SYMPOSIUM E

Semiconductor Defect Engineering–Materials, Synthetic Structures, and Devices

March 28 - April 1, 2005

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TUTORIAL

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 heterostructures and heterojunctions that make them suitable for a wide variety of electronic and optoelectronic applications. A broad range of material system, with special emphasis on III-V alloys, will be used as examples to illustrate the types of band alignment and band-offset determination, and their electrical and 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 organic semiconductor heterostructures 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
Chairs: J. Chevallier and Kin.Man Yu
Tuesday Morning, March 29, 2005
Room 2006 (Moscone West)

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

In the past, some well-known "difficult to dope" systems were largely treated as isolated cases by isolated communities. Thus, n-type doping of diamond, or p-type doping of ZnO, or n-type doping of Chalcopyrites (CuGaSe2) were studied as isolated cases by these three respective communities (synthetic diamond people; transparent conductor people, and photovoltaic people). Yet, it is now becoming clear, largely because of better inter-field communication and theoretical work (which is intrinsically more transferable to other systems than experiment, where investments in specific growth methods are required), that there are some common features and common "rules" concerning doping in semiconductors. I will describe those rules and results, formulating some general "design principles" which should help experimentalists to navigate in this multi-parameter space of optimizing doping in difficult cases. These rules do not address all cases, and do not provide simple cures. But they tell you in which direction you should concentrate your efforts. See recent papers: 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 Eberlein[1], Robert Jones[1], Patrick Briddon[2] and Sven Oberg[3]; [1]School of Physics, University of Exeter, Exeter, United Kingdom; [2]School of Natural Sciences, University of Newcastle upon Tyne, Newcastle upon Tyne, United Kingdom; [3]Department of Mathematics, Luleaa University of Technology, Luleaa, 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 severe problem if the resulting defects are electrically active, resulting in a reduction of the carrier lifetime. It is even possible that the irradiation reduces the electrically active 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 to 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 rapid growth of SiC by CVD methods leads to a deterioration in 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 Doped 4H-SiC Using Optical Admittance Spectroscopy. Wonwoo Lee[1] and Mary E. Zvanut[2]; [1]Materials Science, University of Alabama at Birmingham, Birmingham, Alabama; [2]Physics, University of Alabama at Birmingham, Birmingham, Alabama.

Semi-insulating SiC is an excellent candidate for a variety of applications, including microwave field effect transistors and other devices for high power and high temperature applications. Vanadium doping is one way to make a semi-insulating (SI) material. Vanadium impurity in SiC is important because it 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 $V^{3+/4+}$ acceptor 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. We have 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_{Ph1}) 1.89 ± 0.02 eV and (E_{Ph2}) 2.89 ± 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_c -0.65 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 Mitchel for providing samples. Program is funded by Dr. Colin Wood, ONR.

9:15 AM E1.4
Important Grown-in Defects in Novel Dilute Nitride (Al,In)GaNP: Ga Interstitials. N. Q. Thinh[1], I. P. Vorona[1], I. A. Buyanova[1], Weimin M. Chen[1], Sukit Limpijumnong[2], S. B. Zhang[3], Y. G. Hong[4], H. P. Xin[4], C. W. Tu[4], A. Utsumi[5], Y. Furukawa[5], S. Moon[5], A. Wakahara[5] and H. Yonezu[5]; [1]Dept of Physics and Measurement technology, Linkoping University, Linkoping, Sweden; [2]School of Physics, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima, Thailand; [3]National Renewable Energy Laboratory, Golden, Colorado; [4]Dept of Electrical and Computer Engineering, University of California, La Jolla, California; [5]Dept of Electrical and Electronic Engineering, Toyohashi University of Technology, Toyohashi, Japan.

Novel $(Al,In)_yGa_{1-y}N_xP_{1-x}$ alloys have recently attracted increasing attention due to their fascinating physical properties as well as potential applications in optoelectronics that can be lattice matched to Si substrates. Unfortunately, epitaxial growth of these alloys remains as a great challenge and the crystal quality is known to 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 (Al,In)GaNP-based alloys, from optically detected magnetic resonance (ODMR) studies. Based on the characteristic hyperfine structure, two Ga-interstitial (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 theoretical calculations, both defects are suggested to be complexes involving a Ga_i^{2+}. By taking advantage of the freedom in altering compositions of both cations and anions of the novel alloy, compositional 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 surface adatom mobility of the 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 performance of potential photonic devices based on this materials system. The high thermal stability of these defects observed from studies of post-growth rapid 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. Tiziana Cesca[1], Andrea Gasparotto[1], Adriano Verna[1], Beatrice Fraboni[2], Giuliana Impellizzeri[3] and Francesco Priolo[3]; [1]Physics Department, INFM and University of Padova, Padova, PD, Italy; [2]Physics Department, INFM and University of Bologna, Bologna, BO, Italy; [3]Physics 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^{2+} 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. Post-implantation annealing treatments at temperatures in the range between 300 and 600 °C cause both a reduction of the residual damage and an Fe escape from substitutional sites (2). It is very important to study this process because it determines the final concentration of active Fe^{2+} centers which in turn 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 occuring 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 $1x10^{19}$ cm^{-3} were implanted at 200 °C at energies between 190 and 300 keV and fluences ranging from $5x10^{11}$ up to $5x10^{15}$ 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-PIXE-channeling. Electrical properties related to the activation of Fe^{2+} centers were studied by means of experimental and simulated I-V characteristics or DLTS-PICTS 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 dopant electrons may influence the final location and electrical properties of the implanted atoms. A possible mechanism is discussed to explain the observed behavior at a microscopic level. (1) A. Gasparotto et al., Appl. Phys. Lett. 75, 668 (1999). (2)T. 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 Galtier[1], Jean-Francois Rommeluere[1], Jaime Mimila-Arroyo[2], Michel Barbe[1], Francois Jomard[1] and Yves Marfaing[1]; [1]Laboratoire de Physique des Solides et de Cristallogenese, CNRS UMR 8635, Meudon, France; [2]CINVESTAV, 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 generates a highly n-type conductive layer close to the substrate interface. This could make difficult the achievement a low level of carriers in non intentionally doped ZnO thin films. This could be also a difficulty for measuring p-type conductivity. We report on the electrical activity of ZnO films grown on sapphire substrate using the Closed Space Vapor Transport (CSVT) technique. The n-type conductivity of the epitaxially deposited films has been studied for thicknesses ranging from 0.1 to 60 μm. The carrier concentration, measured by Hall effect, is found to decrease linearly with the film thickness. This result is explained by the dominant contribution of an interface layer to the measured conductivity in relation with Al diffusion from the substrate as demonstrated by Secondary Ion Mass Spectrometry (SIMS). This interface contribution dominates the electrical behavior of the films for thicknesses up to 10 μm. We show that this strong interface conductivity can be compensated on thin films using thermal annealing under oxygen atmosphere at 850°C. Under these conditions, n-carrier concentration in the $10^{14}cm^{-3}$range can be achieved. Furthermore, the effect of this annealing under oxygen is found to be completely reversible after a further thermal annealing under argon atmosphere at the same temperature. The creation of complexes formed by an Al donor and a Zn vacancy (acceptor) whose creation is favored by oxygen annealing is proposed to explain our results. These studies confirm the importance of oxygen treatments on the electrical activity of ZnO and indicate that a suitable thermal annealing can compensate 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 thicknesses below one micron. 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 conditioned by the use of (i) an alternative substrate to sapphire or (ii) a specific buffer layer as barrier to the diffusion of Al.

