom (Oi) is controlled by the optimum configuration of three silicon (germanium) atoms nearest to Oi. The calculated energy values of the Si-O (Ge), Si-O, and Si-O-Si bonds are in a excellent agreement with experimental ones and for the first time describe perfectly an experimental temperature dependence of the Oi diffusion constant in Si crystals (0.046 cm^2 s^-1 at 1500 C). Hydrostatic pressure of 6 GPa results in a linear decrease of the diffusion barrier (δE= -4.38 x 10^{-3} eV kbar^{-1} for Si crystals). The calculated pressure dependence of Oi diffusivity in silicon crystals agrees well with the pressure enhanced initial growth of oxygen-related thermal donors.

E9.21 Contact Free Defect Investigation in As-Grown Fe Doped Si, InP, GaAs, Hahn 1, Hahn 2, Landrigh-Wendrock 3, Kay Dornich 4, Mueller 5, Schwegler 6, and Niklas 7; 1Institute for Experimental Physics, TU Freiberg, Freiberg, Germany; 2Dept. of Materials Science, University Erlangen, Nuremberg, Germany.

InP is a promising semiconductor with properties suitable for many applications, particularly for optoelectronics and high frequency devices. The new experimental methods of microwave detected photo induced current transient spectroscopy (MD-PICTS) and microwave detected photoconductivity (MDP), which we used already successfully e.g. for the investigation of defects in GaAs Wafers, where applied to semi insulating (SI) Fe doped InP samples. These methods allow for defect investigations somehow similar to DUTS, however, without the necessity of special doping, without contacts and high spatial resolution. Several characteristic defect levels were observed in InP doped with iron. One prominent defect center observed to Fe showed a similar behavior like the well known EL2 defect in GaAs. The Fe level in InP:Fe exhibits a positive or a negative PICTS signal depending on the Fe concentration and hence on the Fermi level position. According to solutions of a rate equation system we developed to account for the properties of the EL2 in GaAs this provides strong evidence that the iron center in InP:Fe must have properties of a recombination center. The associated activation energies to the conduction band and to the valence band, respectively, were determined. Beside this major defect we discovered a wide range of shallow defects. The new experimental methods MD-PICTS and MDP allow not only for a non-destructive defect investigation but also for the measurement of spatial distributions of these defects, which were usually not within the spatial resolution of conventional methods like the homogeneity of the samples. This will be also demonstrated.

E9.22 Peculiarities of Defect Formation Processes in ZuSe Crystals
isovalent impurities lead to significant increase of temperature and radiation stability of semiconductor, etc. They are also very important for LED and similar applications because of improving intensity of radiation recombination rate. This paper is dedicated to the analysis of doping technology influence on the ensemble of intrinsic defects for zinc selenide crystals and isovalent tellurium impurities. We used the method of quasi-chemical reactions to calculate equilibrium concentration of intrinsic defects, when isovalent tellurium impurity was introduced in two different ways, namely from the vapor phase and during the crystal growth process. It was shown that in the latter case the tellurium system is dominated by formation of zinc vacancies $V_{Zn}$, together with selenium and zinc atoms occupying interstitial positions in crystalline lattice ($Se_i$ and $Zn_i$). Single-charged defects create associates of $V_{Zn}$ - $Zn_i$, causing intensive radiation band at the energies of about 1.7eV. Annealing of the sample in saturated zinc vapors resulted in the shift of the band to 1.0eV. Recombination processes taking place in the system for this case involve $Zn_i$ impurity levels. Doping of ZnSe with tellurium from the vapor phase led to another shift of the effective radiation band to 2.3eV, caused by tellurium impurities in the donor states. Intrinsc defect concentrations obtained from our calculations are in good agreement with experimental data for luminescent and electrophysical parameters and characteristics. 

E9.23
Electronic Structure of Defects and Defect Clusters in Narrow Band-Gap Semiconductors\[1\] Shubendra D. Mahanti \[1\]; Daniel W. Graphman \[1\] and Vincent G. Kandru \[1\]; \[1\] Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan. 

It is well known that defects profoundly alter the electronic structure near the band gap of semiconductors and control their transport properties. Almost 17 years ago Lent et al. [1] presented a simple chemical bonding description of substitutional impurities in PbTe, a classic narrow band gap semiconductor used for infrared detection and thermoelectric application. This theory explained the origin of resonant defect levels near the fundamental band gap and also predicted resonant level further away from the band gap. They argued that due to the large dielectric constant of PbTe, the Coulomb forces were screened out and local bonding considerations dominated the impurity state formation. These impurity states are referred to as deep defect states. We have carried out ab initio electronic structure calculations within density functional theory to both understand the physics behind the formation of deep defect states and to have a quantitative understanding of these states. [2] We have investigated how these deep defect states get modified when different types of impurity microstructures are present. In particular we will discuss about a class of novel narrow band gap semiconductors and semimetalites $MnSbTe_2$- $ZnSe_2$ where $M$ is Ag, Na, K. We will discuss the details of these calculations. We have found that the electronic structure near the band gap region of PbTe caused by replacing divalent Pb atoms by monovalent M and trivalent Sb atoms preserving the optical exciton energy. Possible reasons behind the superior thermoelectric properties observed in these quaternary systems will be discussed. [2] Work supported by an ONR-MURI grant [1] C. S. Lent et al., Solid State Communications 61, 83 (1987). [2] Daniel Bic et al., Phys. Rev. Lett. 93, 140403 (2004). [2] K. F. Hsu et al., Science 303, 818 (2004). 

