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 28, 2005
1:30 PM - 5:00 PM
Room 2006 (Moscone West)

This tutorial will cover basic concepts of semiconductor heterojunctions and the consequences that make them suitable for a wide variety of electronic and optoelectronic applications. 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-edge deformation, and their electrical and photoelectronic 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. Chevallier and Kin-Man Yu
Tuesday Morning, March 28, 2005
Room 2006 (Moscone West)

8:00 AM *E1.1

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 (CuGaSn2) were studied as isolated cases by these three respective communities. Synthetic diamond (transparent conductor, and photovoltaic material). 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 these 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 Eberleina, Robert Jonesb, Patrick Briddona and Sven Obergb; aSchool of Physics, University of Exeter, Exeter, United Kingdom; bSchool of Natural Sciences, University of Newcastle upon Tyne, Newcastle upon Tyne, United Kingdom; cDepartment of Mathematics, Lulea University of Technology, Lulea, Sweden.

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 serious 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 dopant concentration. Although many of the point defects can be eliminated through thermal annealing, some, however, e.g., the PL D1 and Z1/Z2 centers in 4H-SiC, are stable at high temperatures. In this polytype, D1 and the related Alphabet lines are the most prominent photoluminescence (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 radiation effects lead to a deterioration of defect quality with an increase in electrically active grown-in defects. Among these, the Z1/Z2 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 Dopled 4H-SiC Using Optical Admittance Spectroscopy. Winn Yeo, and Mary E. Zvanut; 1Materials Science, University of Alabama at Birmingham, Alabama; 2Physics, University of Alabama at Birmingham, Birmingham, Alabama.

Vanadium doping is one way to make a semi-insulating (Si) material. Vanadium impurity in SiC is important because it can not 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 V^{4+} electron level thought to be within 1 eV of the conduction band edge and a V^{4+/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 E. 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 (E_P1) 1.89 ± 0.02 eV and (E_P2) 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 E_c -1.5 eV is fairly close to the vanadium donor level and the other level E_v -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 additional samples. Program is funded by Dr. Colin Wood, ONR.

0:15 AM E1.4
Important Grown-in Defects in Novel Dilute Nitride (AlIn)GaNP: Ga Interstitials. N. Q. Thinh, I. P. Vorona, I. A. Buyanova, W. M. Chen, Sukit Limpijumnong, B. Z. Zhang, Y. G. Hong, H. P. Xin, G. W. Yu, A. Utsunomi, Y. Furukawa, S. Matsumoto, A. Wakahara and H. Hasegawa; 1Institute of Condensed Matter Technology, Linkoping University, Linkoping, Sweden; 2School of Physics, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima, Thailand; 3National Renewable Energy Laboratory, Golden, Colorado; 4School of Electrical and Computer Engineering, University of California, La Jolla, California; 5Dept of Electrical and Electronic Engineering, Toyoashi University of Technology, Toyoashi, Japan.

Novel (AlIn)GaNP_N_xP_y 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 deteriorate with 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 (AlIn)GaNP-based alloys, from optically detected magnetic resonance (ODMR) studies. Based on the characteristic hyperfine structure, two Ga-interstitials (Ga_i) defects are positively identified as being common grown-in defects in GaNP and AlGaNP 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 Ga_i and thus a deep-level nature of the defects. Based on comparison with calculations of important grown-in defects in (AlIn)GaNP-based alloys, both defects are suggested to be complexes involving a Ga_i-Ga defect by taking advantage of the freedom in altering compositions of both cations and anions of the novel alloy, compositions. The 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
replace Ga, i.e. it is largely enhanced by the presence of Al in the alloys, but is only marginally affected by In incorporation. The effect is attributed to the differences in the ionization energies of group III atoms involved and their bonding strengths with N. The defects are shown to act as non-radiative recombination centers reducing the efficiency of light emissions from the alloys. They can thus undermine the potential of these materials and thus inhibit the performance of diodes based on this materials system. The high thermal stability of these defects observed from studies of post-growth thermal annealing calls for future efforts to eliminate them by optimizing growth conditions.

9:30 AM E1.5 Role of the Substrate Doping in the Activation of Fe\(^{2+}\) Centers in Fe Implanted InP. **Triziana Cesca**, Andreas Gasparotto,2 Adriano Verna,1 Beatrice Fraboni1, Giuliana Impellizzeri1,2 Francesco Priolo1,2, Physics Department, INFM and University of Padova, Padova, PD, Italy; 2Physics Department, INFN and University of Bologna, Bologna, BO, Italy; 1Physics and Astronomy Department, INFM 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 semi-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\(^{3+}\) centers can be incorporated in InP crystals by high temperature ion 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. One particularly relevant point is Fe\(^{3+}\) annealed 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 centers which in turn controls 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 dopant concentration between 5x10\(^{15}\) and 1x10\(^{16}\) cm\(^{-3}\) were implanted at 150 keV and 300 keV and fluences ranging from 5x10\(^{11}\) up to 5x10\(^{12}\) 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-PFIX-channeling. Electrical properties related to the activation of Fe\(^{2+}\) centers were studied by means of experimental and simulated L-V characteristics or DLTS-PICOTS 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 electrical doping in InP affects 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. 75, 668 (1999). (2)/. Cesca et al., Phys. Rev. B 68, 224113 (2003).

9:45 AM E1.6 Electrical Activity of ZnO Grown by Closed Space Vapor Transport on Sapphire Substrates. **Pierre Gaillier**,1 Jean-Francois Rommelou1,2, Jaime Minilla-Arroyo,2 Michel Barbe,1 Francois Jonnard1 and Yves Marfaing1,2 Laboratoire de Physique des Solides et de Cristallogenie, CNRS UPR 8635, Meudon, France; 2CINVESTAV, 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 n-type conductive layer close to the substrate. It is difficult to control the activation of this layer of carriers in non intentionally doped ZnO thin films. This could be also a difficulty for measuring p-type conductivity. We report here attempts to synthesize p-type conducting zinc oxide.

SESSION E2: Dopant/Defects in Silicon Technology

Chairs: **Yu-Ming Wu**

Tuesday Morning, March 29, 2005 Room 2006 (Moscone West)


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-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 an Al contamination and a Zn vacancy (acceptor) whose formation 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 the n-type conductivity of 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 with a thickness below a few microns. This indicates that, with our experimental conditions, Zn vacancies are only generated close to the surface. We conclude that any attempt to achieve and measure p-type doping on ZnO thin films might be condition by the use of (i) a specific diffusion barrier to suppress or (ii) a specific buffer layer as barrier to the diffusion of Al.
Co-Doping Concepts for p-Type Silicon. Paola Alippi and Giorgia M. Lopez. CNR-IMM, Catania, Italy; IFNM-SILACS and Dept. of Physics, University of Cagliari, Monserrato, Italy.

The extreme miniaturization of ultra-large-scale integration Si-based devices requires the increasing use of silicon - 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 formed by isovalent species and acceptors in Si can produce electrically active p-type centers with reduced ionization energies and higher concentrations. The concept (partially analogous to that envisaged for donors in diamond) is based on the empty p-like states of the isovalent center couple to 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. In this work, we report experimental results demonstrating the formation of such oxygen complexes in Si materials. 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 [10-100]°C/min, a p-type doping leading to the formation of a p type structure is observed by spreading resistance measurement. The lower the cooling rate, the deeper the junction is. On the contrary, there is no influence on the doping level when the samples are exposed to room temperature. In this context, we have observed such a hole trap by DLTS measurement with an energy level situated at 0.42 eV from the valence band. Any positive stress increase the capture cross section of this trap. Such a result occurs also in intrinsic and boron doped silicon materials, rejecting the recombination with phosphorus or boron atoms. To check the impact of the oxygen, we have performed a Pt diffusion at the temperature of 950°C for 10 hours in a very low oxygen concentrated silicon material (σ=10⁻⁷ O/µm³, n-type) from Wacker Siltronic AG. A slow cooling at 1°C/min has been used in the following ones: Phosphorus atoms, which are then cooled slowly in the range [1-10]°C/min, a p-type substitutional platinum atom and another unknown impurity along spreading resistance measurement. The lower the cooling rate, the silicon material is rejected the reaction with phosphorus or boron atoms. By using the Ga-B and In-Ge p-type pairs, we confirm the soundness of the general scheme. The effect is sizable (and in good agreement with experiment) for In - whose 0.19 eV level shifts to 0.10 eV upon cooling to C - whereas it is less significant for B. We also investigated co-doping with other acceptors, considering the Ga-B and In-Ge pairs but none of these is bound, so that acceptor-acceptor co-doping is of no help.

SESSION E3: Interfaces and Strain-Induced Defects

Chairs: T. Tsuda and Wai-Shing Lau

Tuesday Afternoon, March 29, 2005
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 Yamashita, W. Futako and Norikazu Mizuochi. AIST, Diamond Research Center, Tsukuba, Japan; Graduate School of Pure and Applied Science, University of Tsukuba, Tsukuba, Japan; Institute of Library 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 structure of Si oxide/Si interface. Furthermore, we need microscopic information about the dynamic oxidation mechanism. 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 a 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. [1] W. Futako, N. Mizuochi, and S. Yamashita, Phys. Rev. Lett. 92 (2004) 105505.

2:00 PM E3.2
Efficient Quantitative Detection of Oxygen Vacancy Double Donors in Capacitors with Ultra-Thin Tantalum Oxide Films for BNAM Applications by Quantified Current Spectroscopy: Wai-Shing Lau, Linbin Zhong, Taejoon Han and Nathan P. Sandler. School of EEE, Nanyang Technological University, Singapore, Singapore; Lam 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. ZBTSC measurements were performed with a ramp rate of 0.5 K/s as shown in [1]. Our method to fill the defect states was UV illumination at about 90 K. The energy level of the defect was estimated using ET = 23kTm, where Tm is the peak temperature and k the Boltzman constant. The first ionization state of the oxygen vacancy deep double donor (VO⁻) is also known as defect D and is the deepest electron trap detected in the temperature range of 100-400 K [3]. Smaller leakage current can be easily correlated with lower ZBTSC signal from D (0.8 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 (VO⁻), 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 found the most efficient way to fill defect D with electrons is to use the optical illumination and soft X-ray during electron beam evaporation of metal to form the top electrode for sample preparation.

2:15 PM E9.3: An Investigation on the Band Offsets of GaNAsSb/GaAs and GaInNAsSb/GaAs. Homan B. Yuen1, Robert Kudrawiec1, Krzyztof Rycroft2, Seth B. Bank3, Mark A. Wiesty1, Hopley Boe1, 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 longer emission wavelengths 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. These materials issues can be overcome by adding more In to N to GaNAs to reach the technologically important wavelength near 1.55 µm. Sb acts as both a surfactant and constituent when introduced during dilute-nitride growth, forming GaInAsSb and GaInAsSb. These materials exhibit a much smaller gap in the energy and reduction of band gap, by adding Sb, has enabled the development of GaNAs-based lasers out to 1.55 µm. Although dilute-nitride-antimonide lasers have been shown to have great potential telecommunication applications, several limitations are well known. Since these materials are relatively new, there has not been any detailed study of the band properties. A greater understanding of the heterojunction band offsets and effective masses would allow for better design of lasers and understanding of the physical processes in these semiconductor active regions. One powerful method of determining band offsets is photoelectron spectroscopy (PH). By monitoring the spectra obtained from PH, a model of the band offsets, energy levels, and effective masses are obtained. There have been many studies on GaNAs and GaNAs band offsets, however there have been none for GaNAsSb and only a few for GaAsSb. 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 to effects such as band anti-crossing. To determine the GaNAsSb and GaNAsSb band offsets, we performed PH measurements on GaNAsSb/GaAs and GaNAsSb/GaAs quantum wells. These samples were grown by solid-source molecular beam epitaxy utilizing a N long plasma source. Secondary-ion mass spectrometry and high-resolution x-ray diffraction were performed to obtain the compositions of the samples. We find that for the technologically important compositions, Gao.41n.61Ino.02Aso.55Sb0.45/GaAs has a band offset ratio of ∆Ec/∆Ev of 0.9 and Ga0.62Sb0.38Sb0.7/Sb0.3/GaAs a ratio of ∆Ec/∆Ev of 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 in the band structure of dilute-nitride devices is 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 E9.4: Direct Measurements of Trap Density in a SiGe/Si Hetero Interface by New Charge-Pumping Technique. Toshiyuki Terai1, Missako Sakurai1, and Junko Murota2; 1Shinshu University, Matuse, Japan; 2Tokyo University, Senda, 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 the SiGe/Si heterostructures effectively and to establish a good device design methodology, it is important to clarify the relationship between device characteristics and the introduced heterostructure, 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] is a useful tool for the interface trap density (ITD) measurement 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 are strained SiGe-channel pMOSFETs with 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 100-nm thick Si-buffer layers, strained-SiGe-layer, and Si layer by low-pressure chemical vapor deposition (LPCVD). All of the annealing processes were performed at temperatures below 700 C to prevent degradation of the heterostructure surface flatness and of the Ge oxide in the channel region and high Ge fractions. We also measured the low frequency noise power in the drain current flowing in the SiGe-channel [4], and show 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 LTCP 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 these interface-traps. References [1] G. Groeseneken, H. E. Maes, N. Beltran, and B. F. De Keersmaecker, IEEE Tran. Electron Devices, vol. ED-31, no. 7, pp. 435-452, 1994. [2] T. Tsuchiya, Y. Inadama, and J. Murota, IEEE Trans. Electron Devices, vol. 50, no. 12, pp. 2507-2512, 2003. [3] J. Murota and S. Ono, Jpn. J. Appl. Phys., vol. 33, Part I, no. 4B, pp. 2290-2299, 1994. [4] T. Tsuchiya, T. Murota, and J. Murota, Jpn. J. Appl. Phys., vol. 39, no. 7B, pp. 5290-5293, 2001. [5] T. Tsuchiya, M. Sakuraba, and J. Murota, Proc. of IEEE Int’l Reliability Physics Symp., pp. 449-454, 2004.

3:30 PM E9.5: Ultra-Shallow Junctions for the 65nm Node Based on Defect and Stress Engineering. Viktor Moroz1, Mjeced Foad2, Houda Grauf2, Faran Nouri2, Dipo Pranavank2 and Susan Fetch1; 1Synopsys, Inc, Mountain View, California; 2Applied Materials, Sunnyvale, California.

The co-implantation of germanium, carbon, and the optimum implant energies and doses make it possible to create p+/n junctions with the sheet resistance of less than 600 Ohm/sq and the slope of less than 3 nm/dec. 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 boron diffusion and help to make 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 makes the junction slope steeper. The optimum implant energy and dose of the p+ implant 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 have a chance to reach 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 amorphization, the irradiation damage, and 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 medium-state saturation. 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 implant is always accompanied by the non-equilibrium interstitials, coming from either the BICs or the amospherely implanted carbon which 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 E9.6: High Quality Strained-Si Growing Techniques. Young-Pil Kim, Sun-Ghil Lee, Young-En Lee, Jong-Wook Lee, In-Soo Jung,
In a strained-Si/SiGe/Si-sub system, the properties of strained-Si layer depend on the composition of SiGe strain. 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 (B + wafer) and the B + wafer was outgassed for 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 for comparison. The 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. During the growth of SRB, the doped boron in substrate forms a p-n junction 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 E3.7
N+/P and P+/N Junctions in Strained Si on Thin Strain-Relaxed SiGe Buffers: The Effect of Defect Density and Layer Structure. Sung-Kwan Kang, Deok-Hyung Lee, Yong-Hoon Son, Pil-Kyu Kang, Gyeonggi-Do, South Korea. The study their effect on device leakage. The best junctions were found in suitable channel Si layer. In order to prepare a high quality space charge region of transistor junctions, can lead to undesired bulk leakage, and therefore also extra power dissipation, an important problem in current and future technologies. We have fabricated n+/p and p+/n junctions, using standard transistor Highly Doped Drain junction implants and anneals, in strained Si on SRB layers. The SRB layers have been fabricated, using a technique that allows to grow a very thin (200-400nm) SiGe layer. This layer includes a thin carbon-doped layer. Defects in this layer help nucleate misfit dislocation and this high degree of relaxation can 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 their effect on the leakage. 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 these SRBs. Increasing the defect density as well as bringing the carbon-doped layer closer to the junction severely 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 distance of the defect-rich carbon-doped layer, on the current characteristics at elevated temperatures is investigated.