10:00 AM E1.7

The Role of Oxygen Interstitial Defects in Zinc Oxide. Paul Erhart, Karsten Albe and Andreas Klein; Institut fuer Materialwissenschaft, TU Darmstadt, Darmstadt, Germany.

The electronic and optic properties of zinc oxide are to a large extent controlled by the presence of intrinsic as well as extrinsic defects. Therefore, a detailed understanding of its defect physics is essential for successful defect engineering. In the past a number of first-principles studies has dealt with intrinsic point defects in zinc oxide. While these studies have essentially confirmed the importance of oxygen vacancies and zinc interstitials, the role of oxygen interstitials has been insufficiently explored so far. We have performed a careful study of possible oxygen interstitial configurations based on density-functional theory calculations within the local density approximation. The charge state determines which configuration is energetically prefered: (1) if the oxygen interstitial is negatively charged the most stable conformation is the octahedral interstitial; (2) on the other hand, if the oxygen interstitial is neutral or positively charged it assumes a configuration in which two oxygen atoms share one site. This defect is characterized by a strong oxygen-oxygen bond which gives rise to its particular stability. Thanks to the oxygen-dimer-like structure it is able to compensate positive surplus charges in a manner that its formation energy remains almost constant as its charge state changes from neutral to doubly positive and thus acts as an effective donor. In fact, since it involves a surplus of oxygen atoms the oxygen split-interstitial turns out to be the dominant "hole killer" under oxygen-rich conditions. In this context our results are of importance for the interpretation of numerous recent attempts to synthesize p-type conducting zinc oxide.

SESSION E2: Dopant/Defects in Silicon Technology
Chairs: J. Chevallier and Kin.Man Yu
Tuesday Morning, March 29, 2005
Room 2006 (Moscone West)

10:45 AM *E2.1

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

As the semiconductor industry approaches sub-90 nm technology nodes, the trend is to replace cobalt silicide with nickel monosilicide (NiSi) since the use of NiSi for contact metallization shows a number of technological advantages, including its line-width independent low resistivity, less Si consumption and low thermal budget for its formation, and compatibility with Si1-xGex 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 surface contaminants (e.g., residual interfacial oxide). Other than the beneficial effects in enhancing thermal/morphological stability of NiSi as well as alleviating the sensitivity of NiSi to surface contamination for its formation, the incorporation of some elements has also been found to be effective in tuning the work function of NiSi, thus making it a suitable candidate material for the use as metal gate. This talk will present and discuss the details of these experimental results.

11:15 AM E2.2

Co-Doping Concepts for *p*-Type Silicon. Paola Alippi[1] and Giorgia M. Lopez[2]; [1]CNR-IMM, Catania, Italy; [2]INFM-SLACS and Dept. of Physics, University of Cagliari, Monserrato, Italy.

The extreme miniaturization of ultra-large-scale integration Si-based devices requires an ever increasing carrier density - especially for p-type doping. Engineering the coupling of acceptors with other impurities ("co-doping") may offer a route to improving the solubility and ionization, and ultimately the carrier density, for some dopants. Here we suggest that the substitutional-pair complexes 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 idea that 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. Ab initio density-functional calculations on In-C, In-Ge, B-Ge pairs confirm the soundness of the general scheme. The effect is sizable (and in good agreement with experiment) for In - whose 0.19 eV level shifts to 0.10 eV upon coupling to C - whereas it is less significant for B. We also investigated co-doping with other acceptors, considering the Ga-B and In-B pairs: but none of these is bound, so that acceptor-acceptor co-doping is of no help.

11:30 AM E2.3

Study of the $Pt-O$ Complex Formation in Platinum Doped Silicon. Wilfried Vervisch[1,2,3], Laurent Ventura[1], Bernard Pichaud[2], Gerard Ducreux[3] and Andre Lhorte[3]; [1]LMP, Universite de Tours, Tours, France; [2]TECSEN, Universite Aix-Marseille III, Marseille, France; [3]STMicroelectronics, Tours, France.

In this work, we report experimental results demonstrating the formation of a platinum oxygen complex in silicon. We model the reaction of this complex formation and propose a set of parameters according to our experimental results. When platinum is diffused at temperatures higher than 900°C in Cz and FZ n-type silicon samples which are then cooled slowly in the range [1-10]°C/min, a p-type doping leading to the formation of a pn 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 samples are quenched. Moreover, we have experimentally demonstrated that this reaction is reversible. This reaction must be associated with a complex formation between a substitutional platinum atom and another unknown impurity among the following ones: Phosphorus atoms, Pt_i, I, V, C or O_i. We have shown that this reaction occurs also in intrinsic and boron doped silicon materials, rejecting the reaction 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 ($\approx 10^{15}$ O_i/cm^3, n-type) from Wacker Siltronic AG. A slow cooling at 1°C/min has been used in order to favour the complex formation with platinum. Only a slight compensation of the phosphorus doping has been observed in the first microns under the silicide layer, certainly due to the low oxygen concentration. This result strongly suggests the participation of the oxygen in the complex formation with platinum, in Cz and FZ silicon materials. Due to its p-type doping influence, the $Pt-O$ complex must be associated with the formation of an acceptor hole trap. We have observed such a hole trap by DLTS measurement with an energy level situated at 0.42 eV from the valence band [1]. At the junction depth, only this acceptor trap participates to the phosphorus doping compensation, in a fully ionised configuration [2]. We used this property to adjust the simulation parameters of the $Pt-O$ complex formation, for different junction depths corresponding to different Pt diffusion conditions. Hypothetic reactions with other impurities are also simulated before being physically rejected. [1] L. Ventura, B. Pichaud, F. Lanois, A. Lhorte, Japanese J. Appl. Phys. Vol 40 (2001) pp. 3938-3943 Part 1, N°6A, June 2001 [2] W. Vervisch, L. Ventura, B. Pichaud, F. Lanois, A. Lhorte, Solid State Phenomena Vols. 95-96 (2004) pp. 599-604