E9.24
Abstract Withdrawn

E9.25
Micro-Raman Spectra Analysis of the Evolution of Hydrogen Related Defects and Void Formation in the Silicon Ion-Cut Process\[1\] Wolfgang Duengen \[1\], Reinhart Job \[1\], Yue Ma \[1\], Yue Long Huang \[2\], Wolfgang R. Fahrner \[1\], Lars O. Keller \[2\], Achim Wiggershaus \[2\]; \[1\] Electrical Engineering and Information Technology, University of Hagen, Hagen, Germany; \[2\] Electrical Engineering and Information Technology, University of Dortmund, Dortmund, Germany. 

Hydrogen induced exfoliation plays an important role for the silicon-on-insulator (SOI) wafer fabrication. A prominent example is the Smart-cut process. By such processes it is possible to create silicon layers which could be used to form SOI wafers. The properties and evolution of various silicon-hydrogen bonds and atomic hydrogen in hydrogenated silicon wafers is crucial for the growth of platelets and blisters, which pushes the exfoliation of a thin silicon layer. By micro-Raman spectroscopy (RS) we have investigated the hydrogen concentration of hydrogen implanted boron doped (100)-oriented carbon spread on Czochralski silicon (Cz Si) wafers after post implantation annealing. We have studied the evolution of hydrogen related defects, multi-vacancy complexes and hydrogen molecules by the investigation of implanted and subsequently annealed Cz Si samples in dependence on the implantation dose. The formation of blisters, platelets, voids and the saturation of dangling bonds by hydrogen (i.e. Si-H bonds) in dependence on the annealing temperature can be studied by RS. At temperatures above about 400 C the Raman signal of H-molecules located in vacancy complexes at a frequency of about 3820 cm$^{-1}$ disappears and the higher frequency of hydrogen molecules in voids or platelets at 4160 cm$^{-1}$ can be observed. The bigger part of the multi-vacancy complexes (2000 - 2200 cm$^{-1}$) is dissolved at an exfoliation temperature of 600 C but characteristic stable bonds remain at 2110 cm$^{-1}$ and 2170 cm$^{-1}$ even after the annealing process. Further measurements, i.e. atomic force microscopy (AFM) and thickness measurements of exfoliated silicon films indicate that hydrogen bonding on thermally grown silicon oxide or after anodic bonding on sodium doped glass were performed. The distribution of hydrogen related defects was investigated in dependence of the depth in the wafer. The impact of the damage region caused by the hydrogen implantation and the projected ion range on the depth of the ion-cut process is also discussed. 

E0.26
P-N Junction Diodes Fabricated on the Basis of Hydrogen Enhanced Thermal Donor Formation in P-Type Czochralski Silicon. Yuelong Huang, Katrin Meusinger, Yue Ma, Wolfgang Duengen, Reinhart Job and Wolfgang R. Fahrner; Electrical Engineering and Information Technology, University of Hagen, Hagen, Germany. 

Hydrogen is introduced into subsurface layer of the p-type Czochralski silicon wafers by the direct exposure to a high-frequency (110 MHz) hydrogen plasma exposure. Post-hydrogenation annealing at temperatures between 350-450 C leads to the rapid in-diffusion of hydrogen and hydrogen-enhanced thermal donor (TD) formation. Due to the counter doping by TDs, deep p-n junctions are created in a short time. P-n junction diodes (prototypes) are fabricated in a clean room environment. The diodes are characterized by means of spreading resistance probe (SRP), current-voltage (I-V) and capacitance-voltage (C-V) measurements. The working mechanism of the diodes is discussed. The thermal stability of the diodes is investigated. 

E0.27
Hydrogen Diffusion and Crystallization Induced a Structural Change in Boron Doped Hydrogenated Amorphous Silicon Films. Kail Fatilla \[1\]; Hadjadj Aoinar \[2\] and Roca i Cabarrocas Pere \[2\]; \[1\] Laboratoire de Physique des Interfaces et des Couches Minces, Ecole Polytechnique, 91128 Palaiseau, France; \[2\] Laboratoire d’Analyse des Solides, Surfaces et Interfaces, Universite de Reims, 51087 Reims Cedex 2, France. 

We have studied the evolution of the structure of intrinsic and doped hydrogenated amorphous silicon films exposed to a hydrogen plasma. The substrate temperature was fixed at 200 C and the hydrogen plasma was obtained under an RF power of 30 W and a total pressure of 1 Torr. For this purpose we combine in-situ spectroscopic ellometry and secondary ion mass spectrometry measurements. We show that hydrogen diffuses faster in boron doped hydrogenated amorphous silicon, leading to a thick H-rich subsurface layer from the early stages of hydrogen plasma exposure. At longer times, hydrogen plasma leads to the formation of a microcrystalline layer via chemical transport where a silicon is etched by hydrogen from the reactor walls and deposited on the heated a-Si:H substrate. There is no evidence for crystallization of the a-Si:H substrate. Interestingly, we observe that hydrogen content decreases in the boron doped a-Si:H exposed to deuterium plasma and once the microcrystalline layer is formed hydrogen diffuses out of the sample accompanied with decrease of boron content. 