4:15 PM E3.8
Morphology, Defects and Thermal Stability of SiGe Grown on Heteroepitaxy, Benny Perez Rodriguez and Joanna Mirecki Millunchick; 2 Applied Physics, University of Michigan, Ann Arbor, Michigan; 3 Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan. The mechanisms for stress relaxation have been investigated during growth of GaAs/GaAs heterostructures grown by molecular beam epitaxy in a regime where misfit dislocations and surface morphology strongly interact. The real-time stress evolution was obtained using an in situ multi-beam optical stress sensor (MOS) measurement. This real time data has been combined with detailed analysis of data obtained from x-ray diffraction, transmission electron microscopy, and atomic force microscopy. We compared the strain evolution for two different compositions. Several distinct stages of the stress evolution were observed during growth of GaAs/GaAs films that are correlated to the development of dislocation structure, morphology and strain relaxation. The strain relaxation is divided in three regimes: pseudomorphic growth, fast strain relaxation and annihilation. For GaAs/InP/GaAs the strain-relieved shows that for h < 80 Å essentially no strain is relieved. Fast relaxation occurs for 80 Å < h < 600 Å and by 500 Å, 62% of the strain has been relaxed. Beyond 600 Å the rate of the strain continues to decay for the duration of the growth. Similar results were found for GaAs/InP/GaAs, except that the residual strain was found to be lower. This suggests that there is less resistance to the strain relaxation in these films compared to the higher mismatch films. AFM images show that both films have an undulating surface with similar RMS roughness at high thicknesses. Therefore, both films show a better strain relief than other materials.
until the coalescence of islands. Contrary to the observed in other systems, the threading dislocations density is significantly smaller in thinner films. Preliminary TEM/HRTEM images show that the core high V/III ratios exist during the fast relaxation regime. For Ga$_{0.53}$Al$_{0.47}$N/GaN, preliminary TEM shows that the film has more threading dislocations. In conclusion, this data suggests that increasing the $Sb$ composition inhibits the threading dislocations.

 SESSION E4: Poster Session I
 Chairs: Peter Kiesel and R.L. Sopori
 Tuesday Evening, March 29, 2005
 8:00 PM
 Salons 8-19 (Marriott

E4.1 Chromium Diffusion Doping of Commercial ZnSe and CdTe Windows for Mid-Infrared Solid-State Laser Applications. 
Ivy P. Jones
department of Physics, Hampton University, Hampton, Virginia; 2Primrose Corporation, Baltimore, Maryland.

We report on the preparation and optical spectroscopy of diffusion doped Cr: ZnSe and Cr: CdTe polycrystalline windows. Cr$_2$+ 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: CdTe windows provides an attractive method for producing MIR laser materials at low cost. For the advancement of current Cr$_2$+ chalcogenide lasers, however, it is critical to gain a better understanding of the Cr$_2$+ 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 enhanced MIR emission over a larger emission cross-section beyond 3000 cm$^{-1}$. 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 Cr$_2$+ peak absorption coefficients ranging from 1 cm$^{-1}$ to 25 cm$^{-1}$. The estimated Cr$_2$+ concentrations ranged from 5x10$^{17}$ cm$^{-3}$ to 3x10$^{18}$ cm$^{-3}$ with a subsequent wet-etching treatment on the Cr: CdTe. For low Cr$_2$+ concentrations (1x10$^{18}$ 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: ZnSe and 95% for Cr: ZnSe. The effect of Cr concentration quenching on the MIR emission was observed for diffusion doping concentrations above 1x10$^{18}$ 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 Gong2, Yu-Li Tsai1, 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, Chiayi, 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) substrate alternatively to triethylgallium (TEG) and ammonia(NH$_3$) fluxes carried by purified H$_2$ gas. An AlN buffer layer, 75 Å in thickness, was deposited at 500°C followed by the deposition of 0.5 μm-thick GaN film at 1000°C. In this case, the V/III ratio was fixed at 5200. The absorption cross-section of the grown film at wavelength 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 growth surface at a V/III ratio of 5200 presumably due to the existence of a pulse time between successive NH$_3$ 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) sapphire substrates under high V/III ratios grow at temperatures higher than 1000°C by the MOCVD process owing to the fact that high dissociation efficiency of NH$_3$ occurs at very high temperature and high desorption rate of surface adspecies can only be suppressed under high V/III ratios. 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 bandedge PL emissions of GaN films versus V/III ratio indicates 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 density 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. References: [1] T. Suski, P. Perlin, H. Teisseyre, M. Leszczynski, J. Grzegory, J. Jun, M. Bockowski, and S. Porowski, Appl. Phys. Lett. 67 pp.2188-2190 (1995). [2] J. Neugebauer, and C.G. Van de Walle, Appl. Phys. Lett. 69 pp.563-565 (1996).

E4.3 Characteristics of GaN Films Grown on Wet-ETched GaN. Yu-Ji Tsai1, Jyh-Rong Gong2, Kun-Ming Lin1, 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, Chiayi, 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 researchers have introduced epitaxial lateral overgrowth process [1] and patterned substrate techniques [2] have been reported to improve the quality of GaN films significantly. However, the employment of dry etching process may cause 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 overlayer on the e-plane Al$_2$O$_3$ substrate with a subsequent wet-etching treatment on the GaN overlayer at 245°C for 25 min. H$_3$PO$_4$/H$_2$SO$_4$ etching solutions having H$_3$PO$_4$/H$_2$SO$_4$ ratios of 1/3, 1, 2, and 3, respectively, were employed to develop pit-pits on the GaN surface. On each of the etched GaN underlayer, 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). At 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 films were grown on the wet-etched GaN underlayer. In addition, the RT PL intensity ratio (I$_{BE}$/I$_{YL}$) of near BE emission to yellow luminescence (YL) of a GaN film overgrown on an etched GaN underlayer having an average pit size of 2.0 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 1.7x10$^{10}$ cm$^{-2}$ to 3.1x10$^{10}$ cm$^{-2}$ when the pit size of the underlying etched GaN increases from 0 to 2.0 μm. Cross-sectional TEM and STEM TEM show that the improved optical characteristics of the GaN films overgrown on the etched GaN underlayers are due to the selective blocking of threading dislocations at the locations of etch pits, which very few dislocations are observed in the etched overgrown GaN areas. References: [1] T. S. Zheleva, O. H. Nam, M. D. Bremer, and R. F. Davis, Appl. Phys. Lett. 71 (1997) 2472. [2] A. Bell, R. Liu, F. A. Ponce, H. Amado, I. Aksoski, and D. Cherns, Appl. Phys. Lett. 82 (2003) 349.

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-Kwei Lin1, Wei-Tsai Liao1, Yu-Li Tsai1, and Tai-Yuan Lin3, 1Department of Materials Science and Engineering, Feng Chia University, Taichung, Taiwan; 2Institute of Opto-Mechatronics, National Chung Cheng University, Chiayi, Taiwan; 3Institute of Optoelectronic Sciences, 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

110
power electronics and GaN-based LEDs [1, 2]. However, because of the large difference in lattice constant and thermal expansion coefficients, achieving high quality GaN films on Si substrates remains to be a great challenge [3]. GaN films were grown on (111) Si substrates at 1000°C using Al_{0.25}Ga_{0.75}N buffer layers, deposited at 800°C, with the thicknesses of Al_{0.25}Ga_{0.75}N buffer layers being 150, 170, 190, and 210 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 0.2μmol/min, respectively. 29 X-ray diffraction (XRD) measurements were used to identify the orientation relationship among GaN and Si substrate. A 20-nm-thick Pt layer was deposited on the 0.4 μm-thick HT GaN film to reduce the cathode contact. Photoionoluminescence (PL) measurements were used to determine the optical properties of GaN films using the 325nm excitation of a He-Cd laser. The results of X-ray θ-2θ scan of all the grown samples clearly revealed that the GaN film (2000) GaN film were grown on the (111) Si substrate. Rocking curves of XRD patterns in the RT photoluminescence spectrum of GaN films grown on the 200 nm-thick Al_{0.25}Ga_{0.75}N buffer-coated (111) Si substrate shows a strong near-band edge emission and a quenched yellow luminescence with the peak and the linewidth of the near band edge emission being 3.49 eV and 100 meV, respectively. Such a PL result is superior to that achieved in the GaN film grown on a high temperature HT AlN-coated (111) Si substrate using the same growth approach [4]. A reduction (or an increment) of the intermedium temperature Al_{0.25}Ga_{0.75}N buffer layer thickness below (or above) 180 nm led to deteriorate the crystalline quality of HT GaN film. Insufficient accommodation of misfit strain in the GaN film for the case of excess buffer layer thickness and strain relaxation in the GaN film for the case of excess buffer layer thickness are responsible for the quality deterioration of GaN films. References [1] M. Poschenrieder, F. Schulze, J. Blasing, A. Dadgar, A. Diez, J. Christen, and A. Krost, Appl. Phys. Lett. 79 (2001) 1501. [2] E.M. Chumakov, A.T. Fehse, J.A. Smart, Y. Wang, N.C. MacDonald, D. Hogue, J.J. Komiak, S.J. Lichwalla, R.E. Leoni, and J.R. Sheney, IEEE Trans. Electron. 48 (2001) 420. [3] A. Dadgar, M. Poschenrieder, J. Blasing, and K. Fehse, A. Diez, A. Krost, Appl. Phys. Lett. 89 (2001) 2670. [4] J.R. Gong, M.F. Yeh, and C.L. Wang, J. Crystal Growth 247 (2001) 261. 

E4.5

Ferromagnetism in the Diluted Magnetic Semiconductor Phase of ZnO:Co. Marco Aurelio Boselli 1, Iype C. da Cunha Lima 2 and A. Ghazali 2, 1Departamento de Fisica, Universidade Federal de Ouro Preto, Ouro Preto, MG, Brazil; 2Instituto de Fisica, Universidade do Estado do Rio de Janeiro, Rio de Janeiro, RJ, Brazil. 2Groupe de Physique des Solides, UMR 7688-CNRS, Universites 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 temperatures diluted magnetic semiconductor, the case of ZnO is still unclear. Actually, Co has been reported to be non-magnetic in ZnO at room temperature, while the Co concentration is below 3% [2].


E4.6

Electrically Active Defects of GaAs Films on Porous GaAs Substrates and Gettering. Alexander Buyzin 1, Yuri Buyzin 2, Alexander Belyaev 3, Eduard Rau 4 and Albert Lukyanov 2, 1General Physics Institute, Russian Academy of Sciences, Moscow, Russia; 2Institute for Physics of Microstructures, Russian Academy of Sciences, Nizhny Novgorod, Russian Federation; 3Physical Department, Moscow State University, Moscow, Russian Federation. Influence of defects on electric properties of devices is caused structural - admixture compounds - defect-impurity, instead of "pure" crystallographic defects. These defects essentially decrease electric and optical properties of material and characteristics of opto-electronic devices. One of the main issues for structural defects is the use of porous substrate. Porous GaAs substrates were earlier successfully used for production of single crystalline GaAs, AlGaAs, and InGaAs films [1,2]. In present work we investigated opportunity of using increase electric uniformity of GaAs films grown by MBE technique both on porous and conventional monolithic substrates GaAs(100). The basic attention was given to study electrically active defects in SEM by new technique, using scintillating film-detector analogues of SEM system. GaAs (100) substrates doped by Te and Si up to concentration 2x10^{19} cm^{-3} were used. To reveal difference in epitaxial layer defect structure connected with substrate state, only half of GaAs substrates have been electrochemically etched. So porous layer GaAs have been fabricated only on one part of a substrate while other part was untreated. This technique allowed us to carry out comparative research of layers received both on porous and monolithic part of the same substrate under identical conditions of growth. It was shown that epitaxial film to be received on porous substrate as compared with that ones on monolithic substrate would have: - smooth surface with morphological attributes of lateral growth mechanism (hills and valleys); - less density of dislocation walls and density of pyramidal holes was n_{\text{py}}=10^{12} cm^{-2} as compared with density of about 2x10^{10} cm^{-2} in films on a monolithic substrate; - less electrical activity of various structural defects and increased electric uniformity of grown films. Features of lateral growth structure on porous substrate led to higher structural perfection of grown GaAs films. Gettering properties porous substrate has lowered electric activity of defects in films [1]. Yu.N.Buyzin, S.A Gusev, V.M.Danilov, V.3. Anisimov, A. Lebedev, and V. Stolyarev, Applied Physics Lett. 81 (2002) 2988. [2] Yu.N.Buyzin, A.E.Khakhalin, et al., Proc. of Inter. Congress oW-M2001>, Advanced Materials, 25-28 Sept. 2000, Munich, Germany, Article 672. The work was supported by the Russian Foundation for Basic Research, grant N 02-02-17337 and by Office of Naval Research, grant N 00014-01-1-0828. 

E4.7

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. Carbon-based materials include high hardness, low friction coefficient, mechanical and electrical properties can be achieved doping diamond crystals with impurities. Two basics processes, dopant diffusion and ion implantation, are the main mechanisms for introduction of impurities in diamond. The introduction of impurities such as B, Li, 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.
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 used. For (105) reflection, FWHM of the rocking curves for patterned substrate was broader than those for unpatterned substrate, for (110) reflection, however, FWHM for patterned substrate was much narrower than that for unpatterned one. The normalized FWHM for all reflections decreases as the incidence angle of X-ray decreases. The results suggest that the crystalline quality in the surface region of the epi-layer on patterned substrate was especially improved because the penetration depth of X-ray depending on the incident angle is shallower for (110) reflection 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 F.L. peak of 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 GaNAsSb Growth with Insertion of GaAs Prelayers. Sickle Bank, Mark Wiesty, Homan Yuen, Roppel Bae, Lynford Goddard and James S. Harris. Solid State and Photonics Laboratory, Stanford University, Stanford, California.

GaNAs and GaNAsSb, grown on GaAs, have emerged as promising active layer materials for lasers covering the entire low-loss fiber bandwidth from 1.2 to 1.6 μm, but lasing at 1.55 μm has remained illusive. We present an important growth optimization that illustrates the importance of extended and point defects in the growth of high-quality dilute-nitride layers. For a 7% GaAs prelayer, we have observed a large improvement in the crystallinity in the surface region of the epi-layer on patterned substrate. This improvement in the surface region is attributed to the reduced dislocation density which was continued by TEM in-plane. The intensity of F.L. peak of 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.


Gaseous layers of SnO2 are perspective for making chemical sensors. Properties and structure of the SnO2 film can be different from the stoichiometry and on the microstructure. The SnO2 films of 250-400 nm thickness were deposited on glass substrates using ion-beam deposition technique. Pure oxygen ion beam were formed in a ring-like electron system with crossed electric and magnetic fields. Discharge power was 300 Wt (3 kV, 100 mA). The substrate temperature was 200 °C. Pure Sn target was used for the sputtering. Samples obtained were annealed isochronously (during 1 hour) in air in the 200-400 °C temperature range with (100) orientation of SnO2- and SnO3-crystallites was observed. Low temperature (200 °C) formation of great number of chaotic oriented SnO2 crystallites is explained by high concentration of oxygen in the film during deposition and by absorption of oxygen during annealing. Simultaneously textured phases are transformed into polycrystalline SnO2 phase. It is shown that the intensity growth of SnO2 sizes and phase volume of polycrystalline SnO2 during annealing at 350-500 °C is taken place at the expense of mainly amorphous phase and intensive absorption of oxygen. The increase of crystallite sizes at 600 °C is observed mainly due to their coalescence. The preparation of a pure crystal with a polycrystalline grain structure is most important problem. The SnO2 films have received considerable attention due to their potential applications in various areas, such as ultraviolet (UV) emitters and detectors, gas sensors, etc. Optical memory effect has been first observed in metal or oxide capped ZnO thin films. The write-once-read-many (WORM) type of optical memory can be achieved by storing nano-patterns that are fabricated by using a simple write-read route. Detailed experiments will be reported elsewhere. In the present report, the charge transport properties in AlOx capped SnO2 nano-patterns have been systematically studied by conducting AFM (c-AFM) and scanning Kelvin probe microscopy (SKPM). Prior to AFM experiments, the capped layer was irradiated with an energetic e-beam and subsequently removed with only a ZnO thin film remained. It is found that its conductivity dropped dramatically with increasing the e-beam irradiation dose, which is consistent with the cathodoluminescence (CL) observation that the total optical intensity increased as the irradiation dose increased. This optical intensity enhancement and conductivity decrease can be attributed to the recombination enhanced defect reaction. Since the recombination occurs in the defect rich interface, the defect reaction will be reinforced which will largely reduce the number of point defects and eventually decrease the number of non-radiative recombination centers. Interestingly, by exploiting SKPM, it is found that the Fermi level of the uncovered ZnO region moves upwards towards the conduction band after the irradiation. This phenomenon is ascribed to the formation of Al-doped ZnO during the e-beam irradiation. The total conductivity constitutes two parts (the interface between AlOx and the bulk ZnO itself). However, in comparison with the non-irradiated and e-beam irradiated regions, the local conductivity can drop about 3 orders of magnitude with a bias voltage of 4V. This shows that the interface's contribution was negligible, which also means it is feasible to read such WORM optical memory stored nano-patterns electrically.