11:45 AM E2.4

New Additions to the Menagerie of Defects in Silicon. Gerd Duscher[1,2], Alexander Kvit[3], Donovan Leonard[1], Abdennaceur Karoui[1] and Nathan G. Stoddard[1]; [1]Materials Science & Engineering, North Carolina State University, Raleigh, North Carolina; [2]Condensed Matter Science Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [3]Department of Materials Science, University of Wisconsin, Madison, Wisconsin.

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

SESSION E3: Interfaces and Strain-Induced Defects
Chairs: T. Tsuchia 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/SiO$_2$ Interface Defects using in-situ UHV-ESR System. Satoshi Yamasaki[1,2], W. Futako[1] and Norikazu Mizuochi[3,1]; [1]AIST, Diamond Research Center, Tsukuba, Japan; [2]Graduate School of Pure and Applied Science, University of Tsukuba, Tsukuba, Japan; [3]Institute of Library and Information Science, University of Tsukuba, Tsukuba, Japan.

As a typical point defect at the Si/SiO$_2$ interface affecting electrical properties, a three-fold coordinated silicon atom with a neutral charge, the so-called P_b center, has been widely investigated. Electron spin resonance (ESR) is one of the most powerful tools available for investigating P_b centers. However, these studies have been limited to the static structure of Si/SiO$_2$ after Si oxidation, whereas microscopic information about the dynamic oxidation mechanism is required. For above purposes, we have developed an ultra-high-vacuum (UHV)-ESR system, which is a combination of an ESR system and a UHV chamber, and reported the dynamic oxygen and hydrogen termination processes on an Si clean surface. In this talk, we focus on the process of P_b center generation during silicon oxidation following oxygen termination on a clean Si surface, based on which we discuss the microscopic origin of P_b centers [1] in the light of oretical works. [1] W. Futako, N. Mizuochi, and S. Yamasaki, 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 DRAM Applications by Zero-Bias Thermally Stimulated Current Spectroscopy. Wai-Shing Lau[1], Lianbin Zhong[1], Taejoon Han[2] and Nathan P. Sandler[2]; [1]School of EEE, Nanyang Technological University, Singapore, Singapore; [2]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 800oC for 30 s. ZBTSC measurements were performed at a ramp rate of 0.5 K/s as before [1]-[2]. Our old method to fill the defect states was UV illumination at about 90 K. The energy level of the defect was estimated using ET = 23kTm, where Tm is the peak temperature and k the Boltzmann 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 that the most efficient way to fill defect D with electrons is to use the optical illumination and soft X-ray radiation during electron beam evaporation of metal to form the top electrode for sample preparation.

The sample actually became slightly hot and since the capture cross section is thermally activated the electron capture became much faster. In addition, the electron filling was done from the beginning, when the metal was thin such that its light blocking effect is much smaller, to the end of the electron beam evaporation process. With this innovation, defect D was detected as a strong ZBTSC peak at about 380 K. By performing a simple integration, we found that the concentration of oxygen vacancies is of the order of 1E17 cm-3 in decent samples. Thus we demonstrated that ZBTSC can detect O vacancy double donors efficiently and quantitatively for tantalum oxide using our new filling method. However, we noticed that the old filling method (UV illumination at 90 K) is more useful for the detection of Si and C contamination. We can predict that ZBTSC can also be applied to other high-K dielectric materials for next generation microelectronics technology. [1] W.S. Lau et al., Jpn. J. Appl. Phys., 34, 757 (1995). [2] W.S. Lau et al., Appl. Phys. Lett. 71, 500 (1997). [3] W.S. Lau et al., Appl. Phys. Lett. 83, 2835 (2003). [4] F.G. Ullman, J. Phys. Chem. Solids. 28, 279 (1967).

2:15 PM E3.3

An Investigation on the Band Offsets of GaNAsSb/GaAs and GaInNAsSb/GaAs. Homan B. Yuen[1], Robert Kudrawiec[2], Krzysztof Ryczko[2], Seth R. Bank[1], Mark A. Wistey[1], Hopil Bae[1], Jan Misiewicz[2] and James S. Harris[1]; [1]Solid State & Photonics Laboratory, Stanford University, Stanford, California; [2]Institute 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. GaInNAs 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 are even more apparent when adding more In and N to GaInNAs to reach the technologically important wavelengths near 1.55 μm. Sb acts as both a surfactant and constituent when introduced during dilute-nitride growth, forming GaInNAsSb and GaNAsSb. The improvement in material quality and reduction of band gap, by adding Sb, has enabled the development of GaAs-based lasers out to 1.55 μm. Although dilute-nitride-antimonide lasers have been shown to have great potential telecommunication applications, several key electronic parameters are not 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 photoreflectance (PR). By simulating the spectra obtained from PR, a model of the band offsets, energy levels, and effective masses are obtained. There have been many studies on GaInNAs and GaNAs band offsets, however there have been none for GaInNAsSb and only a few for GaNAsSb. Before this study, it was unclear what effect the addition of Sb would have on the GaInNAs and GaNAs band offsets. In the dilute-nitrides, it was not known if Sb would on affect the valence band or if there would be a more complex interaction of the valence and conduction bands due to effects such as band anti-crossing. To determine the band offsets of the GaNAsSb and GaInNAsSb materials, we performed PR measurements on GaInNAsSb/GaNAs/GaAs and GaNAsSb/GaAs quantum wells. These samples were grown by solid-source molecular beam epitaxy utilizing a N rf 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, $Ga_{0.6}In_{0.4}N_{0.025}As_{0.955}Sb_{0.02}$/GaAs has a band offset ratio of ΔEc/ΔEv 0.9 and $GaN_{0.025}As_{0.875}Sb_{0.1}$/GaAs a ratio of ΔEc/ΔEv 0.5. Other results from these samples will also be presented to provide a better understanding of Sb's role in dilute-nitride band structure. The results suggest that the addition of Sb affects the band structure of dilute-nitrides for laser devices by mostly only affecting the valence band. With a greater understanding of the band structure, more advanced GaInNAsSb laser devices can be obtained.