E0.28

As silicon CMOS technology is scaled down to smaller dimensions, the ability to activate greater amounts of dopant atoms is a significant challenge for realization of shallow junctions. Dopant activation is more difficult to achieve in shallow junctions due to higher concentrations of dopants and possible formation of clusters. The high temperatures currently used to activate dopants result in increased
juncture depth, and problems with transient enhanced diffusion, however, lowering of annealing temperature results in lesser dopant activation. On the other hand, high-temperature annealing results in activation in boron implanted at a dose of \(5 \times 10^{14} \text{ cm}^{-3}\) and energy of 5 keV at annealing temperatures of 450 C and below, by the incorporation of atomic hydrogen introduced by exposing the substrate to a hydrogen plasma at 250 C prior to implantation. This effect was attributed to three factors. Firstly, lattice relaxation occurs due to the presence of hydrogen at a vacancy, which reduces the activation energy for boron to enter the site. Secondly, vacancies created in the lattice during the hydrogenation process can act as recombination centers. Finally, hydrogenation during annealing lead to greater activation. It is known that the presence of a vacancy supersaturation in the crystal lattice enhances boron activation. Thirdly, it was postulated that the presence of a large concentration of vacancies close to the surface, and hydrogen movement during annealing could either hinder boron cluster formation or assist cluster breakup. However, it is not clear which of the above factors contribute to boron activation enhancement and to what extent. In this work, further experiments have been carried out to attain a better understanding of the mechanisms responsible for boron activation enhancement. Hydrogenated and unhydrogenated samples, implanted with boron, phosphorus, and antimony, were annealed in a Rapid Thermal Anneal (RTA) furnace for 20 seconds, at 300, 400 and 500 C. The active dopant profile was characterized using Spreading Resistance Profiling (SRP). Effect of varying dopant concentration, and annealing time was also studied. Activation enhancement was observed even at lower boron implant concentration, where cluster formation is likely to be reduced. Activation enhancement with hydrogenation was also observed for both p-type and n-type samples. It is worth mentioning that at lower boron concentrations, unlike boron, diffuses by a vacancy-assisted mechanism. The experimental results shed new light on the interaction between atomic hydrogen, point defects and dopants. We would like to acknowledge the assistance of Solid State Measurements Inc. with obtaining the SRP results.

**E9.30** Hydrogen Ion Implantation Caused Defect Structures in Heavily Doped Silicon Substrates. Minjun Li and Qi Wang; Fairchild Semiconductor, West Jordan, Utah.

The defects caused by hydrogen ion implantation have been studied in detail for heavily arsenic (As-doping level at 2.5 \(10^{15} \text{ cm}^{-3}\)) and phosphorus (P-doping level at 1.3 \(10^{15} \text{ cm}^{-3}\)) doped (100) silicon substrates. At the implantation energy of 170keV and ambient temperature, H\(^+\) ion is known to create a damage zone with a width of about 400nm in both substrates. The depths of the zone are 148nm and 1058nm for the P- and As- doped substrates, respectively. The SEM study shows that the width of damage zone increases with increasing hydrogen ion dose. For example, the width of the defect zone in the As doped substrate changes from 138nm, 315nm, through 415nm when \(10^{11} \text{ ions/cm}^2\) and \(10^{11} \text{ ions/cm}^2\) for P-doped substrates. The experimental results show that the width of damage zone increases with increasing \(H^+\) ion dose. The structure and distribution of hydrogen in the damage zone in these substrates have been studied by TEM and Rutherford Scattering Spectroscopy (RBS) for variety of \(H^+\) ion as well as for 


Hydrogenation is used extensively in solar cell fabrication as a technique to passivate residual impurities and defects. In the most common approach, hydrogen passivation is combined with deposition of AR coating and metallization. This consists of depositing a layer of hydrogenated silicon nitride (SiN\(_H\)) by PECVD process on a wafer with an N/P junction. Next, a metallization pattern is screen-printed over the entire wafer and then fired. During the RTA step of the process. Recent studies indicate that \(H\) transport from plasma to the bulk of the silicon wafer occurs as follows: H is stored at the surface of the Si wafer in the process-induced defects (PDs) generated during the deposition. During the annealing step of the process, H is released from the defects and diffuses into the bulk. One of the important requirements in making a good solar cell is that the PDs must be annihilated during the H\(^+\) step. Remaining defects due to incomplete annealing are responsible for decreased device performance through two mechanisms: high surface recombination velocity and poor junction quality. Thus, a study of the dynamics of these defects and their effects on the surface recombination and junction properties is important to understand the transport of \(H\) and to minimize any residual defects or defect conversion. This paper will describe results of our studies in which samples were hydrogenated by two different PECVD techniques: low-frequency and high-frequency-based plasma. These techniques are known to produce different degrees of passivation, but the mechanisms are not known. The samples were studied under different RTP conditions and then analyzed to determine the effects of different defect profiles and H diffusion profiles. These results verify our previous conclusions that a defect layer mediates H transport from PECVD plasma to the bulk Si. H is stored in the damage produced by the plasma. Low damage levels are measured as clusters of small defects. Higher damage levels form a network of stacking faults (SF) and platelets. RTP processing heals the damage to a large degree, but is also accompanied by formation of SF and platelets. We will discuss the differences in the defect dynamics in the two methods of hydrogenation.
The growth and dopant incorporation during metal-organic vapor phase epitaxy (MOVPE) strongly depends on the orientation of the starting substrates. MOVPE of Si-doped GaSb layers on (100), (111)B, and (111)A substrates were used to investigate the effect of orientation on the growth rate, the surface morphology and the silicon incorporation. Orientation dependence of growth rates was studied as a function of temperature (T) and atomic hydrogen flux (H2). The growth rate on the (111)B oriented substrate decreases, whereas that on the (111)A oriented substrate increases. The surface morphology on different substrates was studied by scanning electron microscopy (SEM) and atomic force microscopy (AFM). Flat-top hexagonal hillocks were observed on (111)B surface, and the growth was by step-flow on these facets. A surface kinetic growth model has been proposed to describe the grown GaSb layers on (111)B surfaces. Finally, the orientation dependence of silicon incorporation was studied by secondary ion mass spectrometry (SIMS) and Hall measurements. It was found that the silicon incorporation rate was four times higher on (100) oriented surface than on (111)B oriented substrate. Although no conduction type switch was found on (111)B oriented substrate, throughout the Si doping range studied, a Ga slightly rich growth condition might be one of the factors accounting for the discrepancy between theoretical prediction and experimental results.