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 apparently varies periodically due to the nucleation and coalescence of 2D islands in the growing front. In this work, the surface morphology and growth dynamics of the GaAs(331)B surface has been studied by both in-situ RHEED and in-situ scanning tunneling microscopy (STM). At first time, the RHEED oscillation is reported on high index GaAs(331)B facetted surface with (110) and (111)B facets. The RHEED oscillation was observed only along the [1-10] direction. Absence of any RHEED oscillations along [110], [111], and [11-10] indicates a growth model for the GaAs(331)B surface 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 report, all deposited material on (110) facets move toward (111)B. In order to form the (111)B facets, it is shown that atomic motion help us to better understand the nature of RHEED oscillation on high index GaAs.

E4.12 Structural and Electrical Characterization of Fe Implanted GaP: Interaction of Fe with Induced Defects and Trap Activation. Tiziana Cesca, Andrea Gasparotto, Adriano Verona, Beatrice Fraboni, Giuliana Impellizzeri, Francesco Priolo, Luciano Tarricone and Massimiliano Longo. Physics 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 mixtype deep acceptor character
it is widely employed to produce highly resistive layers for leakage current blocking and electrical insulation in optoelectronic devices. Moreover, Fe diffusion into an epitaxial layer results in the formation of Fe-related complexes, which act as carrier trapping and recombination centers and deteriorate the device performance. For this work, defect analysis of the Burgers vectors indicates that the initial perfect dislocations have a burgers vector of \( +a/3 \times 1 \times 1 - 2 \times 0 \) type then dissociates optical stacking faults bounded by two partial dislocations with burgers vector of \( -a/3 \times 1 \times 1 - 1 \times 0 \) type. The depth of damage was estimated to be up to 50 nm and was conferred by AFM on a KOH etched surface. High purity CVD grown 4H-SiC epilayer grown on mechanically polished wafers exhibit threading dislocation pairs along scratches on the surface of the epilayer. The linear dislocation density along the scratch is 8 dislocations / micron.


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 electron and holes wave functions in GaN-based fundamental and applicative point of view, related to light emitting electrical properties. In this preliminary report we examined single direction. This polarization led to high interface charge densities and quantum well structures. Our transmission electron microscopy (TEM) and atomic force microscopy (AFM) results show 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 defects related to Fe implantation are studied by current-voltage measurements on mesa devices, and related to the different implantation and annealing temperature treatments. The deep (eoe) properties of the Fe centers were studied by means of Photoinduced transient Spectroscopy (PICTS). The results allow a first analysis of the similarities and differences showed by the Fe implanted InGaN with respect to the InP case. (I) T. Cesca et al., Phys. Rev. B 68, 224113 (2003).


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 punched out up to 400 nm along the scratches during mechanical polishing and a total dislocation density of \( 5 \times 10^{10} / \text{cm}^2 \) is produced.

E4.16 The Influence of Stoichiometry on Growth-in-grown Point Defects and Impurities in PVT Growth 6H-SiC Single Crystals. Qiangu Li 1, Alexander Polyakov 1, Mark Fustin 2 and Marek Skowronski 1; 1Materials 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 shown 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 consequent change in the stoichiometry of the grown crystals toward more C-rich conditions.
structure and luminescence properties of a variety of doped samples have been studied by Positron Lifetime Spectroscopy (PLS) and low-temperature photoemission spectroscopy (LTPES). The pronounced correlation between the PLS results and PL will be discussed. Photoemission study reveals several defect related PL bands which are situated in the spectral range between 1.4 and 0.73 eV and are strongly influenced by the dopant concentration. In addition, CdTe samples have been annealed at 400°C, 450°C, 500°C, and 550°C in inert atmosphere to study the effects of annealing treatment on the defect structure. We have shown that annealing behavior also depends on dopants. This work is being funded by the Natural Sciences and Engineering Research Council of Canada (NSERC) and the Ontario Research and Development Fund (ORDF) under the auspices of the Ontario Photonics Consortium (OPC). STUDENT PAPER, Supervisor: P. Mascher

E4.19 Compositional Changes in the Infrared Optical Properties of Cr Doped CdZnTe Bulk Crystals. Uwe Horner1, Althea G. Blutett, IVY K. Jones*, EIE Nyein*, Sridhir Trivedi2 and Ramesh T. Shah2; 1Department of Physics, Hampton University, Hampton, Virginia; 2Brimrose Corporation, Baltimore, Maryland; 3Applied Physics Dept., University of Baroda, Baroda, India.

We are currently investigating the infrared (IR) optical properties of transition metal doped ternary Cadmium Chalcogenides 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 doped Cd1-xZnxTe bulk crystals with x = 0 (CdTe), 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 or through a thermal diffusion process. The samples exhibited the characteristic IR absorption band peaking between 1800-1900 nm due to the 5T2->5E transition of tetrahedrally coordinated Cr2+ ions. The corresponding Cr2+ IR emission following laser excitation at 1907 nm extended from 2000-3100 nm. The Cr2+ 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. Based on crystal-field theory, the interionic bond length between Cr2+ and its nearest neighbors determines the transition energy of Cr2+ ions. The energy between the 5T2 ground state and 5E excited state of Cr2+ is given by 10Dq, where Dq is the so-called crystal field strength parameter. Dq is directly related to the bond length (l) through Dq = l/5. Therefore, a decrease in the bond-length leads to an increase in the crystal-field strength and the 5T2->5E transition energy. The observed spectral blue shift of the Cr2+ absorption and emission is thus consistent with predictions by crystal field theory. Besides spectral shifts, a slight broadening of the absorption and emission was observed in ternary Cr: CdZnTe compounds compared to the binary systems Cd1-xZnxTe. Moreover, the Cr2+ emission dynamics revealed a non-exponential decay for Cr: CdZnTe crystals, whereas the decay time of Cr: CdTe was nearly single-exponential. The corresponding Cr2+ IR emission following laser excitation at 1907 nm extended from 1800-3000 nm. The Cr2+ 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. Based on crystal-field theory, the interionic bond length between Cr2+ and its nearest neighbors determines the transition energy of Cr2+ ions. The energy between the 5T2 ground state and 5E excited state of Cr2+ is given by 10Dq, where Dq is the so-called crystal field strength parameter. Dq is directly related to the bond length (l) through Dq = l/5. Therefore, a decrease in the bond-length leads to an increase in the crystal-field strength and the 5T2->5E transition energy. The observed spectral blue shift of the Cr2+ absorption and emission is thus consistent with predictions by crystal field theory. Besides spectral shifts, a slight broadening of the absorption and emission was observed in ternary Cr: CdZnTe compounds compared to the binary systems Cd1-xZnxTe. Moreover, the Cr2+ emission dynamics revealed a non-exponential decay for Cr: CdZnTe crystals, whereas the decay time of Cr: CdTe was nearly single-exponential. The spectral broadening and non-exponential decay of Cr: CdZnTe suggests the existence of different Cr2+ ions most likely due to the formation of complexes in substiututional 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.

E4.20 Relaxation Mechanism of SiGe Thin Film on SOI Substrate. Zengfeng Di1,2, Miao Zhang 2, Weili Liu 2, Ming Zhu1,2, Chenglu Lin 2; 1Physics & Materials Science, City University of Hong Kong, Kowloon, Hong Kong; 2The Research Center of Semiconductor Functional Film Engineering Technology & State Key Laboratory of Functional Materials for Informatics, Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences, Shanghai, China.

The strain relaxation mechanism of a SiGe film on SIMOX is studied. After annealing for a short time, the SiGe/Si bilayer relaxes via the gliding motion of dislocations in the SiGe layer. Subsequently, leaving the top SiGe layer relaxed and mostly dislocation free. In addition, Ge diffusion into the top Si layer of SOI substrate is not found at the highest annealing temperature. At low annealing temperature, SiGe is not expected to be viscous, and so the strain ratio is reduced to a linear fashion between 600°C and 900°C. When the annealing temperature becomes higher (for instance, 1000°C that is 58.5% of its melting point of 1710°C), the oxide can reflow and the SiGe/Si bilayer behavior is constrained thin foil slipping on the oxide. In this case, the strain ratio reduction is rapidly enhanced.

E4.21 Phase Field Simulation of Alloying Effects on Metal Silicide Morphology Evolution. Mathieu Bouville1, Dongzhi Chi1, Shenyang Hu2, Long-Qing Chen2 and David J. Srolovitz2; 1Institute of Materials Research and Engineering, Singapore, Singapore; 2Department of Materials Science and Engineering, Pennsylvania State University, University Park, Pennsylvania; 3Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey.

The formation and evolution of thin polycrystalline films formed from the reaction of metals on silicon (metal/crystals) or germanium (germanides) is key to the functioning of semiconductor devices. NiSi is a candidate for replacing CoSi2 because of its lower resistivity and its lower Si consumption, but is less stable at high T. As the NiSi grims agglomerate into islands via grain boundary groving the film may lose connectivity. At elevated temperature a higher resistivity disilicide phase, Ni2Si, will form. We use phase field simulation to predict the evolution of the microstructure and morphology of the disilicide film to determine the controlling mechanisms and key physical parameters to aid in metal silicide optimization. Diffuse-interface, transformation, elastic energy, and interfacial energy all play important roles in the evolution. Experimental observations suggest that alloying Ni with Pt or implanting BF3 increases the resistance of NiSi. We use phase field simulation to study the stability of the silicides and extend these ideas to the case of germanides.

E4.22 Various Methods to Reduce Defect States in Tantalum Oxide Films for DRAM Applications. Wai-Shing Lau1, Alfred T. S. Tan1, Nathan P. Sandier2 and Taejoon Him2; 1School of EEE, Nanyang Technological University, Singapore; 2Lum 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 (I-V) measurements for the same samples. In this way, we observed several different absorption processes which give rise to two main bands. One way to reduce defect states and thus leakage current is to optimize post-deposition annealing. We observed that C/O vacancy complexes are more easily suppressed during post-deposition annealing when the sample is very thin. Rapid thermal annealing before deposition of NiSi helps to suppress SiO/l vacancy complexes. The choice of the top metal is also important. For example, TiN tends to produce less defect states than Al. Another way to reduce leakage current is by Ti doping. However, the mechanism of leakage current reduction by Ti doping is still not very well understood. We can see clearly that SiO/l vacancy complex defects in tantalum oxide films are eliminated resulting in significant reduction in leakage current.

E4.23 A Self-consistent Pseudopotential for Superlattices. Gregory C. Denet1,2, Michael J.文档丢失了，无法显示更多信息。


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 non-monotonic. Some structural and electron-physical properties of the Si–SiO2 system by means of EPR, nuclear magnetic resonance (NMR), surface photo-voltage spectra (SVF) and MOS capacitance technique. It has been established that EPR and SVF (40.68 MHz) methods coincide with the differences between charge in SiO2 revealed in samples oxidized in different ambient. The EPR method indicates the interaction between vacancies and interstitial Si atoms (or its complexes) at the interface, whereas simultaneous increase of these signals indicates that interstitial atoms and vacancies are separated and interaction between them is absent. The effective charge of SiO2 does not depend on the oxide thickness if an interaction between the point defects at the interface occurs, while if it is absent, the effective charge decreases with the oxide thickness, due to compensation of the positive SiO2 charge by negatively charged acceptor centers at the interface. It has been established that the differences between the dependence of the charge in SiO2 on the oxidation time in MOS structures hydrogenated and proton baked by EPR and SVF methods, respectively, coincide with the differences between charge in SiO2 revealed in samples oxidized in different ambient. The 1H NMR line width of the n-type samples is remarkably broader than that of the p-type samples due to the extent of the protonation of the surface to which the movement of adsorbed molecules is hindered and the strength of the magnetic interaction with the paramagnetic impurities of the adsorbent. These results indicate that interaction between grown-in defects and impurities (hydrogen) take place also and must be taken into account at the choice of oxidation conditions.


Admittance spectroscopy measurements on Metal-Oxide-Semiconductor (MOS) devices allow the determination of electronic states at the oxide/semiconductor interface. The contribution of the interface trap conductance 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 model of states, when the tunneling effect is also considered in 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 attempt to evaluate the number of carriers as part of the model. Thus, the interface states for MOS devices on Si substrates were studied. Admittance spectroscopy data were collected for various oxide/Si combinations, including high-k dielectrics such as SrTiO3 and BaTiO3 deposited on Si. Both the S–R–H based and the extended tunneling models were used to analyze the data. The results showed that the shape of the barrier and the detailed analysis of the attenuation mechanisms happening at the interface due to electron/hole moving, together with the experimental determination of the oxide/semiconductor interface can model the conductance response of the device and can be used to calculate the interface states density and the traps time constant.

E4.26 A Pulsed EDMR Study of Charge Trapping at P3 Centers. Felice Friedrich, Christoph Boehme and Klaus Lips; 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 throughout the bandgap. Because of this, P3 defects are important trapping and recombination centers of the c-Si/SiO2 interface. In this study, we present 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 readjustment 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 readjustment can exist in any of four spin eigenstates (three triplet states, one singlet state) and thus, it is not magnetic. The 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. One can 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 sublevels can be explained by readjustment out of different spin configurations of P3 defects. What remains is the question of why different paramagnetic species such as uncharged P3 centers in the ground state (S = 1/2) exhibit identical Landé factors whereas the identical EPR signal can be measured as charged two electrons (S = 1) PB centers in triplet configurations.

E4.27 Strain Relaxation in Semiconductor Thin Films on (001) Oriented Semiconductor Substrates via use of Defected Sub-Surface Layers. A. 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 increasing demand for devices with higher speed and lower power consumption. 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 has been used by utilizing factors up to 30% that contribute to 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 that clarifies some of the aspects of the relaxation mechanism. The analysis assumes that the entire relaxation process of the strained layer is due to formation of dislocations and their interaction. The roles of the 60 degree and 90 degree dislocations typically seen 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 Chung 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. It is considered that identical anisotropy is active in immobilized species which decrease the active concentration of carriers in semiconducting devices. 300nm n-type Cz grown silicon wafers were implanted with boron at a dose of 1x10^{15} cm^{-2} and energy of 500keV into 130nm 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 nitrogen at temperatures of 550-700°C lasting for 10-60 minutes under a 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 depth profiles and 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. Haddara; Department of Electrical and Computer Engineering, McMaster University, Hamilton, Ontario, Canada.

Intermixing at heterointerfaces and the broadening of the SiGe layer in the 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 Si$_x$Ge$_{1-x}$/Si SQW structures grown by MBE and annealed at 900°C, 1000°C, and 1100°C for different anneal times in inert and oxidizing ambiances. 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 on the diffusivities of Si and Ge on the Ge fraction. Table 1 lists the values of intrinsic self diffusivities of Si $(D_{Si, \text{int}})$ and Ge $(D_{Ge, \text{int}})$ as functions of temperature and Ge fraction compared with published values [3]-[6]. In all cases, values of $D_{Si, \text{int}}$ and $D_{Ge, \text{int}}$ as a function of Ge fraction were chosen to match the inert diffusion profile. Once 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 and 1000°C the diffusivity values were very close to published values. At 1100°C the values of $D_{Si, \text{int}}$ and $D_{Ge, \text{int}}$ were much higher than reported values. This may suggest that the vacancy exchange mechanism described by vacancy flux model is the dominant mechanism for interdiffusion of Si and Ge at temperatures below 1000°C. For 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. Grigorie, Ph.D thesis, University of Florida, 1990; [3] N. B. Zangenberg 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. Dinse, An introduction to solid state diffusion, (Academic Press, Boston, 1998).