2:30 PM *E3.4

Direct Measurements of Trap Density in a SiGe/Si Hetero Interface by New Charge-Pumping Technique. Toshiaki Tsuchiya[1], Masao Sakuraba[2] and Junichi Murota[2]; [1]Shimane University, Matsue, Japan; [2]Tohoku University, Sendai, Japan.

Strained-Si and SiGe/Si-hetero CMOS structures are highly promising materials for the construction of advanced high-performance Si CMOS devices. To exploit the advantages of the SiGe/Si heterostructure 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 recognized as a very high precision method of evaluating interface traps between the gate oxide and the semiconductor surface in MOSFETs. In this study, we propose a new charge pumping technique, i.e., low-temperature charge pumping (LTCP) technique, to directly measure the interface trap density in the SiGe/Si heterostructure introduced into the channel region of MOSFETs, without interference from the interface traps between the gate oxide and the semiconductor surface [2]. The devices used in this study are strained SiGe-channel pMOSFETs, which has a relatively 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 layer, strained-SiGe layer, and 6-nm thick capping Si layer by ultraclean low-pressure chemical vapor deposition [3]. All of the annealing processes were performed at temperatures below 700 C to prevent degradation of the heterostructure surface flatness and of the Ge profile in the channel region at high Ge fractions. We also measured the low frequency noise power in the drain current flowing in the SiGe-channel [4], and 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 the generated hetero-interface-traps. Referencess [1] G. Groeseneken, H. E. Maes, N. Beltran, and R. F. DE Keersmaecker, IEEE Tran. Electron Devices, vol. ED-31, no. 1, pp.42-53, 1984. [2] T. Tsuchiya, Y. Imada, 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 1, no. 4B, pp. 2290-2299, 1994. [4] T. Tsuchiya, T. Matsuura, and J. Murota, Jpn. J. Appl. Phys., vol. 40, no. 9A, 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 E3.5

Ultra-Shallow Junctions for the 65nm Node Based on Defect and Stress Engineering. Victor Moroz[1], Majeed Foad[2], Houda Graui[2], Faran Nouri[2], Dipu Pramanik[1] and Susan Felch[2]; [1]Synopsys, Inc, Mountain View, California; [2]Applied Materials, Sunnyvale, California.

The co-implantation of germanium, carbon, and boron with the optimum implant energies and doses makes it possible to create p+/n junctions with the sheet resistance of less than 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 amount of carbon is placed in between the implanted boron and the implant damage, which is located below the amorphized layer. During the annealing, the carbon atoms capture silicon interstitials that are coming from the implant damage and form carbon-interstitial clusters. The analysis demonstrates that it is possible to capture over 95% of the interstitials this way before they 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 below the amorphized layer, the rapid temperature ramp down, 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 solid-state solubility level. We explain this effect as a reduction in formation of BICs due to the lack of interstitial supersaturation. In carbon-free silicon, high concentration boron is always accompanied by the non-equilibrium interstitials, coming from either the implant damage or the BICs even if boron is introduced into silicon by pre-deposition instead of the implantation. Extensive experiments and theoretical analysis based on simulation of the interaction of Ge, C, I, and B atoms, as well as the stress effects, point to the optimized process flow that improves the shape and parameters of the p+/n USJs.

3:45 PM E3.6

High Quality Strained-Si Growing Techniques. Young-Pil Kim, Sun-Ghil Lee, Young-Eun Lee, Jong-Wook Lee, In-Soo Jung,

Sung-Kwan Kang, Deok-Hyung Lee, Yong-Hoon Son, Pil-Kyu Kang, Min-Ku Kang, Yu-Gyun Shin, U-In Chung and Joo-Tae Moon; Process Development Team, Samsung Electronics, Yongin-City, Gyeonggi-Do, South Korea.

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

4:00 PM 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. Geert Eneman[1,3,4], Eddy Simoen[1], Romain Delhougne[1,3], Peter Verheyen[1], Michael Ries[2], Roger Loo[1], Matty Caymax[1], Wilfried Vandervorst[1,3] and Kristin De Meyer[1,3]; [1]Imec, Heverlee, Belgium; [2]MEMC, St. Peters, Missouri; [3]ESAT, K.U. Leuven, Leuven, Belgium; [4]F.W.O., Brussels, Belgium.

Downscaling of transistor dimensions has lead to an important performance increase in microelectronics, combined with a decreasing cost per logical function. To obtain the highest possible gain in performance, several changes of the standard technology are investigated. One of these changes is the use of silicon under a tensile strain (Strained Si) in the channel, grown on a Strain Relaxed Buffer (SRB) of silicon-germanium: strained Si can lead to higher performance for devices, without leading to a substantial increase in the processing cost. One of the most important challenges for fabricating SRBs is the control of defects. Dislocations, crossing the 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 dislocations inducing a high degree of relaxation and simultaneously help reducing the number of threading dislocations. In this experiment, the threading dislocation density in the layers was varied, as well as the distance of the C-rich layer to the surface, allowing to study their effect on device 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 depth 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 SOI. Qianghua Xie[1], Mike Kottke[1], Xiangdong Wang[1], Mike Canonico[1], Ted White[2], Bich-Yen Nguyen[2], Alex Barr[3], Shawn Thomas[4] and Ran Liu[5]; [1]Physical Analysis Laboratory Arizona, Freescale Semiconductor Inc., Tempe, Arizona; [2]Advanced Process Research and Development Laboratory, Freescale Semiconductor Inc., Austin, Texas; [3]Crolles-2, Freescale Semiconductor, Crolles, France; [4]Embedded Systems and Science Research Laboratory, Motorola Inc., Tempe, Arizona; [5]School of Micro-Electronics, Fudan University, Shanghai, China.