E9.34 Photoelectron Emission Technique for the Surface Analysis of Semiconductors. Takahiro Saito1, Yoshikazu Momose2, Masaomi Kudou3 and Keiji Nakayama4; 1Division of General Education, Ashikaga Institute of technology, Ashikaga, Japan; 2Department of Material Science, Ibaraki University, Hitachi, Ibaraki, Japan; 3National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan.

To characterize the state of real surfaces of semiconductor in ambient environments, we have developed an extremely sensitive technique for surface analysis using photoelectron emission. The emitted electrons are detected by a gas-flow Geiger counter with Q gas. This measurement is performed by scanning the wavelength from 350 to 2000 nm of incident light from 12 lamp at different temperatures between 25 and 340 °C. The dependence of the intensity of photoelectron emission Iph on the photon energy of incident light (yield spectrum of photoelectron) is obtained at each temperature. Using this technique, the photoelectron emission characteristics of commercial Si wafer (100) surface are investigated. The thickness of the Si wafer is 0.52 mm and the electric resistance is larger than 1000 Ω. In general, the theory of photoelectric emission from semiconductors predicts a power law from the yield near threshold [I] by the following equation: Iph=C(hw - E0). The value of the exponent n and the threshold E0 depend on the excitation and escape mechanism including ionization and transitions in the bulk. However, it was reported that experimental yield spectra of clean (111) Si surface prepared by cleavage in high vacuum showed that n = 3.0 and E0 = 5.15 eV, likely due to indirect transitions from the top of the valence band to the lowest unoccupied levels. Photoelectron emission from real surfaces of semiconductors is affected by direct optical transition from the surface states. Thus, in order to obtain the correct value of the exponent, it is necessary to separate the contributions of surface states to the shape of the spectrum of the photoelectric emission from the real surface. This was performed using the Gaussian function in the present work, and therefore it was confirmed that the value of n = 2.5 is the best power and there exist three surface states on the Si (100) surface. The surface states are considered to be the three states due to the dangling bond terminated by hydrogen atoms: monomer, buckled dimers, and nonbuckled dimers. Acknowledgement This work was supported by Grant-in-Aid through Ministry of Education, Culture, Sports, Science, and Technology. [1] E. O. Kane, Phys. Rev. 127, 131 (1962) [2] G. W. Golabi and F. G. Allen, Phys. Rev. 127, 141 (1962).


As the semiconductor industry strives to decrease device geometries and increase yield, the critical defect size becomes smaller and identification of defects becomes more challenging. Defect analysis is playing an increasing role in process development, process monitoring and yield enhancements. Auger Electron Spectroscopy (AES) is one of the few techniques that has surface sensitivity and small analysis volume to make it the ideal analytical technique for the compositional characterization of submicron defects. However, due to the size and cross section of the buried defect, Auger analysis provides accurate identification of buried defects that are critical for quickly ramping to higher yields and recovering from yield excursions. This paper reports two recent examples of AES combined with XPS to detect and diagnose processing problems. Defining active and isolation is the first important process step for CMOS devices. If defects are created at this step, they will adversely affect device function and yield. One CMOS product lot failed for high defectivity at the KLA inspection after hundreds of pattern killer defects with a very defined wafer signature were detected after trench etch. Auger and EPR analysis were performed on surfaces of the patterned and buried defects. The results showed they were made of nitride or silicon and located beneath the nitride layer, which indicated that the defects were created before nitride film deposition. Based on the analytical and tool commodity information, the root cause was identified and the failure mechanisms were understood. Magnetoreisitive Random Access Memory (MRAM) is nonvolatile, has unlimited read and write endurance, and can operate at high speed and low voltage with densities comparable to conventional memories. Copper is chosen as the interconnect metal for MRAM because of its low resistivity and electromigration resistance. The digit line fabrication process includes copper deposition and a CMP process with an alumina abrasive first step slurry and a silica abrasive second step slurry. The black spot defects were found on the surface voids in the copper filled with Al, Si, O. This suggests that the defect could have been the product of copper corrosion caused by residual slurry from first-step polishing, and a possible incompatibility of the first- and second-step slurries as pad wear increases. As result of this finding, evaluation of different combinations of first- and step-step slurries has been initiated.