### E4.80

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

Matthias Bauer1, Stefan Zollner1, David Theodore2, Michael Canonic2, Pierre Tomassini1, Bich-Yen Nguyen1 and Chantal Arena1; 1 ASM America Inc., Phoenix, Arizona; 2 Freescale Semiconductor, Tempe, Arizona.

Arsenic doped Si films were grown epitaxially using RTCVD from trisilane, monomethylsilane and arsine as source gases with growth rates as high as 260, 60 and 40 nm/min for 600, 550 and 500°C, respectively. A strong dependence of the impurity (C, As) incorporation on growth rate was observed, caused by a growth rate dependent surface segregation behavior of C and As. High electrical active dopant levels of 5×10²⁰ cm⁻³ with resulting resistivities as low as 0.35-0.4 mΩcm were achieved. High-resolution x-ray diffraction measurements of the films find a vertical lattice constant as low as 5.234 Å, which corresponds to a biaxial stress of up to 1.8 GPa and a C content up to 2.3% according to the work by Berti et. al. or Girinders et. al. Films with a low thickness-strain product show pronounced interference fringes in x-ray or spectroscopic ellipsometry spectra, which for these films grown in films with thicknesses of 0.206-0.002.

### E4.31

**Transmission Electron Microscopic Studies of Strained Si CMOS.**

Qianghua Xie1, Peter Fejes:j, Mike Kottke2, Xiaoguang Wang3, Mike Canonic3, David Theodore4, Ted White5, Marian Sadaka6, Victor Vartanian7, Aaron Thean8, Bich-Yen Nguyen1, Shawn Thomas1, Ran Liu9, and Felix Bar1. 1 Physical Laboratory Arizona, Freescale Semiconductor Inc., Tempe, Arizona; 2 Advanced Process Research and Development Laboratory, Freescale Semiconductor Inc., Austin, Texas; 3 Crolles-2, Freescale Semiconductor Inc., Crolles, France; 4 Ioffe Institute, St. Petersburg and Science Research Laboratory, Motorola Inc., Tempe, Arizona; 5 School of Micro-electronics, Fudan University, Shanghai, China.

Strained 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. Nevertheless, stress-related defect generation can generally 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 (thready, 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 SiGe/strained Si 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.

### E4.32

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

Ukyo Jeong, Jinming Liu, Baonian Guo, Kyuha Shim and Saedpeh 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 iron implantation process introduces extensive interstitials. While the amorphous region is completely re-grown into single crystal during subsequent anneal without leaving behind residual 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 transparent 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.

### E4.33

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

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

The HgTe/HgCdTe superlattice (SL) is of fundamental interest as it allows 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 wave length, 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 $17.0 \pm 1.0 \mu m$ 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.
better than 1.0 %, a difficult task. The same wavelength criterion can be satisfied with a \( \text{HgTe/HgCdTe} \) SL with a \( \text{HgTe} \) well width of 4.8 nm and a precision of 2.0 %. This gives the SL a slight advantage; however, the potential to reduce leak currents and to suppress auger recombination is much more important. These SL’s can be designed to reduce leak currents perpendicular to the two dimensional layers of \( \text{HgTe} \) and perpendicular to the substrate. The dislocation densities extracted from XRD Williamson-Hall analysis of various small miscuts of (0001) sapphire substrate (\( \pm 1^\circ \)) have been employed in very long wavelength photodetectors [2,3]; even though more work on p-type doping is required. [1] J. N. Schulman, and High-resolution X-ray diffraction (HRXRD), we report a study of the effect of various small miscuts of (0001) sapphire substrate (\( \pm 1^\circ \)) and the way to further improve the material quality. A set of AIN and AIN/AlxGa1-x Superlattices (SLs) were grown by Migration-enhanced Metalorganic Chemical Vapor Deposition (MEMOCVD) on vicinal (0001) sapphire substrates. The threading dislocation density was found to be very sensitive to the miscut angles. The etch pit density reduced to \( 7 \times 10^6 \text{ cm}^{-2} \) for normal-oriented (0°-off) from the starting value of \( 7 \times 10^7 \text{ cm}^{-2} \) for 0.5°-off. The dislocation densities extracted from XRD Williamson-Hall Plot are consistent with the chemical etching method. We found that the surface morphologies can be easily controlled by the different substrate miscut angles. The 1-2 Mondlayers (MLs) step flow morphology for normal-orientated substrate changed to step bunches of 10 MLs height for 0.5°-off substrate. Correspondingly, AFM Root Mean Square (RMS) increased from 1.52 to 9.15 nm at a scan area of \( 5 \mu \text{m} \times 5 \mu \text{m} \). Thermal dynamic and kinetics during the growth are the key factors that are responsible for the surface morphologies. This finding may help enhance the quality of the Ge NCs. The density of the Ge NCs is strongly affected by the ion dose and the ion source conditions. Steady state PL results show a peak at 2.1 eV originating from nc-Ge and another peak at 2.3 eV arising from ion-beam induced defects in the SiO2 matrix. Time-resolved PL studies reveal double exponential decay dynamics in the nanometer time scale. The decay of the sample with time constant 1.3 ns is attributed to indirect transitions in the Ge NCs. The decay of the sample with time constant 10 ns is attributed to the radiative recombination at the Ge NCs. 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.

**E4.34** Radiative Versus Nonradiative Decay Processes in Germanium Nanocrystals Probed by Time-resolved Photoluminescence Spectroscopy, P. K. Chil1, R. Kesavanloorth 2, B. K. Panigrahi 2 and K. G. M. Nair 2; 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 bandgap nature and stronger confinement effects and has great potential for optoelectronic and memory device applications. However, 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 defects in the photoluminescence (PL) from ion-beam synthesized Ge NCs embedded in SiO2 using steady state and time resolved PL measurements. Ge nanocrystals of diameter 4-13 nm were grown embedded in thermally grown SiO2 layer by Ge ion implantation and subsequent annealing. X-ray diffraction and Raman (optical and low frequency) measurements were performed to study the evolution NCs as a function of ion dose and annealing conditions. Steady state PL spectra show a peak at 2.1 eV originating from nc-Ge and another peak at 2.3 eV arising from ion-beam induced defects in the SiO2 matrix. Time-resolved PL studies reveal double exponential decay dynamics in the nanoseconds time scale. The decay of the sample with time constant 0.8 ns is attributed to indirect transitions in the Ge NCs. The decay of the sample with time constant 10 ns is attributed to the radiative recombination at the Ge NCs. 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.

E4.38 Elastic Stress Relaxation at Nanoscale: A Comprehensive Theoretical and Experimental Investigation of the Dislocation Loops Associated with As-Sb Nanoclusters in GaAs.

Vladimir Chulkov, L. Rosenblatt, A. E. Romanov1, 2Toffe Institute, Saint Petersburg, Russian Federation; 2Institute of Problems of Mechanical Engineering, Saint Petersburg, Russian Federation.

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 temperature and subsequently annealed. A model was developed for the elastic stress relaxation, self-energies and interactions in such cluster-loop nanosystem. 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 prism-like nanoclusters nearby the nanoclusters. Our theoretical model explains 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 conduction band minimum of the inclusion due to diminishing dilatation and the interaction between the dislocation loop and inclusion are important in the relaxation phenomena at stressed nanoscale inclusions in semiconductors.


Tin dioxide is a wide band gap semiconductor whose technological applications largely depend on 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 monolithic aerogels by synchrotron-based soft x-ray absorption near-edge structure (XANES) spectroscopy at 0 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 nanofoam skeleton, and (iii) the dose of soft x-ray irradiation. Both bulk-sensitive fluorescence and surface-sensitive electronic 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 electrical states of f and e 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, LLNL 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\(^{-1}\) and 2277 cm\(^{-1}\) varied according to the 12C and 13C concentration. These results demonstrate conclusively that the impurities originated from the precursors. Isotachon annealing results revealed that the CO2 molecules are stable even 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. Physics, 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 Foundation and the ACS Petroleum Research Fund.

SESSION E5: Novel Materials, Synthetic Structures and Nanomaterial Devices and Defects/Dopants

Chair: S.R. Schofield and M. Tabo

Wednesday, Nov 2005 Room 2006 (Moscone West)

8:30 AM *E5.1 Electrical Transient Based Defect Spectroscopy in Polymeric and Organic Semiconductors. Yoshowata N. Mohapatra1, 2, 3, Vishal Varshney1, Vineet Rao1, 3, Samarendra P. Singh1, 3 and Girija S. Samal1, 2, 3, 4.

1Santac Centre for Display Technology, Indian Institute of Technology Kharagpur, Kharagpur, 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, especially 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 activity in organic devices and structure 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/Al, and similar structures wherein 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 mechanisms traceable to dielectric nature and trap like behavior in organic semiconductors.

9:00 AM *E5.2 Rare-Earth Doped Silicon Nanoclusters for Microphotonics. Francesco Priolo1, Domenico Pacifici1, Giorgio Frano2 and Fabio Iacono2.

1Dept. Physics & Astronomy, MATIS-INFM & Univ. Catania, Catania, Italy; 2IMM, CNR, Catania, 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 nanocrystals 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 sensitizing action of Si nanoclusters. In this work we will show that upon introduction of the rare earth through ion implantation, the Si nanocrystals are completely amorphized and the subsequent annealing at 900 C is not able to recrystallize them. Indeed it is demonstrated that both the electronic properties as well 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 amorphization centers. Aim of this work is to underline 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...

9:30 AM E5.3 Efficient Spin Injection from NiFe/CoFe into GaAs in Spin-LED Structures. Shin Kim1, Jung Ho Choi2, Donggi Choi2, Kwon Il Kim3, Kyoung Won Kim1, Dong Geun Oh3; 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 LED (light emitting diode) 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, the exciton transition was dominant at lower temperatures and at higher temperatures free exciton transition became dominant. The circular polarization of the free exciton transition was about 15% at 20 K, whereas that of the bound exciton was almost negligible. At relatively higher 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 photo-electro-optical modulator together with a monochromator. After 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 E5.5 Atomically-Precise Positioning of Phosphorus in Silicon using STEM. Steven Richard Schofield1, Neil J. Curson2, Hugh F. Wilson3, Nigel A. Marks4, Oliver Wanschow4, Frank J. Rue1, Toby Hall1, Paul Tops1, Martin W. Radny1, Michelle Y. Simoons4, David R. McKenzie4, and Robert G. Clark5; 1School of Mathematical and Physical Sciences, University of Newcastle, Callaghan, New South Wales, Australia; 2Centre for Quantum Computer Technology, School of Physics, University of New South Wales, Sydney, New South Wales, Australia; 3Centre for Quantum Computer Technology, School of Physics, University of Sydney, Sydney, New South Wales, Australia.

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 nm accuracy. [1] This report constitutes the first demonstration of the atomically-precise positioning of individual atoms in a semiconductor surface and opens an exciting new path to fabricate a broad range of atomic-scale devices in Si, e.g., quantum cellular automata, mesoscopic devices such as single electron transistors and the key functional element (qubit) of a solid-state quantum computer [2]. The strategy that we use is as follows. A highly-confined electron beam generated from the tip of a scanning tunnelling 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 are then incorporated to the top layer 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-layer deposition technique. The P atoms replace a Si atom to form a P-Si heterodimer. In order to demonstrate the above process it was first necessary to obtain a detailed understanding of the surface physics and chemistry of the interaction of PH3 with Si(001). With this system as a test case, a variety of experiments 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 STEM with detailed first-principles calculations to outline a mechanism for the dissociation of PH3 and the substitutional incorporation of P to Si(001). The strategy that we use is as follows. A report [1] by R. Schriefel, National Inst. Med. Res. Rev. Lett. 91, 136104, 2003. [2] B. E. Kane. Nature, 395, 153, 1998. [3] J. W. Lyding, et al. J. Vac. Sci. Technol. B, 12, 5735, 1994. [4] J. L. O'Brien, S. R. Schriefel, et al. Phys. Rev. B, 64, 101401, 2001. [5] J. R. Tucker and T. C. Shen, Solid-State Electron., 42, 1061, 1998. [6] H. F. Wilson, O. Warschow, N. A. Marks, S. R. Schriefel, et al. Accepted for publication in Phys. Rev. Lett. (2004)

10:45 AM E5.6 Imaging Electrically Deactivating Defects in Si One Impurity at a Time. Paul Voyles1, David Muller2 and John Graul2; 1Materials Science and Engineering, University of Wisconsin, Madison, 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 Si-doped Si [1]. These images showed that the electrically deactivating defect in low-temperature MBE grown Si-doped Si must consist of at least two Si atoms. Further comparison of low-angle, strain profiles with TiN contacts using 0.15 μm technology. Polysilicon 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 4.8 V pulse. A diode rectification of 10% at ±2 V is achieved after high voltage pulse. When TiSi2 is used to contact the p+ cell diode terminal instead of Ti, and the silicon is first oxidized, memory switching is eliminated, with equivalent high forward current in the diode before and after an +8 V pulse. Transmission electron microscopy reveal a remarkable difference: diodes with memory switching (Ti contact) have high density of grain boundaries and twin defects, whereas 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 Si. These defects are barriers to current flow in the diode, and play a major role in polysilicon 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 Herring, Carole Jahn and Don Kidwell; Matrix Semiconductor, Santa Clara, California.

Polysilicon memory switching is demonstrated in vertical n-i-p diodes with TiN contacts using 0.15 μm technology. Polysilicon 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 4.8 V pulse. A diode rectification of 10% at ±2 V is achieved after high voltage pulse. When TiSi2 is used to contact the p+ cell diode terminal instead of Ti, and the silicon is first oxidized, memory switching is eliminated, with equivalent high forward current in the diode before and after an +8 V pulse. Transmission electron microscopy reveal a remarkable difference: diodes with memory switching (Ti contact) have high density of grain boundaries and twin defects, whereas 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 Si. These defects are barriers to current flow in the diode, and play a major role in polysilicon memory switching. The defect-based barriers are reduced by high voltage pulse.

11:30 AM E5.7 Analysis of Nanoscale Deformation in GaAs(100): Towards Patterned Growth of Quantum Dots. Curtis Raymond Taylor1, Eric Stacho2, Ajay Makale3 and Gregory Salamo3; 1Microscopy centre for Photonics, University of Arkansas, Fayetteville, Arkansas; 2Material Science, Purdue University, West Lafayette, Indiana; 3Department of Physics, University of Arkansas, Fayetteville, Arkansas; 4Department of Mechanical Engineering, University of Arkansas, Fayetteville, Arkansas.

It is widely known that the nucleation of epitaxial quantum dots is mediated by strain mechanisms. Nanoinclusions are created in the GaAs(100) surface to act as strain sources for nucleation and patterning of InAs quantum dots. A systematic approach is taken to understand the indent deformation processes that may lead to precision patterning capabilities for a broad range of nanostructures. In particular, studies of mechanical deformation approaching quantum dot size scales (< 100 nm) are scarce. Deformation of GaAs has been studied in the past using high load (50-200 nN) and low load (0.2-8 nN) indentation combined with transmission electron microscopy (TEM) characterization of the
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 minimize damage to the indent. 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 nanoindent was studied by cross-sectional transmission electron microscopy (STEM) in a probe-forming beam system used to delicately 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 other deformation transformation. Comparison of plastic zone size with the residual indent impressions indicate that the plastic zone extends approximately 5-6 times the indentation depth and 1.5 times the width. These results are currently being confirmed by the plastic deformation on the indentation sites. The success of this work could lead to a relatively simple and inexpensive process for the development of various nanoelectronic-photonic devices, for example, on-chip optical communication using quantum dots.

11:45 AM E5.5
Hydrogen in GaMnAs: Engineering of Magnetism by Defects. Martin S. Brandt1, Christoph Bihler1, Hans Huebl1, Sebastian T. B. Goennenwein3 and Whadimir Schuch2; 1Walter Schottky Institute, Garching, Germany; 2Universitaet Ulm, Ulm, Germany; 3TU Delft, Delft.