We will present a systematic study of the strain, defect and morphology of SiGe (Ge composition from 20-40%) layers grown on silicon on insulators (SOI). For low Ge composition (20%), the strain relaxation in SiGe layer is minimal as determined by Raman spectroscopy (delayed by the increased critical thickness for dislocation formation in SiGe on SOI). The misfit dislocation density is below the detect limit of transmission electron microscopy (TEM). For higher Ge content (32%), the tensile strain in a Si capping layer grown on top of SiGe/SOI is 0.46% to 0.65% (a stress of 0.81 GPa to 1.17 GPa). The misfit dislocation linear density observed in cross sectional TEM is 17/ μm and 23/μ m which is consistent with the strain relaxation of the SiGe layer as determined by Raman. Upon thermal annealing, increased surface roughness, dislocation density and strain relaxation in the SiGe layer are observed. TEM also reveals that the misfit dislocations are confined mostly at SiGe/SOI interface and move down to the Si/oxide interface. Based on this, a new compositionally downgraded scheme having a higher-Ge (upto 40%) buffer layer grown first has been devised. This layer adsorbs most of the misfit defects and is partially relaxed. Then a thin layer of SiGe of lower Ge composition (20%-25%) is grown on this artificial substrate achieving high strain relaxation and low defect density in this layer. This stack serves as the substrate upon which a tensilely strained silicon capping layer can be grown to realize strained Si CMOS devices.

4:30 PM E3.9

Characterization of Ultrathin Strained-Si Channel Layers of n-MOSFETs Using Transmission Electron Microscopy. Dalaver Hussain Anjum[3,1], Robert Hull[1], Jian Li[1], Judy L. Hoyt[2] and Guangrui Xia[2]; [1]Materials Science & Engineering, University of Virginia, Charlottesville, Virginia; [2]Electrical Engineering & Computer Science, Massachusetts Institute of Technology, Cambridge, Massachusetts; [3]The Burnham Institute, La Jolla, California.

Strained-Si based FETs have enabled improvement of carrier transport in MOS-based devices, both in the ON state of the device and in the sub-threshold region. This leads to devices with higher ratios of on-to-off current, and to the development of new concepts aimed at dramatically improving the device sub-threshold slope, enabling much lower voltage operation. However, in order to understand the fundamental physics of these devices, it is imperative to address the stress conditions of the strained-Si channel layers after device processing, particularly after the ion-implantation process. In this work, we have studied Si+ self ion-implantation and thermally annealed strained-Si channel layers in n-MOSFETs. The n-MOSFETs were fabricated with various channel lengths, implant doses and thermal budgets. Neutral Si implants were used to study the impact of the implant damage on mobility separately from ionized impurity scattering effects. It has been observed that the density of defects in the strained-Si layer depends upon implant dose as well as thermal treatment. Using the EDS spectra, it is determined that the average concentration of Ge in the strained Si layer is about 4 at.%. The presence of Ge in strained Si channel layer causes the relaxation of strain. This is verified by Convergent Beam Electron Diffraction (CBED) technique by measuring the lattice constant of the strained Si lattice. It is concluded that the electron mobility enhancements can be degraded in n-MOSFETs due to presence of both Ge up-diffusion and defects.

4:45 PM E3.10

The Defect Formation and Strain Relaxation in GaAsSb/GaAs Heteroepitaxy. Benny Perez Rodriguez[1] and Joanna Mirecki Millunchick[2]; [1]Applied Physics, University of Michigan, Ann Arbor, Michigan; [2]Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan.

The mechanisms for stress relaxation have been investigated during growth of GaAsSb/GaAs (001) 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 (MOSS) 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 GaAsSb/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 saturation. For $GaAs_{0.5}Sb_{0.5}$/GaAs the strain-relieved shows that for $h_f < 80$ $\AA$ essentially no strain is relieved. Fast relaxation occurs for 86 $\AA < h_f < 600$ $\AA$ and by 500 $\AA$, 62% of the strain has been relaxed. Beyond 600 $\AA$ the rate of the strain continues to decay for the duration of the growth. Similar results were found for $GaAs_{0.64}Sb_{0.36}$/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 surfaces can relieve about the same amount of strain. For $GaAs_{0.5}Sb_{0.5}$/GaAs the TEM images shows that a high density of dislocation does not form until the coalescence of islands. Contrary to the observed in other system, the threading dislocations density is significantly smaller in thinner films. Preliminary HRTEM shows that pure edge dislocations exist during the fast relaxation regime. For $GaAs_{0.64}Sb_{0.36}/GaAs$, 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 B.L. Sopori
Tuesday Evening, March 29, 2005
8:00 PM
Salons 8-15 (Marriott)

E4.1
Chromium Diffusion Doping of Commercial ZnSe and CdTe Windows for Mid-Infrared Solid-State Laser Applications.

Ivy K. Jones[1], Uwe Hommerich[1], EiEi Nyein[1] and Sudhir Trivedi[2]; [1]Dept. of Physics, Hampton University, Hampton, Virginia; [2]Brimrose Corporation, Baltimore, Maryland.