E9.36 Abstract Withdrawn


In a study attempting to link visible light emission with structure and defects, near-stoichiometric a-SiC:H films have been subjected to vacuum anneals. The a-SiC:H films were deposited by reactive magnetron sputtering of silicon in an (Ar+CH4) gas mixture. Quartz and silicon wafers were used as substrates. The films were analyzed by means of Auger-electron spectroscopy (AES), atomic force microscopy (AFM), optical absorption spectroscopy in visible/infrared region, optical reflectance, paramagnetic resonance (EPR), photoemission (PL) and Raman scattering. Thermal annealing was performed in vacuum (10^{-10} Pa) for 15 minutes over the temperature range 200 - 850 °C. As-deposited film showed weak room-temperature PL and a high concentration of paramagnetic centers N, (3.4 x 10^{15} cm^{-3}). The PL band was centered at 2.3 eV and covered the entire visible range. After a 450 oC anneal, there was almost a decade change in the PL intensity, while Ns decreased by a similar order to 3.8 x 10^{18} cm^{-3}. For annealing temperatures above 450 °C, the PL intensity decreased and Ns increased monotonically. Analysis of the EPR line showed that the few techniques that has surface sensitivity and small analysis that were used to detect the as-deposited films the spin was mostly related to carbon dangling bonds (g=2.0026), whereas silicon dangling bond signals (g=2.0039) appeared after thermal annealing. The peak position and peak width (FWHM) of the PL band was almost unchanged after annealing while the optical band gap decreased significantly from the as-deposited value of 2.6 eV to 1.8 eV after annealing at 850 °C. We believe this to be evidence of inhomogeneity of the structure now composed of wide bandgap and low bandgap regions. Radiative recombination takes place in the wide gap regions while fundamental absorption edge is determined by low gap regions. Raman scattering measurements of the films annealed at high temperatures indicated formation of free amorphous carbon clusters. Chemical bonding of hydrogen in the films was analyzed by FTIR measurements in transmission geometry. As-deposited film had H/C ratio of about 0.61, while the film annealed at 850 °C had 0.83 cm^{-1}, 1100 cm^{-1} and 2100 cm^{-1}; we ascribe these to the Si-C stretching, C-Ha wagging and Si-Ha stretching modes respectively. The FTIR measurements also showed that the concentration of Si-H bond was steadily decreased during annealing, at the same time the intensity of the C-Ha absorption band changed in
good correlation with the temperature dependence of PL intensity, N, and optical band gap. We draw the following conclusion from our experimental data: At low annealing temperatures, the weak hydrogen bonds (including Si-H bonds) start to break. Released atomic hydrogen is trapped by carbon dangling bonds because the C-H bonds are still stable at such temperatures. Redistribution of hydrogen leads to a decrease of N, and an increase of PL intensity. At higher annealing temperatures all forms of hydrogen bonds become unstable and the light-emitting property of the films deteriorates.


It is well known that many common fabrication processes will produce some kind of defects in semiconductors. At the same time, these processes will also induce stresses in the semiconductor structures. It is therefore not surprising that these process-induced defects and stresses are associated with each other. Recently, we have developed a high sensitivity stress measurement technique based on the infrared photoelastic method using a low level birefringence detection system [1]. This system has been applied to study the local stress distribution in Si under thin oxide layers. Because of the high sensitivity of this system, for the first time it was clearly shown that the local stress distribution under the thin oxide layer deviated from what predicted by the metallic model [2], and that stress due to defects is detected in Si substrate during the oxidation process. In the future, we shall report more of our recent results to demonstrate how we can probe process-induced defects in Si using this method. For example, we have prepared silicon oxide and silicon nitride layers of various thickness on Si substrate under various conditions and studied the stress distribution in the substrate, hence obtaining information on the defects associated with these processes. We have also prepared shallow-implanted samples and used this stress measurement method to probe the defect distribution in the substrate. Details of the measurement system and quantitative analysis of the correlation between the process-induced defects and stresses will be presented and discussed. [1] G. J. H. Peng et al., Rev. Sci. Instr. 74 (2003) 4745. [2] X. Li et al., Mat. Res. Soc. Symp. Proc. 821 (2004) P8.8.

**E9.39** Defect Reduction in Si-based Metal-Semiconductor-Metal Photodetectors with Cryogenic Processed Schottky Contacts. Minya Li and Wayne A. Anderson; Electrical Engineering, SONY at Buffalo, Buffalo, New York.

Metal-Semiconductor-Metal photodetectors (MSM-PD's) were fabricated using a low temperature (LT) technique to greatly reduce the device dark current. Low temperature (LT) processing for metal deposition increases growth rate by improving the interface between metal and semiconductor to reduce the leakage current of the device. The structure consists of a 20 Å oxide on the active area to passivate surface states, a thicker oxide under contact pads to reduce dark current and the interdigitated Schottky contacts. A comparison was made for Schottky metal deposited with the standard room temperature (RT) metal deposition technique. The dark current for the LT film was found to be two orders lower in magnitude compared to the film deposited at RT. The dark current was significantly reduced from 4.06 to 0.009 nA. The active area for the device was determined to be 40 x 50 μm² with 4 μm electrode width and 2 μm electrode spacing. Additionally, LT-MSM-PD's exhibited an excellent linear relationship between the photovoltage and photocurrent. The band gap height was found to be 0.73 eV. However, this value was 0.1 eV more than that of the same device fabricated at RT. The paper will discuss current-voltage temperature (IVT) analysis to reveal changes in the interface due to LT processing.

**E9.40** Optical and Electrical Characterization of Quantum Dot Infrared Photodetectors. Young-Deok Hong, Dong-Hwan Hwang, B. B. Nielsen, B. B. Nielsen, Physics and Astronomy, University of Aarhus, Aarhus, Denmark.