Manganese acceptors in GaAs provide both the localized magnetic moments as well as the itinerant holes necessary to obtain a ferromagnetic semiconductor. Recently, Bouzain-Rabhi, Lemaire 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 by 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 ∆a/a = 0.6 x 10^-2 cm^-1 [H]. This increase is markedly lower than the corresponding increase in hydrogenated Si:B of 2.4 x 10^-2 cm^-1 [H], where H is incorporated into deep-center traps. This difference suggests that H is built into GaMnAs on a lattice site that leads to a small lattice dilatation only such as the antibonding site. The effective indiffusion of hydrogen is determined via measurements of the ferromagnetic resonances of the thin films. Due to an inhomogeneity 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 modes upon hydrogenuation 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.

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 acceptor element, boron: (i) the dissociation of interstitial iron-substitutional boron (Fe:B) pairs and (ii) the formation of recombination-active boron-antimony 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 degrading effect is 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 these effects are not directly involved. However, in contrast to the Fe:B-related lifetime degradation, which also occurs upon 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. Recently, 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. This contribution reviews the present physical understanding of both degradation effects and discusses different approaches for reducing or even completely avoiding them. Special attention is paid to a recently presented defect reaction model [J. Schmidt and K. Bothe, Phys. Rev. B 80, 024107 (2009)] of the boron-oxygen degradation, in which a fast-consuming oxygen dimer (O2i) is trapped by B, to form a B:O2i complex, acting as a highly effective recombination center. Results of theoretical calculations using density functional theory (DFT) for B:O2i suggest that it is bistable 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:O2i 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. Narayanan2 and Dave Carlson2; 1National Renewable Energy Laboratory, Golden, Colorado; 2National Renewable Energy Laboratory, Golden, Colorado; 3BP Solar, Fredrick, Maryland; 4BP 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 cluster formation occurs during crystal growth when local thermal stress exceeds yield stress of some preferred grain orientations, causing the stress relief through local generation of defect networks. This phenomenon results in patches of well-separated defective regions, which can be several millimeter wide. This methodology allows simulation of the stress field. This paper describes characteristics of defect clusters and presents a comparison between experimental and theoretical dependencies of cell performance on the distribution of defect clusters in a wafer. For the experiments, wafers were selected from different regions of a mc-Si casting, and separated into two "sister" groups of adjacent wafers. Wafers from one group were defect-mapped to determine distributions of defect clusters, and defect-clustered regions were TEM analyzed to determine nature of precipitations. Sister wafers were processed into cells; their I-V characteristics and photoreponse maps (LBIC) were generated to correlate local photoreponse/recombination properties with the cell performance. The theoretical modeling was done using a Network-Model, which synthesizes a large-cell from a large number (1000) of local cells representing the measured defect distributions. The input data to the model comes from LBIC measurements, defect maps, and a data bank that relates dark current components on the diode and the interconnect density. The output of the model consists of terminal I-V characteristics of the total cell and spatial distribution of cell voltage and currents for any terminal voltage. Excellent agreement between calculated and the measured parameters of cells is obtained. The most important results of our analysis are: (i) Defect clusters are the primary sites of impurity precipitation, and hence are not gittered by conventional gettering treatments of P diffusion and Al alloying. (ii) Defect clusters act as "shunts", creating "internal sinks," which dissipate power within the cell. (iii) The loss depends on several factors: the nature of the impurity precipitates, distribution and total area of defects compared to the cell area; quality of the base material (the regions with no defects in which cell performance is limited by the base material only), and cell processing technology. (iv) Defect clusters

SESSION E6: Defects in Devices
Chairs: Peter Kiesel and W.C. McGolgin
Wednesday Afternoon, March 30, 2005
Room 2006 (Morocro East)
1:30 PM E6.1
Electronically Stimulated Degradation of Crystalline Silicon Solar Cells. Jan Schmidt1, Karsten Bothe1, Daniel Macdonald2, James Adey1, Robert James3 and Derek Palmer3; 1Institute of Solar Energy Research Hameln/Emmerthal (ISFH), Emmerthal, Germany; 2Department of Engineering, Australian National University (ANU), Canberra, Australian Capital Territory, Australia; 3School of Physics, University of Exeter, Exeter, United Kingdom.

Carrier lifetime degradation in crystalline silicon solar cells under illumination with white light is a frequently observed phenomenon. The 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 minimize damage to the indent. 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 nanoindent was studied by cross-sectional transmission electron microscopy (STEM) in a probe-forming beam system used to delicately 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 other deformation transformation. Comparison of plastic zone size with the residual indent impressions indicate that the plastic zone extends approximately 5-6 times the indentation depth and 1.5 times the width. These results are currently being confirmed by the plastic deformation on the indentation sites. The success of this work could lead to a relatively simple and inexpensive process for the development of various nanoelectronic-photonic devices, for example, on-chip optical communication using quantum dots.
produce an efficiency loss of 3 to 4 absolute points in efficiency. To reduce the influence of defect clusters, techniques for dissolving the precipitates during impurity gettering must be developed.

2:15 PM E6.5
Silicon Wafer Defect Self-Characterization with CCD Image Sensors

Today’s CCD image sensors can provide very high image quality. However, used as a tool, they can also provide a sensitive window into defects in silicon, either intrinsic to the starting wafers or introduced during fabrication. In this paper, we will examine some cases of known silicon wafer defects and show how they can appear in, and be studied by, CCD imagers. As examples, we will discuss epi-layer defects, slip-dislocation defects, and dark-current rings. Epi stacking faults occur when an imperfection at the substrate surface propagates upwards through the epilayer as the epi layer is deposited. We ignore those stacking faults with complex topography that interfere with lithography in device fabrication and consider only simple stacking faults, which typically have less than 100 nm of topography. We then show that the epi-layer defects can be made to look worse, but that high defect current is generated at the site, especially at the stacking fault corners. However, simple growth hillocks of the same size tend not to add dark current. Slip dislocations are also well known in semiconductor fabrication and are generally avoided through careful process design and fabrication practices. However, the ability of imagers to amplify small differences through extended integration (exposure) time means that residual slip effects can be imaged that would be difficult to detect otherwise. We will give an example of slip extending inward from the wafer edge with reduced dark current along the slip line, but with a small cluster of brighter pixels at the ending dislocation. Fault arc patterns can sometimes be observed in the interface diffraction pattern of images as viewed on the wafer, the area are seen as portions of concentric rings on the wafer. This suggests that the source lies in the substrate wafer growth process, even though the imagers are built in an overlying epi layer. We have observed such arcs in epi on n and p+ wafers, including silicon from different wafer vendors. Striations in imagers have been previously reported, but the explanations do not seem to apply in our case. We will show the extent to which these data-current patterns are correlated with visible striations.


2:30 PM E6.4
Silicon Light Emissions from Boron Implanted-Induced Extended Defects
Gran Z. Paul, Roman P. Ostroumov, Yuguang Lian, Liping P. Ren and Kiang L. Wang; Microfabrication Laboratory, University of California at Los Angeles, Los Angeles, California; 2 Device Research Laboratory, and MARCO Focus Center on Functional Engineered Nano Architectonics-FENA, University of California at Los Angeles, Los Angeles, California; 3 Nanophotonics 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^{-2} [2]. There are types of extended defects that evolve 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, [115] rodlike defects along <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/3<111> [3]. Here, a is the lattice constant of silicon. We studied the photoluminescence (PL) and transmission electron microscopy (TEM) of boron-implanted p-n junction silicon light-emitting diodes in correlation with the implant-induced defects of different types. By varying the implant annealing conditions to tune the extended defects of different types and by using plan-view transmission electron microscopy (TEM) to identify them, we found that there are 113 defects along <110>Si the ones that result in strong silicon light emissions. These are p-n junction silicon light-emitting diodes with a Burgers vector of a/2<110>, [111] perfect prismatic and faulted Frank dislocation loops. The EL and PL peak intensity at 1.1 eV from [113] defect-engineered LEDs is about twenty-five times higher than that from dislocation defect-engineered LEDs. This is the first time we observed such high defect density silicon light-emitting diodes and high-efficiency silicon light-emitting diode LEDs for monolithic Si nanophotonics. Measurements of both EL and PL at low temperatures indicated that the emissions from extended defects are related to silicon band gap radiative recombination. The high emission results 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 rate localizing them in the damage-repaired defect regions. 1. L.C. Kimerling, The Electrochemical Society Interface 9, 28 (2000). 2. W.I. Ng, M.A. Lourenco, R. M. Gwilliam, S. Ledain, G. Shao and K.P. Homewood, Nature 410,192 (2001). 3. G.Z. Paul and K.N. Tu. Appl. Phys. 82, 601 (1997).

3:15 PM E6.5
Conductivity Enhancement in Thin Silicon-on-insulator Layer Embellishing Artificial Dislocation Network
Yasuhiro Ishikawa1, Kazuaki Yamauchi1, Ruto Nuryadi1, Hiroyo Ikeda1, Michiharu Tabe1, Yukinori Ono2, Masao Nagase2, Massali Arita3 and Yasuo Takashashi1; 1Research Institute of Electronics, Shizuoka University, Hamamatsu, Japan; 2NIST Basic Research Laboratories, Atenji, Japan; 3Graduate School of Information Science and Technology, Hokkaido University, Sapporo, Japan.

Formation of nanometer-scale potential-arrayed structures is important for ultrasonic devices such as single-electron transistors with multiple tunnel junctions. In this work, from the viewpoint of nanodevice applications, a dislocation network sandwiched by thin Si layers is artificially formed using a wafer bonding technique, and the effect of the periodic structure, or perhaps the periodic potential, on the conductance property is examined. The dislocation network sandwiched by thin Si layers was artificially formed using a wafer bonding a pair of (001) Si-on-insulator (SOI) wafers, which had the top p-Si layer (10 cm) of 25 -180 nm on the buried SiO2 (BOX) layer of 400 nm. Since no SiO2 layer was inserted at the bonding interface, a periodic array of screw dislocations was induced at the Si/BOX interface. The lattice mismatch caused by the small misalignment of in-plane crystalline direction between the wafers [1]. After the high-temperature annealing and the selective etching of the Si substrate and the BOX layer in the front-side SOI, a new two-layer structure was formed with the top Si layer (180nm) embedding the dislocation network. The transmission electron microscopy clearly revealed the formation of a dislocation network in the bonding interface in the top Si layer. Furthermore, the dislocation network was found to increase the conductivity of top Si layer by more than two orders of magnitude in comparison with the top Si layer without the dislocation network. From the SOI thickness dependence, this enhanced conductivity is probably derived from the formation of quantum channels around the top Si layer. Although the periodic structure has not yet clarified, the MOSFETs using the Si layer embedding the dislocation network will be also presented. [1] J.L. Kouvou, K. Rousseau, F. Fournel and H. Moret, Appl. Phys. Lett. 77 (2000)1135; Appl. Phys. Lett. 80 (2002) 4321.

3:30 PM E6.6
Physical Mechanisms of Negative-Bias Temperature Instability, Ionisha Dereck1, X. J. Zhou2, D. M. Fleetwood2, R. D. Schirmid2 and S. T. Pantelides1; 1 Department of Physics & Astronomy, Vanderbilt University, Nashville, Tennessee; 2 Department of Electrical Engineering and Computer Science, Vanderbilt University, Nashville, Tennessee.

The negative bias temperature instability (NBTI) phenomenon is a critical reliability issue for electronic devices. Though several explanations have been proposed for NBTI, a comprehensive account of the available experimental data remains elusive. In this work we report new results, obtained by first-principles density-functional theory calculations, that allow us to elucidate the atomistic-scale mechanisms of NBTI. 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 passivate dangling bonds. Hydrogen release from dopants is greatly enhanced in the depletion region, when the substrate is driven into inversion as happens during NBTI stress. The released hydrogen atoms diffuse rapidly in the substrate and capture a hole in the inversion layer to become positively charged (protons). Thereupon, they are swept to the interface because of the applied negative bias. Once at the interface, these protons can either depassivate Si-H bonds to create interface traps, or enter the oxide to contribute to oxide trapped charge. The combined effects of the drift of the electric field and the oxidation of the oxide and the depassivation 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 how different observed kinetics, both reaction-limited and diffusion-limited, are 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 finally discuss the effect of the polarity of the substrate (n-type, p-type), the polarity of the applied bias, and the possible role of water.
or hydrogen molecules, on the overall degradation.

**3:45 PM E6.7**

**Silicon Single-Electron Pump and Turnstile: Interplay with Crystalline Imperfections.** Yukinori Ono, Yasuo Takahashi and Hiroshi Inokawa: NTT Basic Research Laboratories, NTT, Atsugi, Kanagawa, Japan; Graduate School of Science and Technology, Hokkaido University, Sapporo, Hokkaido, Japan.

The single-electron-tunneling device (SED), which has quantum dots in its channel circuit, is an example of the control of electron charge due to the presence of an elementary charge. The single-electron pump and turnstile are members of the SED family and enable single-electron transfer synchronized with the gate clock. They have the potential for extremely low-power electronic transfer and 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 turnstile [2]. They are composed of one silicon quantum dot and two tiny MOS gates and have achieved 30-kV operation, which is the highest-temperature operation ever reported. This opens up the possibility of the practical use of the pump and turnstile. 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 crystalline 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 turnstile, 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 simple dopant levels in silicon. This work was performed under the Grant-in-Aid for Scientific Research (C) of Japan Society for the Promotion of Science. [1] Y. Ono and Y. Takahashi, Appl. Phys. Lett. 82, 1221 (2003). [2] Y. Ono, N. M. Zimmerman, K. Yamazaki and Y. Takahashi, Jpn. J. Appl. Phys. 42, L1109 (2003).

**4:15 PM E6.8**

**Random Telegraph Signals in Carbon Nanotube Field Effect Transistors.** Fei Liu, Mingqiang Bao, Kang L. Wang and XiaoLei Liu, Chao Li and Chongwu Zhou: 1 EE, UCLA, LA, California; 2 EE, USC, LA, California.

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 dielectric 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 synthesized single-wall carbon nanotubes were applied on electrodes on top of the nanotube, followed by Ti/Al deposition as the contacts. The following measurements were carried out 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 (Ids) biases. The amplitude of the RTSs is up to 60% of the total current at 4 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 1.3 nm. At certain gate biases, the observed RTSs show 4-level switching due to trapping and de-trapping of the two defects inside SiO2 or at the interface between the CNT and SiO2. The switching magnitude of RTSs is low due to a large low frequency (1/1) 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 RTSs in the CNTs may be used as the single defects that produce telegraph signal-to-noise ratio. The RTSs 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).  

**4:45 PM E6.10**

**A Novel Method to Synthesize Blue-photoluminescent Doped GaN Powders.** Rafael Garcia 1, Abigail Belli 1, Fernando A. Poncè 1 and Alan C. Thomas 2: 1 Physics & Astronomy, Arizona State University, Tempe, Arizona; 2 Roger 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 electroluminescence lighting industry. Currently electroluminescent (EL) powders are based on ZnS:Cu,Ci and can be found in many applications including keypads lighting in cellular phones containing, 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 ammonia in a horizontal quartz tube reactor at 1100 °C. Si doped powders were prepared by reaction between a homogenous Ga-Si alloy and ammonia 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 ammonia 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 a 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 peak at 390 nm (8200 cm-1) is the most intense peak at 4.2K. At room temperature 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.
Our results allows to...
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 generate 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 cavity and its surface on the overall cavity morphology. For this 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 chosen from 90 to 127 nm 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 constant the local He⁺ concentration at all tuned-Rp. Consequently, the cavities nucleated in as-grown samples were assumed to be the same but the distance of cavities from the silicon surface. Indeed, the closer the Rp 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 673 K to 1323 K. 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 change in the nature and 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 with the computer code von Miessner, R. S., 1992a, 1992b, allows both the cavity equilibrium shape to be understood, and the chemisorption hypothesis [3] 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. Letters, 70, 1643 (1993) [2] R. Kern, P. Mueller, J. Cryst. Growth, 146, 193 (1995) [3] G. A. Petersen, S. M. Myers, O. M. Follstaedt, Nucl. Inst. and Meth. B 127/128, 301 (1997)

10:30 AM E7.7 Theory of Fluorine-Induced Suppression of Transient Impurity Diffusion in Silicon. Vincenzo Fiorentinì, Giorgia Lopez1 2, Giulia Impellizzeri2, Salvatore Mirabelli2 and Enrico Napolitani1, 1 Dept. of Physics, University of Cagliari, Monserrato, Italy; 2INFN-SLACs, Cagliari, Italy; 3INFN-Matia, Catania, Italy.