We report on the preparation and optical spectroscopy of diffusion doped Cr: ZnSe and Cr: CdTe polycrystalline windows. Cr2+ doped II-VI semiconductors have recently emerged as a new class of room temperature operated and widely tunable (2-3 μm) mid-infrared (MIR) solid-state lasers. The demonstration of efficient lasing from diffusion doped polycrystalline Cr: ZnSe windows provides an attractive method for producing MIR laser materials at low cost. For the advancement of current Cr2+ chalcogenide lasers, however, it is critical to gain a better understanding of the Cr2+ incorporation and infrared optical properties in II-VI hosts. In this work we present results on Cr diffusion experiments performed on commercial ZnSe and CdTe windows. Compared to Cr: ZnSe, Cr: CdTe offers the advantage of an extended MIR emission with a larger emission cross-section beyond 3000 nm. Cr doping was achieved in both window materials through a thermal diffusion process controlled by temperature (750-850C) and time (0.25-6 days). Commercial CrSe powder (99.5% purity) was used as the dopant source. Various samples of Cr: ZnSe and Cr: CdTe were prepared with Cr2+ peak absorption coefficients ranging from 1 cm-1 to 25 cm-1. The estimated Cr2+ concentrations ranged from 5x10Î7cm-3 to 3x10Î9cm-3 assuming absorption-cross sections of 0.9x10-̂18cm2 for Cr: ZnSe and 1.1x10-̂18cm2 for Cr: CdTe. For low Cr2+ concentrations (1x10Î8cm3) the room-temperature decay time varied between 5-6 μs for Cr: ZnSe and 2-3 μs for Cr: CdTe. Based on low temperature (15 K) lifetime data, the emission efficiencies were estimated to be 75% for Cr: CdTe and 95% for Cr: ZnSe. The effect of Cr concentration quenching on the MIR emission was observed for doping concentrations above 1x10Î9cm3. 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 Liao[1], Jyh-Rong Gong[2], Yu-Li Tsai[1], Cheng-Liang Wang[1], Keh-Chang Chen[1] and Tai-Yuan Lin[3]; [1]Department of Materials Science and Engineering, Feng Chia University, Taichung, Taiwan; [2]Institute of Opto-Mechatronics, National Chung Cheng University, Chiayi, Taiwan; [3]Institute of Optoelectronic Sciences, National Taiwan Ocean University, Keelung, Taiwan.

GaN films were grown on (11-20) sapphire substrates at 1000 °C under various V/III ratios. Growth was conducted by exposing the (11-20) sapphire substrate alternatively to trimethylgallium(TMG) 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 a 0.6 μm-thick GaN film at 1000 °C. In this case, the V/III ratios of TMG and NH_3 are 4100, 5200, 6800, 8300, and 10400, respectively. It appears that the OM surface morphology of the GaN film grown on a (11-20) sapphire substrate improves with the increment of V/III ratio. Room temperature (RT) PL spectrum of the GaN film grown under a V/III ratio of 5200 shows strong near bandedge emission along with prominent yellow luminescence. An increment of V/III ratio up to 10400 was found to enhance near bandedge emissions and to quench yellow luminescence. It is believed that the amount of reactive N-H radicals may not be high enough to support sufficient overpressure on the grown surface at a V/III ratio of 5200 presumably due to the existence of a pulse time between successive 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 can only be achieved under high V/III ratios and at a growth temperature 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 adsorbates can only be suppressed under high V/III ratio. Thus, it is believed that sufficient supply of the reactive N-H radicals at a V/III ratio of 10400 is crucial for the growth of high quality GaN films on (11-20) sapphire substrates in this study. A plot of the linewidth of the RT near 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 defect 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, I. 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.503-505 (1996) .

E4.3
Characteristics of GaN Films Grown on Wet-Etched GaN.

Yu-Li Tsai[1], Jyh-Rong Gong[2], Kun-Ming Lin[1], Wei-Tsai Liao[1], Cheng-Liang Wang[1] and Tai-Yuan Lin[3]; [1]Department of Materials Science and Engineering, Feng Chia University, Taichung, Taiwan; [2]Institute of Opto-Mechatronics, National Chung Cheng University, Chiayi, Taiwan; [3]Institute of Optoelectronic Sciences, National Taiwan Ocean University, Keelung, Taiwan.

It is well known that the reliability of light-emitting devices, particularly laser diodes, can be greatly deteriorated by the presence of structural defects such as dislocations. Many approaches including epitaxial lateral overgrowth process [1] and patterned substrate techniques [2] have been reported to improve the quality of GaN films remarkably. However, the employment of dry etching process makes the fabrication process less cost-effective. In this study, we report the improvement of optical properties of GaN films by using a simple wet-etching technique. Typically, a GaN sample was prepared by growing a 2 μm-thick GaN underlayer on the c-plane Al_2O_3 substrate with a subsequent wet-etching treatment on the GaN underlayer at 245°C for 25 min. H_3PO_4/H_2SO_4 etching solutions having H_3PO_4/H_2SO_4 ratios of 1/3, 1, 2, and 3, respectively, were employed to develop etch pits on the GaN surface. On each of the etched GaN underlayers, an 1.5 μm-thick GaN film was grown afterward. For comparison, a GaN film, 1.5 μm in thickness, was also grown on the 2 μm-thick GaN underlayer without wet-etching treatment. All the overgrown GaN films were etched again by molten KOH at ~260°C for 10 min to reveal the etching pit densities (EPDs) of the GaN films. The grown samples were characterized by using optical microscopy (OM), scanning electron microscopy (SEM), photoluminescence (PL) spectroscopy, and transmission electron microscopy (TEM). Room temperature (RT) PL measurements of the overgrown GaN films show a remarkable increment in PL intensity and a considerable reduction in emission linewidth of the near bandedge (BE) luminescence when GaN films were grown on the wet-etched GaN underlayers. 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 2.9 μm increases by one order of magnitude when compared with that of the GaN film grown on a GaN underlayer without wet-etching process. OM images of the etched overgrown GaN films indicate that the EPD of the film reduces from 1.7×10^7 cm^{-2} to 3.1×10^6 cm^{-2} when the pit size of the underlying etched GaN increases from 0 to 2.9 μm. Cross-sectional TEM observations 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 above which very few dislocations were observed in the laterally overgrown GaN areas. References: [1] T. S. Zheleva, O. H. Nam, M. D. Bremser, and R. F. Davis, Appl. Phys. Lett. 71 (1997) 2472. [2] A. Bell, R. Liu, F. A. Ponce, H. Amano, I. Akasaki, and D. Cherns, Appl. Phys. Lett. 82 (2003) 349.

E4.4
On the Properties of GaN Films Grown on (111) Si Substrates using Intermediate Temperature AlGaN Buffer Layers.