Hydrogen atoms interact strongly with native defects in crystalline silicon, as well as in other semiconductor materials. The primary reason is that native defects possess dangling bonds, and that a hydrogen atom inside the material may lower its energy significantly by saturating a dangling bond attached to a semiconductor host atom. Hydrogen-defect complexes may be studied by a range of experimental techniques among which Fourier Transform Infrared (FTIR) spectroscopy, Electron Paramagnetic Resonance (EPR) spectroscopy, and Deep Level Transient Spectroscopy (DLTS) have been particularly useful. In this talk, I will review our studies on hydrogen-defect complexes in crystalline silicon. The vacancy in this material can accommodate up to four hydrogen atoms whereas the self-interstitial can bind up to two. The local vibrational modes of hydrogen are studied by FTIR spectroscopy, and the results reveal information about how the Si-H bonds are perturbed by their surroundings. For hydrogen atoms in the vacancy, the Si-H stretch-mode frequencies increase substantially with the number of hydrogen atoms, because the Si-H bonds interact repulsively. In contrast, the Si-H stretch mode frequencies change only moderately when the charge state of the hydrogen-defect complexes is changed. This suggests a rather weak coupling between the Si-H bonds and the electronic levels within the band gap. These findings are confirmed by EPR measurements, which demonstrate that band-gap states are largely formed as bonding and antibonding combinations of dangling-bond orbitals. Although a Si-H bond usually requires about 3 eV to dissociate, we find that the hydrogen atoms in the vacancy jump rather freely among the dangling bonds at temperatures below 200 K. In particular, the vacancy with...
Two hydrogen atoms reorient thermally at about 150 K but under illumination, the reorientation sets in below 8 K. The implications of these observations will be discussed briefly.

8:30 AM E10.2
Void Formation in Hydrogen Implanted and Subsequently Plasma Hydrogenated and Annealed CZochralski Silicon. Reinhard Job 1, Wolfgang Duengen 1, Yue Ma 2, Yue-long Huang 3, Lars O. Keller 3, Achim Wiggershaus 1 and John T. Horstmann 2; Electrical Engineering and Information Technology, University of Hagen, Hagen, Germany; 2Electrical Engineering and Information Technology, University of Dortmund, Dortmund, Germany.

The formation and evolution of voids in hydrogen implanted and subsequently plasma hydrogenated and annealed (Cz) silicon wafers is studied by depth resolved micro-Raman spectroscopy. Standard (100)-oriented Cz Si wafers were used for the investigation. Hydrogen was implanted with an energy of 40 keV and a dose of 1E16 /cm2. During the implantation the wafers did not exceed a temperature of about 30 °C. Radio frequency hydrogen plasma treatments were applied for 10 min in a standard PECVD setup (50 W, 13.56 or 110 MHz). The plasma hydrogenations were applied at several different substrate temperatures between room temperature and 250 °C. The final annealing was done for 10 min in a forming gas atmosphere under normal pressure at temperatures up to 600 °C. For the analysis depth resolved micro-Raman spectroscopy (RS) was carried out on the Cz Si samples, which were bracketed by low angle on a rotating quartz plate. The Raman vibration modes of H-molecules in vacancies (at 3820 1/cm) and in voids (at 4150 1/cm) are analyzed to provide information about the evolution of vacancies and voids along with the corresponding vibrational features during the hydrogenation and annealing processes. The vibrations at 3820 cm1 are not observed during the plasma exposure.

8:45 AM E10.3
Study of the Hydrogen Effect on Dopant Activation for the Plasma Doping and Ion Implantation. Sungkewon Baek 1, Sunghee Heo 1, Donggyu Lee 2, Won-Ju Choi 2, Kiju Im 2, Chang-Geun Eo 1, Gwan-Ju Dortn 1, and Meinhard Hugl 1; 1Material Science & Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea; 2Future Technology Research Division, Electronics and Telecommunications Research Institute, Daedeon, South Korea.

The ITRS roadmap projected the junction depth of less than 10nm for sub-32nm MOSFET devices, which is the extreme limit of defect engineering. To meet this goal, the ultra-shallow junction, the understanding and control of point defects are important. For the ion implantation, the interstitials are generated by dopant atoms in the junction tail region, which is related to the enhanced diffusion and dopant deactivation. For the plasma doping, additional defects are generated by co-implanted hydrogen and helium. The hydrogen and helium have been used for the dilution. Recently, it was reported that hydrogen in the ambient reorders the solid phase epitaxial growth rate for arsenic-implanted samples. Therefore, for the ultra-shallow junction less than 10nm, the control and understanding of hydrogen contained in the ambient and co-implanted during the plasma doping are necessary. In this study, the hydrogen was incorporated into the P, and As-implanted samples by hydrogen plasma doping. For the exact role of hydrogen, ion implantation energy and dose were divided into two regions. One is for containing the hydrogen profile (high energy & high dose), and the other is for overlapping the hydrogen profile with dopant profile (low energy & low dose/high dose). At the various annealing temperature of 600 900°C, the activation behavior was examined. The activation study shows the hydrogen reduce the dopant activation significantly when the hydrogen profile is overlapped with dopant profile. In addition, it is noted that the reduced activation could be restored and improved by low-temperature pre-annealing. The physical damage by hydrogen plasma doping also could be annealed out by low-temperature pre-annealing, confirmed by TEM/PTM analysis. For the plasma doping of P, the hydrogen was doped simultaneously. The similar role of hydrogen was observed for the plasma doping. By applying the low-temperature pre-annealing, the activation improvement and the reduction of junction depth could be obtained. In addition, the mechanism for the dopant behavior in the RTA and laser annealing for plasma-doped samples was proposed. Finally, the sub-10nm p+n ultra-shallow junction could be fabricated by plasma doping and low-temperature annealing prior to laser annealing.

9:00 AM E10.4
Hydrogen Donors in Zinc Oxide. M. D. McCluskey and S. J. Jokela; Department of Physics, Washington State University, Pullman, Washington.