The transient enhanced diffusion of acceptor impurities affects severely the reliability of ultra-high doping region of miniaturized Si-based devices. Fluorine co-doping is an efficient method that can suppress this transient diffusion, but the mechanism underlying this effect is not understood. It has been proposed that fluorine-impurity, or fluorine-atmosphere, 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 formation of fluorine-atmosphere dangling bonds and the consequent 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 instead 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 interfait districted-assisted transient diffusion, however, in view of the effect of fluo-rine assisted trapping, we suggest that fluorine will also suppress vacancy-assisted diffusion, which is most relevant for donors.

10:45 AM E7.8 Fluorine Behavior in Preamorphized Si: Segregation and Point Defect Interaction. Giulia Impellizzeri1, Salvatore Mirabella1, Lucia Romano1, Maria Grazia Grimaldi1, Francesco Priolo1, Enrico Napolitani1 and Alberto Carres1.

Recently, grown the higher the probability to recombine vacancies with Nitrogen K-edge XAFS and emission (XES) spectroscopy is used to investigate modifications to the conduction band (CB) and valence 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 fluences (0.07-3x10¹⁴ F/cm²). We observed always 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)x10⁻¹⁴ cm²/s at 580 °C. The above phenomenon is accompanied by a SPE rate retardation and to a consistent F loss through the surface. Moreover, the concentration of F implanted in our samples increased by increasing the SPE temperature. In samples doped with B atoms (1x10¹⁴ B/cm², 10 keV), we observed also an anomalous F accumulation at the B implantation peak during the SPE step. As we demonstrated, with a custom-designed experiment, the absence of any F chemical bonding during SPE and post-SPE annealings [4], we believe that the above increased F incorporation is due to the increase of the SPE velocity induced by B. We investigated also the low of F during a post-SPE annealing. 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 self-interstitials (IS) during the post-SPE annealing. We evidenced a Fickian-deviated F diffusion promoted by the above I flux, together with a complete TED suppression of a shallow B profile. We verified that the IS emission from the EOR region is not affected by the F implanted in the amorphous layer. Fluorine is also able to suppress the B thermal diffusion (TD). In conclusion, our data support the idea of an interaction between F and IS, leading to a non Fickian F diffusion and to an increase of the TED and TD reduction. This F-IS interaction causes a very effective lowering of the IS population. [1] D. F. Downey, J. W. Chow, E. Ishida and K. S. Jones, Appl. Phys. Lett. 73, 1263 (1998). [2] A. Mokhiber, R. Kasnov, P. B. Griffin and J. D. Plummer, Appl. Phys. Letters, 80, 5350 (2002). [3] R. Kern, P. Mueller, J. Cryst. Growth, 146, 193 (1995) [4] G. A. Petersen, S. M. Myers, O. M. Follstaedt, Nucl. Inst. and Meth. B 127/128, 301 (1997)

11:00 AM E7.8 Clustering Analysis in Boron and Phosphorus Implanted (100) Germanium by Soft x-Ray Absorption Spectroscopy. Mehmet Alper Sahiner1, Parviz Ansari1, Malcolm S. Carroll2, Yong S. Suh3, Roland A. Levy3, Temel H. Buyukkhalil4 and Mark C. Croft3.

Recently, germanium based semiconductor device technology gained renewed interest due to new developments such as the use of high-k dielectrics for high mobility Ge MOSFETs. However, a systematic local structural investigation of clustering of dopants is still lacking. In this study, we present a detailed analysis of boron and phosphorus implanted Ge wafers. We have used Ge K-edge x-ray absorption fine-structure spectroscopy (XAFS) in order to probe the local structural modifications around the Ge atom under various implantation parameters and post-implantation treatments. The (100) Ge wafers were implanted with B or P using energies ranging from 20 keV to 320 keV and doses of 5x10¹³ to 5x10¹⁴/cm². Pieces of the implanted wafers were subjected to thermal annealing at 400°C or 600°C for three hours in high purity nitrogen. Secondary ion mass spectrometry (SIMS) and spreading resistance profiling (SRP) measurements on these wafers were used to correlate the dopant activation behavior with the local structural information obtained from XAFS. The local structural information on the nature of the formed clusters under heavy dose of B or P implantation will be presented in correlation with the theoretical XAFS calculations using B or P doped Ge crystal models.


We show that irradiation of InN with 2 MeV He ions produces a highly conducting n-type material. Electron concentration saturates at about 4x10²⁰ cm⁻³ for the ion dose of 800 μC. Nitrogen K-edge soft x-ray absorption (XAS) and emission (XES) spectroscopy is used to investigate modifications to the conduction band (CB) and valence
The electronic structure of InN containing these very high concentrations of free electrons and defects. XAS, a probe of unoccupied CB states 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. XAS, a probe of unoccupied CB states of states near threshold 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 is consistent with a bound state 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, 20403 (2002).

Electronic and Optical Properties of High Energy Particle-Irradiated In-rich InGaN Alloys. Sonny X. Li1,2, Kim Man Yu1, Rebecca E. Jones2, Junqiao Wu1, Whadek Walukiewicz1, Joel W. Ager1, Wei Shan1, Eugene E. Haller1, Hai Lu1, William J. Schaff3 and William Kemp3, 1Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California; 2Department of Materials Science and Engineering, University of California in Berkeley, Berkeley, California; 3Department 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 cells in space applications is the radiation resistance of the materials. We have carried out a detailed study of irradiation effects 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 (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 1022 MeV/g). The saturation of carrier density is attributed to the Fermi level pinning at the Fermi Stabilization Energy (EFs), as predicted by the amphoteric native defect model [2]. Electromechanical capacitance-voltage (ECV) measurements reveal a surface electron accumulation whose concentration is determined by pinning at EFs. Using the room temperature photoluminescence intensity as a indirect measure of minority carrier lifetime, it is shown that InN-GaN 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. Walukiewicz, Physica B 302 – 303, 123 (2001).

Intrinsic and N-related Defects in Hydrogen-Free ZnO Films Fabricated by Plasma Immersion Ion Implantation. Y. F. Mei1, Y: K. Yung1, Paul K. Y. Nakamura1, W. K. Ge2, 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. Undoped and doped ZnO films 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, the 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. Charge- and band-gap-increasing influence of nitrogen in the band structure and low doping enthalpy. The doping bottleneck is generally due to intrinsic defects, unintentional hydrogen impurities, and low N solubility. In this work, a dual plasma technique comprising zinc arc plasma and mixture gas (oxygen, nitrogen, and hydrogen) 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: S. Johnson and P.M. Vryes
Thursday Afternoon, March 31, 2005
Room 2006 (Moscone West)

1:30 PM E8.1
Mutual Passivation in Dilute GaN, Asx1-y, Alloys. Kin Man Yu1, Whadek Walukiewicz1, Junqiao Wu1, D. E. Mars2, Michael A. Scarpulla1,2, and Oscar D. Dubon1,1 Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California; 1Department of Chemistry and Chemical Biology, HARVARD University, Cambridge, Massachusetts; 2Agilent Laboratories, Palo Alto, California; 4Department of Materials Science and Engineering, University of California, Berkeley, California.

The dilute GaN, Asx1-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 Inx-0.5N0.5Asx-0.5 pairs. The passivation of the shallow donors and the N4_1 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 n of a highly Si-doped GaN [Si:1019 cm-3] (with Si concentration of 9x1015 cm-3) decreases to a net 1016 cm-3 after an annealing of 950°C for 10 sec. The same time annealing causes an enhancement for photon excitation at the localized defect level and the non-elastic CB emission is consistent with a band gap narrowing of 0.3 eV. [3] J. Wu et al., J. Appl. Phys. 94, 6477 (2003). [4] W. Walukiewicz, J. Appl. Phys. 94, 6477 (2003).

Quantitative Modeling of Self-Interstitial Diffusion in Silicon. N. A. Modine, 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 and directed dimer methods within the DFT to find the reaction pathways 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.

2:00 PM E8.2
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 dopant concentrations in excess of 10^{20} cm^{-3} to approach 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 these donors introduced during the wafer manufacturing process are compensated during the wafer manufacturing process. Co-doping is considered to be one method that could potentially forestall donor deactivation. Prerequisite for its investigations is a deep understanding of the diffusion mechanism of such donors 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 (d3 for short), 2. donor-vacancy clustering, and 3. ultimately precipitation of donors on interstitial sites. We have evaluated 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. In this talk, we will present the interaction of interstitials with arsenic and arsenic-vacancy complexes based on density functional theory calculations within the generalized gradient approximation. We have identified the structure and diffusion of arsenic-interstitial and arsenic-pairs. For arsenic-interstitial pair diffusion, our DFT calculations predict two pathways, with overall barriers of 0.28 (1.40) eV and 0.46 (1.13) eV in the neutral (charged) state, respectively. The arsenic-interstitial binding energy with respect to substitutional arsenic and interstitial is calculated to be approximately 0.4-0.6 eV, depending on their charge states. Di-nuclear 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 will assist in improving current models for arsenic junction formation.

2:00 PM 8E4.4 Determination of Diffusivities of Si Self-Diffusion and Si Self-Interstitials using Isotopically Enriched Single- or Multi-30Si Epitaxial Layers. Satoru Matsumoto1, Shun Seto2, S. Abe2, S. Aid1, T. Sato3, N. Nakabayashi1, K. Toyoura2, Shinya Fujii1, K. Tsuchiya1, M. Sakamoto1, M. Murakami1, J. Wada5, and T. Abe2 1Electrical Engineering, Keio University, Yokohama, Japan; 2Tokohama University, Sendai, Japan; 3MIT, Cambridge, Massachusetts; 4Shin-Etsu Handotai, Isogo, Japan.

In order to understand the point of impacts (vacancy, Si self-interstitial) to Si, it is important to clarify diffusivity of Si self-diffusion over a wide temperature range. We used highly isotopically enriched Si epitaxial layers as diffusion samples. 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 Kurchakoff Laboratory. Diffusion was performed under very pure Ar(99.999%) atmosphere at 867-1300°C. 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 error. Dsd can be described by an Arrhenius equation with one single approximation. We have identified the structure and diffusion of silicon. DV and DI are the diffusivity of vacancy and self-diffusion or self-interstitial (for good passivation) are

2:30 PM 8E5.5 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 silicon matrix by high-temperature thermal annealing. In this talk, we will present the interaction of interstitials with arsenic and arsenic-vacancy complexes based on density functional theory calculations within the generalized gradient approximation. We have identified the structure and diffusion of arsenic-interstitial and arsenic-pairs. For arsenic-interstitial pair diffusion, our DFT calculations predict two pathways, with overall barriers of 0.28 (1.40) eV and 0.46 (1.13) eV in the neutral (charged) state, respectively. The arsenic-interstitial binding energy with respect to substitutional arsenic and interstitial is calculated to be approximately 0.4-0.6 eV, depending on their charge states. Di-nuclear 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 will assist in improving current models for arsenic junction formation.

3:45 PM 8E6.6 Effects of Silicon Nitride Passivation Layer on Mean Dark Current and Quantum Efficiency of CMOS APS Sensors. D. Benoit1, P. Morin2, M. Cohen3 and J. L. Regolini1; 1STMicroelectronics Crolles1, 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 layers. The SiN layers were characterized by Spectroscopic Ellipsometry (SE) and Fourier Transform Infra Red (FTIR) spectroscopy to get the optical indices and the hydrogen content of the films, respectively. For the films light absorption, the [Si-Si] bond concentration has been determined supposing a linear dependence with the extinction coefficient value at 350 nm. This relationship was justified by simulation results according to the Si-centered tetrahedral model [1, 2]. Thanks to these data and the gravimetric density results, we have also determined the [Si-N] bond concentration and therefore the [Si-N]/[Si-Si] ratio. Hydrogen desorption 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 [3] 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 these two indices on the quantum efficiency of the SiN passivation layers is proposed. Requirements to minimize the mean dark current and to maximize quantum efficiency are somewhat different. In principle, high [Si-H] bond concentration is essential, while low [Si-N] bonds concentrations (for good passivation) are generally observed in silicon nitride films, which contains a 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 annealing and preserving a transparent and passivating layer.
Origin of Vacancy and Interstitial Stabilization at the Amorphous-Crystalline Silicon Interface. Scott A. Harrison, Taras A. Kirichenko, Decai Yu, Thomas F. Edgar, Sanjay K. Banerjee and Gyeong S. Hwang. Chemical 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 p-n junctions. Currently, ultrashallow junction formation followed by high-temperature thermal annealing is widely used due largely to bond rearrangement arising from interstitial integration of donor dopants. It is well known that native defects (such as vacancies and interstitials) created during ion implantation are mainly responsible for dopant transient enhanced diffusion (TED) and hence influence dopant electrical activation/deactivation. It is therefore necessary to develop a detailed understanding of their diffusion and annihilation behavior. Ion implantation at high doses may lead to amorphization of the implanted section. The behavior of native defects in the amorphous regions would be different from that in the crystalline regions. This can in turn affect the density and spatial distribution of defects. For instance, if there is a difference in formation energy between the amorphous and crystalline regions, the relative density of interstitials and vacancies will change. 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 early 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 poster, 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 effects 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.


The wideband gap material of GaN has attracted for the high power 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.


Silicon carbide PIN diodes with planar edge termination have been fabricated using a direct write laser doping and metallization technique. Trichloroethylene (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 diode can be improved dramatically compared to that of diodes without edge annealing. An annealing technique is also used to tailor the performance of the diodes.

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

A2B6 semiconductors and their solid solutions (ZnSe, ZnTe, CdTe, ZnCdHgTe) are matter of choice for near- and far-infrared optoelectronics. The importance of minimally reducing the degree of defects for these materials is not subjected to discussion. However, preparation of high quality barrier structures based on these compounds by means of MBE, laser technology or liquid phase technology is not always successful due to lattice parameters mismatch, and a good selection of a proper buffer layer may also pose some unavoidable problems. From this point of view the nanindentation as a tool of defect engineering can be effective for fabrication of surface barrier structures. The abstract presents first experimental results and numerical simulation of experimental data obtained under investigation of nanindentation effect on electric characteristics (in particular, current-voltage and capacitance-voltage) of CdTe/CdHgTe/Cd(Zn)HgTe heterostructures at the room temperature. It is shown that nanindentation 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 LPE technology. Experiments demonstrated dramatically changes in the capacitance properties of the heterostructure as well as drastically changed energy band diagram. Appearance of quasi-triple barriers seems to be dependent on the composition of the eplayer 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 modes at room temperature can be used for previous barrier construction before growth of the film.

Aiming at the Deformation-Induced Damage in Silicon Detected by Oxygen Agglomeration. Nikolai Yarykin and Ellen Hieckmann. 1Physics, University of Technology, Kaiserslautern, Germany; 2Institute of Microelectronics Technology RAS, Chernogolovka, Moscow Region, Russian Federation; 3Dresden 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 deformed 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 samples subjected to post-deformation annealing at temperatures up to 1150°C. The kinetics of the decay was measured in a wide temperature range of 500 to 1300°C. It is shown that the decay is determined by the oxygen diffusion and agglomeration at the deformation-induced defects; rate of the process serves as a measure of the remaining defects. The overall concentration is observed to significantly decrease during annealing around 900°C, while the dislocation density is more stable over the temperature range studied. The results are analysed in conjunction with the literature data on annealing and agglomeration of oxygen in silicon. [1] N. Yarykin and E. A. Steinman, Physica B 340-342, 756 (2003).

**E9.6** Comparison of the Deep-Level Spectra Produced by Particles of Different Mass in p-Type Silicon Crystals. Nikolai Yarykin

and George A. Rozgonyi. 1 Institute of Microelectronics Technology RAS, Chernogolovka, Moscow Region, Russia; Federation; 2Materials 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 recently. In the latter case observations fitted lines upon 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 implantation, we also compare the results 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 irradiation. 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., Phys. Rev. Lett. 55, 1312 (1985). [2] C. R. Cho et al., Appl. Phys. Lett. 74, 1263 (1999).