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Recently, there has been a considerable interest in the growth of GaN films on (111) Si substrates for applications in AlGaN/GaN high power electronics and GaN-based LEDs [1, 2]. However, because of the large difference in lattice structure and thermal expansion coefficient, the growth of 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 $Al_{0.58}Ga_{0.42}N$ buffer layers , deposited at 800°C, with the thicknesses of $Al_{0.58}Ga_{0.42}N$ layers being 150 ,170 ,180 ,190 and 205 nm, respectively. In this case, a 0.4 μm-thick HT GaN film was deposited with the admittances of TMG and NH_3 being 34 μmol/min and 0.2μmol/min. θ-2θ X-ray diffraction (XRD) measurements were used to identify the orientation relationship among GaN film, $Al_{0.58}Ga_{0.42}N$ buffer layer and Si substrate. Photoluminescence (PL) measurements were conducted to obtain the optical properties of GaN films using the 325nm excitation of a He-Cd laser. The results of X-ray θ-to-2θ scan of all the grown samples clearly reveal (0002)GaN, (0004) GaN and (0002)$Al_{0.58}Ga_{0.42}N$ diffracted peaks along with the (111) Si diffracted peak at 28.4°. There is no other diffracted peak from the GaN film grown on the $Al_{0.58}Ga_{0.42}N$-coated (111) Si substrate. Room temperature (RT) photoluminescence (PL) spectrum of a GaN film grown on the 180 nm-thick $Al_{0.58}Ga_{0.42}N$-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 3.40 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 intermediate temperature $Al_{0.58}Ga_{0.42}N$ buffer layer thickness below (or above) 180 nm was found to deteriorate the crystalline quality of HT GaN film. Insufficient accommodation of misfit strain in the GaN film for the case of reduced 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. 81 (2002) 1591. [2] E.M. Chumbes, A.T. Schremer, J.A. Smart, Y. Wang,N.C. MacDonald, D. Hogue, J.J. Komiak, S.J. Lichwalla, R.E. Leoni, and J.R. Shealy, IEEE Trans. Electron. 48 (2001) 420. [3] A. Dadgar, M. Poschenrieder, J. Biasing, and K. Fehse, A. Diez, A. Krost, Appl. Phys. Lett. 80 (2002) 3670. [4] J.R. Gong, M.F. Yeh , and C.L. Wang, J. Crystal Growth 247 (2003) 261.

E4.5

Ferromagnetism in the Diluted Magnetic Semiconductor Phase of ZnO:Co. Marco Aurelio Boselli[1], Ivan C. da Cunha Lima[2] and A. Ghazali[3]; [1]Departamento de Fisica, Universidade Federal de Ouro Preto, Ouro Preto, MG, Brazil; [2]Instituto de Fisica, Universidade do Estado do Rio de Janeiro, Rio de Janeiro, RJ, Brazil; [3]Groupe de Physique des Solides, UMR 7588-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 shown to be more interesting than Mn in what concerns the magnetism of this compound. As in other ferromagnetic semiconductors, two key issues are the occurrence of clustering and the presence of free carriers [2,3]. These two factors are determined, in principle, by the Co concentration in the growth process. We have adapted a spin-polarized quasi-2D RKKY formalism [4] to treat the wurtzite structure. The indirect exchange matrix resulting of this indirect interaction is then used in a temperature dependent Monte Carlo simulation to obtain the average magnetization and the magnetic susceptibility. The Co concentration and the density of free carriers providing the interaction between the magnetic moments are treated as independent parameters. Therefore, we do not have to assume a definite origin for the carriers mediating the interaction, neither effects like compensation. Every Co atom participates of the interaction, either being ionized or not. The Co distribution is assumed to be homogeneous allover the sample. In terms of the Monte Carlo simulation this is equivalent to assume that a Co atom is equally likely to occupy any Zn site in the structure. Samples containing 5%, 15% and 25% were simulated both for a thin film and a layered system. The magnetization curve as function of temperature shows the typical shape appearing in other quasi-2D DMS systems [5]. We show how the transition temperature varies with the Co concentration and the density of free carriers. [1] T. Dietl, H. Ohno, and F. Mtsukura, Phys. Rev B 63, 195205 (2001) [2] Jung H. Park, Min G. Kim, Hyun M. Jang, Sangwoo Ryu, and Young M. Kim, Appl. Phys. Lett. 84, 1338 (2004). [3] K. Rode, A. Anane, R. Mattana, J.-P. Contour, O. Durand and R. LeBourgeois, J. Appl. Phys. 93, 7676 (2003). [4] M. A. Boselli, I. C. Cunha Lima, and A. Ghazali Phys. Rev. B 68, 85319 (2003) [5] M. A. Boselli, I. C. da Cunha Lima, J. R. Leite, A. Troper, and A. Ghazali, Appl. Phys. Lett. 84,1138 (2004)

E4.6

Electricfly Active Defects of GaAs Films on Porous GaAs Substrates and Gettering. Alexander Buzynin[1], Yuri Buzynin[2], Alexander Belyaev[2], Eduard Rau[3] and Albert Lukyanov[3]; [1]General Physics Institute, Russian Academy of Sciences, Moscow, Russian Federation; [2]Institute for Physics of Microstructures, Russian Academy of Sciences, Nizhny Novgorod, Russian Federation; [3]Physical Department, Moscow State University, Moscow, Russian Federation.

Influence of defects on electric properties of devices is caused structural - admixture complexes defect-impurity, instead of "pure" crystallographic defects. These defects essentially decrease electric and optical properties of material and characteristics of opto- and microelectronic devices. Perspective way of improvement of heteroepitaxial layer quality 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 opportunities of 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 so-called õRau-detector≫ (contactless analogue of SEM-EBIC mode). GaAs (100) substrates doped by Te and Si up to concentration $2{*}10^{18}cm^{-3}$ were used. To reveal difference in epitaxial layer defect structure connected with substrate state, only one half of GaAs substrate 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: - more smooth surface with morphological attributes of lateral growth mechanism (lines of layers); - less density of structural defects - there were no dislocation walls and density of pyramidal holes was $\approx 2{*}10^{5}cm^{-2}$ as compared with density of about $2{*}10^{7}cm^{-2}$ in films on a monolithic substrate; - less electrical activity of various structural defects and increased electric uniformity of grown films. Features of lateral growth mechanism 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.Buzynin, S.A Gusev, V.M.Daniltsev, et al., Technical Physics Letters V.26, No.4, p.298, (2000) [2]. Yu.Buzynin, A.Belyaev, A.Akhsakhalyan, et al., Proc. of Inter. Congress õMW-2001≫, Advanced Materials, 25-28 Sept. 2000, Munich, Germany, Article 672. The work was supported by the Russian Foundation for Basic Research, grant N 03-02-17337 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 their unique properties. Several applications that include high hardness, low friction coefficient, mechanical and electrical properties can be achieved doping diamond crystals with impurities. Two basics processes, dopant diffusion and ion implantation, are the main methods to study the diffusion of impurities in diamond. The introduction of impurities such as B, Li, S, 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 it characterization. Author: Adrian E. Mendez, Ph.D student. Advisors: Mark A. Prelas Ph.D., Tushar Ghosh Ph.D.