Zinc oxide (ZnO) has shown great promise as a wide-bandgap semiconductor with a range of optical, electronic, and mechanical applications. The presence of compensating donors, however, is a major roadblock to achieving p-type conductivity. Recent first-principles calculations and experimental studies have shown that hydrogen acts as a shallow donor in ZnO, in contrast to hydrogen’s usual role as a passivating impurity. The presence of hydrogen during growth and processing, it is important to determine the structure and stability of hydrogen donors in ZnO. To address these issues, we performed vibrational spectroscopy on bulk, single-crystal ZnO samples annealed in hydrogen (H2) or deuterium (D2) gas. Using infrared (IR) spectroscopy, we observed O-H and O-D stretch modes at 3320.3 cm1 and 2470.3 cm1 respectively, at a sample temperature of 10 K. These frequencies indicate that hydrogen forms a bond with a host oxygen atom, consistent with either an antibonding or bond-centered model. In the antibonding configuration, hydrogen attaches to a host oxygen and points away from the Zn-O bond. In the bond-centered configuration, hydrogen sits between the Zn and O. To discriminate between these two models, we measured the shift of the stretch-mode frequency as a function of hydrogen pressure. By comparing our measurements with calculations, we conclude that the antibonding model is the correct one. Surprisingly, we found that the O-H complex is unstable at room temperature. After a few weeks, the peak intensity decreases substantially. It is possible that the hydrogen forms O-H2 molecules, which have essentially no IR signature. Electrical measurements show a corresponding decrease in electron concentration, which is consistent with the formation of neutral H2 molecules. The correlation between the electrical and spectral measurements, however, is not perfect. We therefore speculate that there may be a second "hidden" hydrogen donor. One candidate for such a donor is a hydrogen-decorated oxygen vacancy. This work was supported by the National Science Foundation (DMR-0208382).

9:30 AM E10.5
Unusual Effects of Hydrogen in GaNP Alloys: A General Property of Dilute Nitrides. Irina A. Buyanova 1, M. Izadifard 1, G. Ivanov 1, J. Birch 1, Weimin M. Chen 2, M. Felici 2, A. Polimeni 2, M. Capizzi 2, Y. G. Hong 3, H. P. Xin 3 and C. W. Tu 3; 1Linkoping University, Linkoping, Sweden; 2University of Rome "La Sapienza", Rome, Italy; 3University of California, La Jolla, California.

Hydrogen, the simplest element with a light mass, high diffusivity and strong chemical activity, is a common impurity that is abundantly present in most steps of semiconductor growth and device processing. Due to its high chemical reactivity, hydrogen interacts with practically all types of defects in materials including shallow impurities, dangling bonds, and deep defect centers. This causes substantial changes in electrical and optical properties of semiconductors upon hydrogen incorporation, whereas the structure of host lattices usually remains intact. In this work we report dramatic effects of hydrogen incorporation on the electronic structure and lattice properties of GaNP1-x alloys with x < 0.008 grown by gas source molecular beam epitaxy. By employing photoluminescence (PL) excitation spectroscopy we show that post-growth hydrogenation not only leads to passivation of various N-related isoelectronic centers, starting from the one which has the deepest energy levels in the bandgap, but also re-opens the band gap of the GaN alloy and efficiently reduces the N-induced coupling between the Γ, X, and L conduction band states. By Raman spectroscopy, these effects are shown to be accompanied by hydrogen-induced breaking of the Ga-N bond in the alloy, evident from disappearance of the corresponding vibrational mode. According to the performed Raman and X-ray diffraction measurements, the hydrogenation is also found to cause strong expansion of the GaNP lattice which changes tensile strain in the as-grown GaNP epilayers to compressive strain in the post-hydrogenated structures.

SESSION E11: Defect Characterization
Chairs: Reinhard Job and Matthew D. McCluskey
Friday Morning, April 1, 2005
Room 206 (Moscone West)
10:15 AM E11.1
Three Dimensional Hydrogen Microscopy in Diamond.
Guenter Dollinger, Fakultat fur Luft- und Raumfahrttechnik, Institut fur Angewandte Physik und Messtechnik, Neubiberg, Germany.

We introduce proton-proton scattering at a microprobe of 17 MeV protons to quantitatively image three-dimensional hydrogen distributions in metal and semiconductor photovoltaic diamond films at a lateral resolution better than 1 μm and high sensitivity. The images show that most of the hydrogen in a <110>-textured undoped polycrystalline diamond film is located at grain boundaries. The average amount of hydrogen is 8±1.5·10^{18} atoms/cm² along the grain boundaries which corresponds to about 0.05% of the diamond thickness. The content within the grain is below the detection limit of 1·10^{16} atoms/cm² (0.08 at-ppm).

10:45 AM E11.2 Non Destructive Electrical Fault Characterisation and Topography of Silicon Wafers and Epitaxial Layers.
Kay Donnich, T. Hohn and J. R. Niklas; Experimentelles Physik, Technical University Bergakademie, Freiberg, Germany.

Recent progress in the development of experimental technology made it possible to improve the sensitivity of microwave detected photoconductivity (MDP) by several orders of magnitude. This opens completely new possibilities for a contact less non-destructive electrical fault characterisation on silicon wafers and even on epitaxial layers. Electrical properties such as lifetime, mobility and diffusion length can be measured also at low injection levels with a resolution only limited by the diffusion length of the charge carriers. The doping level of the material plays no major role. Recently, it was for the first time possible to extend such investigations also to epitaxial layers with 1μm thickness. Depending on the wavelength of the laser used for optical excitation, it was possible to distinguish between defects in the bulk of an epitaxial layer and defects at the interface to the substrate. Besides the possibility to deliver lifetime, diffusion length and mobility mapping the technique offers a completely new kind of experiment. Owing to the high sensitivity, at sufficiently low injection levels thermal excitation of charge carriers out of defect levels filled during the photo pulse can be observed. This leads to new defect specific photo conductivity transients which can be used like DLTS transients to gain specific information about the defect under investigation. This enables one to obtain pieces of information similar to DLTS, e.g. energies of defect levels and capture cross sections, however, again contact-less, non-destructive, and highly spatially resolved. Moreover, in contrast to DLTS, doping is not a critical parameter and the investigations are not restricted to just deep levels. We called this technique "microwave detected photo induced current transient spectroscopy (MD-PICTS)". MDP and MDP-PICTS may have the potential to become a powerful tool for the investigation of semiconductor materials. Besides a detailed characterisation of starting materials it is a challenge to apply these techniques also to follow process induced defects during device fabrication. First steps in this direction are also reported.