**E9.7** He Implant Energy Dependence of Thermal Growth of Nanocavities in Si. Pakiser Ntsoenzok, Rachid El Bouayadi, Gabrielle Regula2, Bernard Pichaud2 and S. Ashok1; CNRS-CERI, Orleans, France; 2TECSEN, Case 151, Faculte des Sciences St-Jerome, Marseille, France; 3Department 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 1.9 MeV in increments of 0.1 MeV, with the ion flux maintained between 5 x 1012 and 1 x 1013 He cm-2 s-1. Cavities might then be created at depths varying from 2.8 to 9.1 microns according to TRIM (Transport of Ions in Matter) simulations. 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 recently. In the latter case observations fitted lines upon 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 implantation, we also compare the results 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 irradiation. 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., Phys. Rev. Lett. 55, 1312 (1985). [2] C. R. Cho et al., Appl. Phys. Lett. 74, 1263 (1999).

The optical and structural properties of H or He implanted ZnO was investigated using low temperature photoluminescence (PL), Rutherford backscattering spectroscopy (RBS), and infrared spectroscopy (IR). H implantation changed the relative ratio of the luminescence from the donor bound excitons and the overall intensity of the PL spectrum. The PL spectrum for the He implanted ZnO and the RBS spectra for H implanted ZnO demonstrated that implantation damage was partially responsible for these variations. IR spectra of H implanted and ZnO have shown that the increase in the relative ratio of the 3.601 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.

**E9.8** Blistering and Splitting in Hydrogen-Implanted Silicon. Pakiser Ntsoenzok, Hanan Assaf1 and S. Ashok1; CNRS-CERI, Orleans, France; 2Department of Engineering Science and Mechanics, the Pennsylvania State University, University Park, Pennsylvania.

Production of ultra-thin silicon top layers by means of hydrogen implantation is obviously under estimated 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). Secondly, 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 can well describe the phenomenon. And surface annihilation speed is increased. In order to understand the surface sink possibility, simulation comparison of annealing at different surface conditions are simulated. Experimental data (Edmund G. Seebauer IEEE ICSICT 2004) is well reproduced by applying different 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.
E9.12 Defect Structure in ZnO Studied by ab-initio Calculation. Naoki Ohadi and Hajime Haneda; Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Ibaraki, Japan.

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 trap 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 Al acceptor at zinc site with vacancy at 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 varied with impurity element. For example, local structure around Al acceptor was obviously different from that of Ga 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 Followed by Low Temperature Annealing. Kiju Im1, Won-Ju Cho2, Chang-Geun Ahn2, Jong-Heon Yang2, In-Bok Baek1, Seongjae Lee1, Sungkwon Baek1 and Hyunsang Hwang2; 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 requires implantation process showing that 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 high ion current and dose rate capability at very low implantation energy equipment. High throughput structure and low production costs. To get minimum dopant diffusion the novel 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.


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 application of Ge wafer on the substrate 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) p-type Germanium wafer with resistivity of 15 23 Ohmcm was used as a substrate. Prior to plasma doping, the wafer was cleaned. The plasma doping system was performed using PHS(1%) 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 plasma 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, with nbt was resulted to the leakage current. The laser annealed sample in the energy of 300mJ/cm2 at 1 pulse showed the sheet resistance of 280ohm/sq and the activated carrier concentration of 2.5E14/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 lower leakage current of 2 orders of magnitude than annealed by RTA at 500°C for 10min. The n+p junction on Ge formed by plasma doping and laser annealing showed the superior electrical characteristics, and could be applied to the fabrication of the next generation device.


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, pI-Gate structures are promise 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 wafer are exposed to high density plasma directly. Novel plasma dopant doping efficiency and silicon fins compared with widely used combination of tilted-angle ion implantation and high-temperature post annealing. Due to its low process temperature it is very attractive to applications of high-k dielectric and metal gate. We fabricated several tens nm width fins and 60 nm gate length FinFETs, and measured their I-V characteristics. Fins and FinFETs using novel plasma dopant show good current drivability and low subthreshold slope. However without proper thermal annealing, this process generates material defects as well as hydrogen ions on the interface and inside silicon, and 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. Halyna M. Khl yap1 and Roman M. Peleshchuk2; 1Physics, University of Technology, Kaiserslautern, Germany; 2Physics, State Pedagogical University, Drohobych, 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 very good instrument for material engineering in order to form isotopic or anisotopic 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+S[Al] due to electron-deformation effects. The model recognizes self-consistent solution of the following set of equations: calculated charge distribution; 2) equation of mechanical equilibrium; 3) Poison 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, Yoshio Ashizawa2 and Hidetaka Oma1; 1Fujitsu R&D Center Co. Ltd, Beijing, China; 2Fujitsu Laboratories Ltd., Akirosu, Japan.

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 CATS using the GGA functional and ultra-soft pseudopotentials. All the calculations were performed in a 64-atom supercell with periodic boundary conditions and 2**3x2**3x2 Monkhorst-Pack k-point sampling with an energy cutoff of 160 eV. We have calculated pathways and barriers using Linear Synchronous Transit (LST) method. For the structure and formation energy of interstitials, 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 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. It is clear that the structure of the site to be most stable at midgap. Different diffusion paths in 0, +1, +2 charge state are investigated. The migration barriers in 0, +1 and +2 charge states are 0.25eV, 0.44eV and 1.2eV respectively. Next the structure and formation energy of vacancy in different charge states are studied. The ionization levels for vacancy are in agreement with experimental results and previous studies. The migration barriers are 0.1eV, 0.36eV, 0.52eV and 0.75eV 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 was found recently. The migration energy of FFCD is 0.5eV and 0.86eV 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 0.37eV much smaller than that given by previous tight-binding calculation. Our calculation shows that FFCD is the IV complex proposed by previous tight-binding calculation. Its migration barrier can be considered as IV recombination barrier in agreement with the values used in many analytical models of IV recombination. Our value 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 is 1.6eV. The migration barriers of divacancy in -1, 0 and +1 state are about 1.4eV in good agreement with experimental results.

E9.18 Impacts of Back Surface Conditions on the Behavior of Oxygen in Heavily Arsenic Doped Czochralski Silicon Wafers. Qi Wang1, Manmohan Dagarbuti1, Hossein Paravi1, Rong Yu*1, Xiaofeng Zhang2,1Fairchild Semiconductor, West Jordan, Utah; 2Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California.

The precipitation and diffusion of oxygen in heavily arsenic doped Czochralski (CZ) silicon wafers (with resistivity of 3mΩ·cm) with an interstitial oxygen concentration of 7×10¹⁰/cm³ have been studied for different thermal budgets and different back surface treatments. After annealed at 1200°C for 45 minutes and 800°C for 13hrs sequentially, the wafers with damaged back surface showed rodlike and platelike SiO₂ precipitates. These defects extended about 1μm into silicon bulk from the back surface. They all have a habit plane of [111]. This morphology has only been observed at low temperature (<900°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 polycrystalline oxygen precipitates were observed at the interface between the polycrystalline 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 exposed to silicon nitride. The kinetics and structure 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 epilayer layer has been significantly reduced in the wafers with damaged back surface, compared with those with polycrystalline sealed back surface. This diffusion difference shows significant impact to the performance of the devices built on these substrates.


Local defects in thin gate oxide films used for sub 100-nm devices play a very simple 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-dielectric and the remained 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 structural characteristic of SiO₂, we performed a quantum chemical molecular dynamics analysis for SiO₂-2, structure under strain by 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-cristobalite with oxygen vacancies was used for the simulations. The simulation enabled us to predict the effect of the strain on both oxygen vacancies on the atomic level. We found that oxygen vacancies in SiO₂ 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 SiO₂. The calculated band gap of SiO₂ 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 for SiO₂ with an oxygen vacancy. This result indicates that the insulating property decreases in the SiO₂ 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 SiO₂ film. [1] K. Suzuki, Y. Kuroiwa, S. Takami, M. Kubo, A. Miyamoto and A. Imaunura, Solid State Ionics, 152-153 (2002) 273-277.

E0.20 General Model of Diffusion of Interstitial Oxygen in Silicon and Germanium Crystals. Vasiliy Gogosov, Institute of Solid State and Semiconductor Physics, Minsk, Belarus.

A theoretical modeling of the oxygen diffusivity in silicon and germanium crystals both at normal and high hydrostatic pressure has been carried out using molecular mechanics, semi-empirical 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 values of the activation energy (∆E = 2.05 eV and pre-exponential factor D0( Si) = 0.28 cm² s⁻¹, D0( Ge) = 0.39 cm² s⁻¹) are in a good agreement with experimental ones and for the first time describe perfectly an experimental temperature dependence of the Oi diffusion constant in Si crystals (T = 300 - 1500 C). Hydrostatic pressure (P) results in a linear decrease of the diffusion barrier (δP = -4.38 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.

E0.21 Contact Free Defect Investigation in As-Grown Fe Doped Si. Sabrina Hahn1, Torsten Hahn1, Bianca Groendiek-Wendrock1, Kay Dorrich1, G. Mueller2, P. Schwies2 and J. Niklas2; 1Institut für Experimental Physik, 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 were developed 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 DLTS, however, without the necessity of special doping, without contacts and with high spatial resolution. Several characteristic defect levels were observed in InP doped with iron. One prominent defect center attributed 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 ferri 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 recombinaction 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 furnishes additional information like the homogeneity of the samples. This will be also demonstrated.

E0.22 Peculiarities of Defect Formation Processes in ZnSe Crystals
with Isovalent Te Impurity. Victor Makhnyi, Peter Gorley, Irene Tkachenko, Paul Horley, Yuri Vorobiev and Jesus Gonzalez Hernandez; 1Electronics and Energy Engineering, Chernivtsi National University, Chernivtsi, Chernivtsi, Ukraine; 2Unidad Queretaro, CINVESTAV-IPN, Queretaro, Mexico.

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 impurity. We used the method of quasi-chemical reactions to calculate equilibrium concentration of intrinsic defects, when isovalent tellurium impurity was introduced in the different ways, namely from the vapor phase and during the crystal growth process. It was shown that in the latter case the defect subsystem is mostly determined by formation of vacancy complexes $V_{Zn}$ together with selenium and zinc atoms occupying interstitial positions in crystalline lattice ($S_e$ and $Zn_i$).

Single-charged defects create associates of $(V_{Zn} - Zn_{i})$, causing intensive radiation band at the energies of about $1.7\text{eV}$. Annihilation of the sample in saturated zinc vapors resulted in the shift of the band to $1.0\text{eV}$. Recombination processes taking place in the system for this case involve $Zn$ impurity levels. Doping of $ZnSe$ with tellurium from the vapor phase lead to another shift of the effective radiation band to $2.3\text{eV}$, caused by transitions with participation of single-charged zinc vacancies. Isovalent 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]: Subhendra D. Mahanti[1], Daniel Wei[1], and Marcus G. Kauzmann[1]; 1Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan; 2Department of Chemistry, 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 model of intrinsic lattice impurities in PbTe, a classic narrow band gap semiconductor used for infrared detection and thermoelectric applications. This theory explained the origin of resonant defect levels near the fundamental band gap and also predicted resonant levels further away from the band gap. They argued that due to the large dielectric constant of PbTe, the Coulombic 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 these deep defect states and mapped out when different types of impurity microstructures are present. In particular we will discuss about a class of novel narrow band gap semiconductors and semimetallic $\text{MSbF}_2(2n)-(\text{Te})_2(2n)$, where $M$ is $\text{Ag}$, $\text{Na}$, $\text{K}$. We will discuss how these defects may influence electronic structure near the band gap region of PbTe caused by replacing divalent Pb atoms by monovalent $M$ and trivalent $Sb$ atoms preserving the overall charge neutrality. Possible resonances behind the superior thermoelectric properties observed in these quaternary systems [2] will be discussed. [2] Work supported by an ONR-MURI grant [I] C. S. Lent et al., Solid State Communications 61, 83 (1987). [2] Daniel Blicic et al., Phys. Rev. Lett. 93, 140403 (2004). [3] 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. Wolfgang Duengen[1], Reinhart Job[2], Yue Ma[1], Yuelong Huang[1], Wolfgang Fahrner[2]; 1Department of Chemical Engineering and Information Technology, University of Hagen, Hagen, Germany; 2Department of Engineering Science, Pennsylvania State University, State College, Pennsylvania.

Hydrogen is introduced into subsurface layer of the p-type Czechoslovakian 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 cleanroom 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.

**E9.26**

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

Hydrogen is introduced into subsurface layer of the p-type Czechoslovakian 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 cleanroom 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.
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 ions (H+) implantation have been studied in detail for heavily arsenic (As-doping level at 2.5m \text{cm}^3) and phosphorus (P-doping level at 1.3m \text{cm}^3) doped silicon substrates. At the implantation energy of 170\text{keV} and an ambient temperature, H+ ions produce a damage zone with a width of about 400nm in both substrates. The depths of the zone are 1489nm and 1585nm 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 H+ ion implant dose increase from 1x10^{10} \text{ion/cm}^2, 3x10^{10} \text{ion/cm}^2, through 5x10^{10} \text{ion/cm}^2, respectively. This is opposite to the trend in H+ ion implant dose increase, in which the defect zone decreases 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 implant dose and annealing conditions. A discussion is given rise to the H+ ion straggling in the heavily boron, arsenic, and phosphorous doped silicon substrates.


Hydrogenation is used extensively in solar cell fabrication as a technique to passivate residual impurities and defects. In the most common approach, hydrogenation 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 nitride layer and then fired through the RTP step. This releases the hydrogen, point defects and dopants. We would like to acknowledge the assistance of Solid State Measurements Inc. with obtaining the SRP results.

E9.30

E9.31


AlGaN/GaN high mobility transistors have a strong potential for high power and high frequency applications because of their high breakdown voltage and their excellent transport properties. However, these devices can suffer from damage created by trap or by the interaction of hydrogen with the defects in the active layer. This trapping effect leads to distortions of the I-V characteristics. In addition, defects are a source of noise generation. Hydrogen is known to passivate deep level defects in a number of semiconductors and first indications have been presented that, under post-hydrogenation, certain defects are passivated in n-GaN. However, besides this H-defect interaction aspect in n-GaN, it is necessary to investigate the effect of hydrogen diffusion on the electrical characteristics of the 2D electron gas present in the AlGaN/GaN heterointerface. A series of C(V), Hall effect, and conductivity experiments have been performed on AlGaN/GaN heterostructures before and after deuterium plasma exposure. The typical deuterium plasma conditions were: T=460 C, P=3-30 W, t=20-90 min. SIMS analysis show that deuterium diffusion occurs in the whole AlGaN/GaN heterostructure for P=30 W, t=20 min. In such plasma conditions, the deuterium concentration is a few 10^{19} \text{cm}^{-2} in the GaN active layer. From C(V) experiments, we observe a decrease of the pinch-off voltage and of the sheet carrier concentration after deuteration. For instance, after deuteration at 460 C, 30 W, 30 min, the pinch-off voltage decreases from -4.5 V to -1.8 V and the carrier concentration decreases from 6.5x10^{12} \text{cm}^{-2} to 2.5x10^{12} \text{cm}^{-2}. From Hall effect and conductivity measurements, we find that, under deuterium diffusion, both the sheet carrier concentration and the mobility decrease. The decrease of the mobility is smaller than the decrease of the carrier concentration. Under rapid thermal annealing at 800 C, 300 C, 30 min, both the sheet carrier concentration and the electron mobility are mostly restored. This reversibility effect is a strong indication that deuterium is responsible for the modifications of the electrical characteristics of the AlGaN/GaN heterostructures. The above modifications induced by deuterium are interpreted as being the result of the acceptor behaviour of deuterium in n-GaN. The deuterium atoms trap the electrons of the 2D gas present in the AlGaN/GaN interface. The resulting H+ specie acts as scattering centers for the electrons which reduce their mobility.

E9.32

Binding of N Interstitials with MgH Complexes in p-type GaN. Ryan Rich Wixom and Alan F. Wright; Sandia National Laboratories, Albuquerque, New Mexico.