11:00 AM E11.3 Direct High-resolution Determination of Vacancy-type Defect Profiles in Ion-implanted Silicon. Andy Peter Knights 1, S. H. Guo 1, M. van Dyken 1, R. E. Mason 2 and P. G. Coleman 2; 1Engineering Physics, McMaster University, Hamilton, Ontario, Canada; 2Physics, University of Bath, Bath, United Kingdom.

Variable-energy (beam-based) positron annihilation spectroscopy (VEPAS) has for two decades been applied successfully to the non-destructive study of open-volume point defects in thin films and in the first few microns beneath the surface of solids. Control of the energy of the implanted positrons, typically between 0.5 and 30 keV, allows one to gain some semi-quantitative information non-destructively on the depth profile of the defects. However, positron implantation profile broadening with increasing energy and pre-annihilation positron diffusion limit the detail one can obtain from these measurements. Here we demonstrate a significant enhancement in the depth profiling capabilities of VEPAS by combining conventional measurement with non-destructive chemical etching. Using this approach we have determined the depth distribution of open-volume point defects created by room-temperature implantation of Cr silicon by 100 keV B+ ions at a dose of 3·10^{14} cm². The depth resolution of PAS is maintained at 50nm by using positrons implanted at energies below 2 keV to probe each layer as it is brought close to the surface by the etching process. The etch depth dependence of the PAS profiles to another depth dependent profile. The results are in good agreement with Monte Carlo simulations, particularly in the traditionally difficult-to-measure deep tail region. Further we compare the distribution of vacancy-type defects created by room-temperature implantation of Cr ions into Si with a dose of 5·10^{13} cm² to Cr, FZ and epitaxially grown silicon.

11:15 AM E11.4 Electrical Characterisation of MOS Structures and Wide Bandgap Semiconductors by Scanning Kelvin Probe Microscopy. Seong-Eun Park 1, Stoyan Jeliazkov 2, Joseph J. Kopanski 3, John Suehle 3, Eric Vogel 3, Albert Davydov 4 and Holger-Keel Shin 2; 1Semiconductor Electronoics Division, Naval Research Laboratory, Washington, DC; 2Metallurgy Division, National Institute of Standards and Technology, Gaithersburg, Maryland; 3School of Mines, Golden, Colorado; 4Institut fur Angewandte Physik und Messtechnik, Neubiberg, Germany.

Electronic properties of Al (Ag, Cr)/SiO2/Si MOS structures and wide bandgap semiconductor materials such as GaN, InGaN, AlGaN, and SiC were determined by scanning Kelvin probe microscopy. From contact potential difference (CPD) between probe tip and sample, both work functions and surface barrier height (SBHs) were calculated. Measurements of metal work function and SiO2 surface barrier height were sensitive to respective material surface condition. The oxidation or contamination of surfaces led to a decrease in the CPD. Furthermore, variations in work functions and SBHs were studied as a function of In or Al content in InGaN and AlGaN films. Variations in CPD at the interface of Al or Bi implanted SiC films were imaged to estimate doping levels.

11:30 AM E11.5 Comparison of Techniques for Measuring Recombination Lifetime in Semiconductors. Richard K. Ahrens 1, 2, Jamyann Deolador 1, Steven Johnston 1 and Wyatt Motzger 1; 1Measurement and Characterization Division, National Renewable Energy Laboratory, Golden, Colorado; 2Department of Physics, Colorado School of Mines, Golden, Colorado.

There are four techniques that are routinely used in our laboratory for recombination lifetime measurement. These are (A) time-resolved photoluminescence (TRPL); (B) microwave reflection (mR); (C) resonant-coupled photoconductive decay (RCPD); and (D) quasi-static photoconductance (QSPC). They are three of the techniques that are especially sensitive to shallow (temperatures close to 200K) carrier states. For the latter situation, the data must be properly massaged in order to extract real recombination lifetimes. Three of the techniques (A, C, and D) are suitable for measuring lifetime over a wide range of injection levels (injection-level spectroscopy, ILS). However, the photoconductance techniques (C and D) must include an algorithm to account for the variation of carrier mobility with injected carrier density. Although the TRPL technique provides the most unambiguous results for ILS studies, it is a functional lifetime-measurement technique only for the direct-bandgap semiconductors. Techniques A, B, and C are readily adaptable to the measurement of temperature-dependent lifetime. The latter has proven to be invaluable in identifying the dominant recombination defect or mechanism for the entire range of materials. The advantages and limitations of all techniques will be discussed as applied to a variety of common semiconductors.
over a broad spectral range (0.7-1.7 eV) revealing a different spectral signature (and consequently a different joint density-of-states) than for bulk defect dominated films. We argue that the technique can be used in a wide-variety of thin film materials. The technique can also be employed in situ and in real-time during growth by modifying the linear optical cavity scheme into a folded cavity scheme in which the thin film is probed by the evanescent wave at the total internal reflection interface. Preliminary results obtained with this folded cavity will be presented.