Recent experiments at Sandia National Laboratories suggest that N interstitials, created by proton irradiation of Mg doped GaN, become mobile during subsequent annealing and bind to MgH resulting in a small positive shift of the H strained-mode vibration frequency. Motivated by these experiments, we have used density-functional theory and the generalized gradient approximation for exchange and correlation to study N interstitials and their interaction with MgH. Formation energies and dynamic configurations for relevant charge states of these defects will be discussed. In support of experimental evidence, N interstitials and MgH are found to be strongly bound in p-type GaN. The binding energies and estimates of the H local vibration modality for this complex will be discussed in comparison with the experiments.

E9.33

Effect of Substrate Orientation on the Growth Rate. Surface junction depth, and problems with transient enhanced diffusion, however, lowering of annealing temperature results in lesser dopant activation. Our group has reported on the effect of boron activation in boron implanted at a dose of 5E14 per cm3 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 for 60 min. 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 by implantation and diffusion are passivated by hydrogen. This movement among 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 Annealing (RTA) furnace for 20 seconds, at 300, 400 and 500 C. The active dopant profile was characterized using Scanning 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 phosphorus and antimony. It is worth mentioning that antimony, 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.

The growth and dopant incorporation during metal-organic vapor phase epitaxy (MOVPE) strongly depends on the orientation of the starting GaAs substrate. 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 the photothermal conductivity (PTC). It was found that the growth rate on the (111)B-oriented substrate decreases whereas, that on the (111)A-oriented substrate increases. The surface morphology of different substrates was studied by scanning electron microscopy (SEM). The surface morphology of the (111)A substrate is flat, whereas the growth on the (111)B substrate is affected by the formation of a large number of hexagonal hillocks observed on (111)B surface, and the growth was by step-flow on these facets. A kinetic growth model has been proposed to describe the growth features observed on (111)B surface. Finally, the influence of the thickness of the Si layer on the 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-rich slightly rich growth condition might be one of the factors accounting for the discrepancy between theoretical prediction and experimental results.

E9.34 Photoelectronic Emission Technique for the Surface Analysis of Semiconductors. Takahiro Takeda 1, Yoshihiro Mond2, Masanori Kudou 3 and Keiji Nakayama 4; 1Division of General Education, Ashikaga Institute of technology, Ashikaga, Japan; 2Department of Material Science, Ibaraki University, Hitachi, Japan; 3National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan.

To characterize the state of real surfaces of semiconductors in ambient environment, 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 a Q gas. This measurement is performed by scanning the wavelength from 300 to 2000 nm of incident light from 12 lamp at different temperature 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 photoemission 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 E1 by the following equation: Iph= C(hν - E1)^n. The value of the exponent n and the threshold E1 depends on the excitation and escape mechanisms involved. For photoemission from the bulk, n = 2 and E1 = 0. However, it was reported that experimental yield spectra for (111) Si surface prepared by cleavage in high vacuum showed that n = 3.0 and E1 = 5.15 eV, likely due to indirect transitions from the top of the valence band to the vacuum level. Photoelectronic 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 contribution of the surface states to the yield 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 for Scientific Research on Priority Areas (A) Semiconductor Physics (Nos. 15017007 and 16017007) and the Ministry of Education, Culture, Sports, Science, and Technology of Japan.


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 enhancement. 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, the intensity and yield of the 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 using AES combined with FIB to 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. Our CMOS product lot failed due to high defectivity at inline KLA inspection after hundreds of pattern killer defects with a very defined wafer signature were detected after trench etch. Auger and FIB analyses were performed on surface and buried defects. The results showed the formation of silicon and local silicon signature, which indicated that the defects were created before nitride film deposition. Based on the analytical and tool commonality information, the root cause was identified and the failure mechanisms were understood. Magnetoresistive 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 an abrasion second step slurry. In this example, after copper CMP and abrasive second step slurry deposition, inline AIT inspection detected black spot defects on some of CMP wafers which are intermittent wafer to wafer. Auger and FIB analysis revealed that the black spot defects were surface voids in the copper filled with Al, Si, O. This suggests that the defects 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 second-step slurries has been initiated.


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, photoelectron emission technique for the surface analysis of semiconductors (PETS) 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 Nv (3.2 x 10^15 cm^-3). The PL band was centered at 2.3 eV and covered the entire visible range. After a 450 °C anneal, there was almost a decade change in the PL intensity, while Nv decreased by a similar order to 3.8 x 10^18 cm^-3. For annealing temperatures above 450 °C, the PL intensity decreased and Nv increased monotonically. Analysis of the EPR line showed that in as-deposited films the spin was mostly related to carbon dangling bonds (g=2.0028), whereas silicon dangling bond signals (g=2.0055) appeared after thermal annealing. The peak position and half-width of the (FWHM) of the PL band was almost unchanged after annealing while the optical band gap decreased significantly from the as-deposited value of 2.8 eV to 1.8 eV after annealing at 450 °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. FTIR 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 films showed bands assigned to C-H stretching, wagging and Si-H stretching modes respectively. The FTIR measurements also showed that the concentration of Si-H bonds rapidly decreased with increasing annealing temperature. On the other hand the intensity of the C-H 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 in the absorption intensity. At higher annealing temperatures all forms of hydrogen bonds become unstable and the light-emitting property of the films deteriorates.

**E9.38** Probing Process-induced Defects in Si Using Infrared Photothermal Stress Measurement Technique. X. H. Liu 1, 2, J. H. Peng 1, N. Ke 1, 3 and Shounan Zhao 1; 1Electronic Engineering, Chinese University of Hong Kong, Shatin, N.T., Hong Kong; 2Applied Physics, South China University of Technology, Guangzhou, China; 3Materials Science and Technology Research Centre, Chinese University of Hong Kong, Shatin, N.T., Hong Kong.

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 photothermal induced 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 bimetallic [2], and it is found that point defects injected into the Si substrate during the oxidation process. In this work, 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 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 ion-implanted samples and used this 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 at this conference [3].


**E9.39** Defect Reduction in Si-based Metal-Semiconductor-Metal Photodetectors with Cryogenic Processed Schottky Contacts. Meiya Li and Wayne A. Anderson; Electrical Engineering, SUNY 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 yield by improving the interface between metal and semiconductor to reduce the leakage current of the device. The structure consists of a 20 Å oxide over 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 4.08 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 photo-current and the incident light power. The Schottky barrier height was found to be approximately 0.73 eV. However, the barrier height value was 0.1 eV more than that of the same contact obtained by RT processing. 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 Fabricated with Hydrogen-Plasma. Hyong Do Nam 1, 2, Song-Ho Hwang 1, Ju Young Lim 1, 2, N. K. Cho 1, S. P. Ryu 1, J. D. Song 1, Won Jun Choi 1, J. S. Yang 1, W. J. Cho 1, J. I. Lee 1 and H. S. Yang 2; 1Nano Devices Research Center, KIST, Seoul, South Korea; 2Dep. of Physics, Chung-Ang University, Seoul, South Korea.

We have carried out hydrogen-plasma (H-plasma) treatments on a quantum dot infrared photodetector (QDIP) structure, whose absorption region consists of a stacked InAs dots in an InGaAs well structure. H-plasma treatment has been carried out at 150 oC for 10 min-10 min under 400 sccm of H2 gas flow rate and 10 W of RF power. After H-plasma treatments, PL intensities of the as-grown samples were slightly reduced compared to that of as-grown sample, without any changes in their PL peak position. Though the reduction in PL intensity after H-plasma treatments implies the introduction of defects in quantum dot structure, I-V measurement showed that the dark currents of H-plasma treated samples were smaller than that for as-grown sample. The sample exposed to H-plasma for 10 min showed lowest dark current, which was 8 order of magnitude smaller than that for as-grown sample even at 200 K. Since the performance of QDIP is strongly dependent on the dark current, this result implies that the H-plasma treatment can be used to make high performance QDIP.

**E9.41** Mechanism of Phosphine Dissociation on the Si(001) Surface. Oliver Warcholew 1, Hugh F Wilson 2, Nigel A Marks 3, Steven R Schofield 4, Neil J Curson 4, Phil V Smith 4, Marwan W Radzy 6, Daniel H McKenzie 4 and Michael Y Simmons 4; 1Centre for Quantum Computer Technology, School of Physics, The University of Sydney, Sydney, New South Wales, Australia; 2Centre for Quantum Computer Technology, School of Physics, University of New South Wales, Sydney, New South Wales, Australia; 3School of Mathematical and Physical Sciences, University of Newcastle, Callaghan, New South Wales, Australia.

The continued down-scaling of electronic devices to the atomic scale increasingly demands an atomic-scale understanding of the elementary processes of semiconductor doping. We present a combined theoretical and experimental investigation into the dissociation mechanism of phosphine (PH3) on the Si(001) surface. A comprehensive ab initio density functional survey of possible dissociation structures, their energetics and simulated STM images, we have been able to assign the STM contrast to the most prominent image features observed in STM. Here we present quantum chemical calculations of these observed and other short-lived transient intermediates as well as the transition states and kinetic barriers between them. This leads us to formulate complete step reaction mechanisms for the two pathways of PH3 dissociation. These mechanisms are consistent in both kinetic and thermodynamic aspects with the dissociation processes observed and provide a comprehensive explanation of all common intermediate species seen in STM.

**SESSION E10: Hydrogen-Defect Interactions**


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 on 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 frequencies change only moderately when the charge state of the hydrogen-defect complex 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 Cadzovski Silicon.
Reinhart Job1, Wolfgang Duengen1, Yue Ma2, Yuelong Huang1, Lars O. Keller2, Achim Wiggershaus3 and John T. Horstemann1; 1Electrical 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 Czochralski 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 1E14 cm2. During the implantation the wafers did not exceed a temperature of about 90 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 beveled under low angle on a rotating quartz plate. The Raman vibration modes of H-molecules in vacancies (at 3820 cm-1) and in voids (at 4150 cm-1) are analyzed to provide information about the evolution of vacancies and voids under various process conditions. During the hydrogen implantation vacancies are created serving as nuclei for voids, which are formed during the subsequent hydrogen treatments and annealing. After the plasma hydrogenation H-molecules trapped in vacancies can be observed at 3820 cm-1, while H-voids have a corresponding appearance at 4150 cm-1. According to the Raman spectra, the hydrogenation of Si wafers does not lead to formation of voids. H-molecules are trapped in the substrate due to the high hydrogen concentration in the plasma. For the higher temperatures of 250 C, a few voids can be indirectly observed by RS. At lower annealing temperatures (T < 400 C) the 3820 cm-1 mode (H-molecules in vacancies) is observed, while at higher temperatures the 3820 cm-1 mode disappears and only the 4150 cm-1 mode is observed. H-molecules in voids can be found in the Raman spectra. This can be well explained by the growing and/or clustering of vacancies towards voids.

8:45 AM E10.3
Study of the Hydrogen Effect on Dopant Activation for the Plasma Doping and Ion Implantation.
Sungwoo Baek1,2, Sunghee Heo1, Dongkyun Lee2, Won-Ju Cho3, Kiju Im2, Chang-Geum Ahn2, In-Bok Baek1, Seogjoo Lee1 and Hyunrang Huang1; 1Material Science & Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea; 2Future Technology Research Division, Electronics and Telecommunications Research Institute, Daejeon, South Korea.

The ITRS roadmap projected the junction depth of less than 10nm for sub-32nm MOSFET device, which is extreme limit of defect engineering. In 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 retards the solid phase epitaxial growth rate for amorphous-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 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 600 000°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 analysis. For the plasma doping of P+ and B2I6, 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. Given the omnipresence of hydrogen during growth and processing, it is important to determine the structure and stabilize the hydrogen donor 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) reflectance spectroscopy, we observed O-H and O-D stretch modes at 3292.3 cm-1 and 2470.3 cm-1 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 partial pressure. By comparing with first-principles 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 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 spectroscopic 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-0209392).

9:30 AM E10.5
Irina A. Buynovska1, M. Laidloff1, I. G. Ivanov2, J. Birch1, Weimin M. Chen3, M. Felici3, A. Poliniemi2, M. Capizzi1, Y. G. Hong3, H. P. Xie2 and C. W. Tu1; 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 reactivity, is a common impurity that is abundantly present in most steps of semiconductor growth and device processing. Due to its high chemical reactivity, hydrogen is known to efficiently interact 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. Incorporation of hydrogen into host lattices usually remains intact. In this work, we report dramatic effects of hydrogen incorporation on the electrical and structural properties of GaNP-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 isostructural centers, starting from the ones which have the deepest energy levels in the band gap, but also opens the band gap of the GaNP alloy and efficiently reduces the N-induced coupling between the Ga-N bond and 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.
We introduce proton-proton scattering at a microprobe of 17 MeV energy 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 sensitive quantitative 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 contrast-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 photoconductivity (MDP)" by several orders of magnitude. This opens completely new possibilities for a contrast less non-destructive electrical defect 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 of less than 10 μm 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 techniques offer another 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 carrier capture cross sections, however, again contrast-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 photoinduced current transient spectroscopy (MD-PICTS)". MDP and MD-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.

Direct High-resolution Determination of Vacancy-type Defect Profiles in Ion-implanted Silicon. Andrew Peter Knights1, S. H. Gou1, M. van Dyken1, R. E. Mason2 and P. G. Coleman2; 1Engineering Physics, McMaster University, Hamilton, Ontario, Canada; 2Physics, University of Bath, Bath, United Kingdom.

Variable-energy (beam-based) positron annihilation spectroscopy (VEPAS) has for 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 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 100 keV B+ ions at a dose of 5x1014 cm-2. The depth resolution of VEPAS 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 is verified by the measured B+ ion depth distribution. 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 ion implantation with that of Si implantation at a dose of 5x1013cm-2 into Cr, FZ and epitaxially grown silicon.

Electrical Characterization of MOS Structures and Wide Bandgap Semiconductors by Scanning Kelvin Probe Microscopy. Seong-Eun Park1, Sooyun Jeliazkov2, Joseph J. Kopanski1, John Suehle3, Eric Vogel1, Albert Davydov1 and Hyun-Kee Kim3; 1Semiconductor Electronics Division, National Institute of Standards and Technology, Gaithersburg, Maryland; 2Metallurgy Division, National Institute of Standards and Technology, Gaithersburg, Maryland; 3Gwangu Techno Park, LTD/LED Packaging Service Center, 958-5 Daejeong-dong, Buke-gu, Gwangju 500-706, South Korea.

Electricity 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 heights (SBHs) were calculated. Measurements of metal work function and SiC 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 implanted SiC films. Variations in CPD at the interface of Al or Bi implanted SiC films were imaged to estimate doping levels.

Comparison of Techniques for Measuring Recombination Lifetime in Semiconductors. Richard K. Ahronland1,2, Jamiyana Dashoro3,4, Steven Johnston1 and Wyatt Metzger5; 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 (RCPCD); (D) quasistatic photoconductance (QSPC). Here we will present a comparison of these techniques for the determination of electron lifetimes. Moreover, we present a discussion for a variety of semiconductor materials, measured by the four techniques. The samples range from direct-bandgap GaAs to indirect-bandgap silicon. Techniques A, B, and C are suitable for direct-bandgap semiconductors such as GaAs and InGaAs. Techniques B, C, and D are suitable for single-crystal and multicrystalline silicon. Comparisons of the data and the application of transport theory show that both photoconductive techniques (C and D) are especially sensitive to shallow (temporarily) trapped defects. 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 recombination 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 valuable 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.


Due to the shrinking critical device dimensions in the fields of integrated circuits, microsystems, and large-area electronics, the device performance is more and more determined by interface and surface defects. Metrology capable of detecting these low concentrations of defects is therefore essential, especially for indirect and absolute defect of defects without the need for calibration procedures would be very beneficial. We have employed the cavity ring-down technique to obtain a highly-sensitive and absolute defect absorption spectroscopy technique for thin films. The technique has been fully characterized using hydrogenated amorphous silicon thin films (ranging between 4 and 1031 nm in thickness) in which electronic defects lead to (very low) absorptions at near-infrared wavelengths. In this context, we present how the technique will be addressed such as the minimal detectable absorption (10-7 per single laser shot) and interference effects within the thin films. Results for the a-Si:H thin films investigated showed an increase in the absorption coefficient with increasing film thickness. A high defect concentration at the surface and interface, which is in agreement with observations made with other (indirect) techniques. The high-sensitivity to surface and interface defects is illustrated by mapping the absorption profiles of an a-Si:H film of only 4 nm thick.
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.