E4.8

Structural Characterization of GaN Epilayers Grown on PSS(Patterned Sapphire Substrate). Chang-Soo Kim[1], Sang-Jun Lee[1], Sam-Kyu Noh[1], Kyuhan Lee[2], Je Won Kim[2], Ji-Hyun Moon[3], Byung-Sung O[3] and Jay P. Song[4]; [1]National Research Laboratory, Materials Evaluation Center, Korea Research Institute of Standards and Science, Taejon, South Korea; [2]Photonic Device Group, Samsung Electro-Mechanics, Suwon, South Korea; [3]Department of Physics, Chungnam National University, Taejon, South Korea; [4]SongJee Industrial Corporation, Sungnam, South Korea.

The structural properties of GaN epitaxial layers grown on PSS(patterned sapphire substrate) by MOCVD have been investigated using HRXRD(high-resolution X-ray diffraction), GIXRD(grazing incidence X-ray diffraction), PL(photoluminescence) and TEM(transmission electron microscope). A 30 nm thick low-temperature GaN nucleation layer and a 3 μm thick GaN layer were grown on both patterned and unpatterned (00 1) sapphire substrates. For X-ray characterizations rocking curves for GaN (10 5), (00 2), (11 4) and (11 0) reflections for which incident angles of

X-rays are 30, 17, 11 and 0.3°, respectively, were measured. For (11 0) reflection which is perpendicular to the sample surface, GIXRD technique was employed. For (10 5), (00 2) and (11 4) reflections FWHMs of the rocking curves for patterned substrate were broader than those for unpatterned substrate, for (11 0) reflection, however, FWHM for patterned substrate was much narrower than that for unpatterned substrate. The normalized FWHM for all reflections decreases as the incidence angle of X-ray decreases. The results suggest that the crystalline quality in the surface region of the epilayer on patterned substrate was especially improved because the penetration depth of X-ray depends on the incident angle, and the depth for (11 0) reflection is about 40 nm. The improvement of the crystallinity in the surface region is attributed to the reduced dislocation density which was confirmed by TEM image. The intensity of PL peak of the epilayer for patterned substrate increased compared to that for unpatterned substrate and the result is consistent with the XRD results. A mechanism for the reduction of dislocation density at the surface region will be discussed.

E4.9

Defect Modification in GaInNAsSb Growth with Insertion of GaAs Prelayers. Seth Bank, Mark Wistey, Homan Yuen, Hopil Bae, Lynford Goddard and James S. Harris; Solid State and Photonics Laboratory, Stanford University, Stanford, California.

GaInNAs and GaInNAsSb, grown on GaAs, have emerged as promising active layer materials for lasers covering the entire low-loss fiber bandwidth from 1.2-1.6 μm, but lasing at 1.55 μm has remained illusive. We present an important growth optimization that illustrates the importance of both extended and point defects in the preparation of high-quality dilute-nitride layers by molecular beam epitaxy. A rf plasma cell was employed to generate reactive nitrogen, as is typical for dilute-nitride growth. Substantial defect generation and surface roughness have been observed when the sample surface is exposed to the plasma during ignition. We investigate the role and optimization of GaAs prelayers inserted between this plasma damaged surface and the active layer. Room temperature optical efficiency was increased 2.9x by insertion of a 15 nm GaAs prelayer. By optimizing the arsenic overpressure in the GaAs layer with reflection high-energy electron diffraction, another 2.3x improvement was realized. Fully optimized structures showed a total photoluminescence efficiency enhancement of 7x. High-resolution X-ray diffraction ω-2θ measurements indicate structural improvements to the GaInNAsSb quantum well with the inclusion of the GaAs prelayer, but little change with the arsenic overpressure. It is postulated that the GaAs prelayer both spatially separates the active layer from the defect-rich interface and smoothes the growth front to reduce defect formation in the quantum well. Similar samples were also characterized by secondary ion mass spectrometry and no contaminants were found at the relevant interfaces. These growth improvements are validated by the first demonstration of lasing at 1.55 μm from a GaAs-based device.

E4.10

Structural Properties of Thin Oxide Films (ZnO and SnOx) Deposited on Glass and Silicon Substrates.
Serekbol Zharylgap-uly Tokmoldin, Bulat N. Mukashev, Nurjan B. Beisenkhanov, Azamat B. Aimagambetov and Irina V. Ovcharenko; Solid State Physics, Institute of Physics and Technology, Almaty, Kazakhstan.

Gas sensitive layers of SnO2 are perspective for making chemical sensors. Properties of tin dioxide films depend on their deviation from stoichiometry and on the microstructure. The SnOx 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 electrode system with crossed electric and magnetic fields. Discharge power was 300 Wt (3 kV, 100 mA), the substrate temperature was 200 C. Pure (99,99%) Sn target was used for the sputtering. Samples obtained were annealed isochronously (during 1 hour) in air in the 200-600 C temperature range with 100 C step. It is shown by X-ray diffraction that immediately after the deposition a preferred orientation of SnO2- and Sn2O3-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 intensive growth of crystallite sizes and phase volume of polycrystalline SnO2 during annealing at 400-500 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 perfect structure is a most important problems. Exciton photoluminescence is very sensitive to the quality of crystal structures and to the presence of defects. The perfect structure of a crystal makes more probable the observation of free-exciton photoluminescence. The ZnO films of 150 nm thickness deposited by DC reactive magnetron sputtering on silicon substrate were exposed to cyclic annealing at 400 C in vacuum, then in air at the same temperature, then in vacuum again. A remarkable photoluminescence band at 375 nm was observed in spectra of the obtained low-resistivity transparent ZnO films exited by He-Cd laser radiation at liquid-nitrogen and room temperatures.

E4.11

Charge Transport Properties in AlO$_x$ Capped ZnO Thin Films by Scanning Probe Microscopy. Jin An^{1,2}, K. C. Hui^{3,2}, K. Xue^{1,2}, Daniel H. C. Ong^{3,2} and J. B. Xu^{1,2}; ^{1}Electronic Engineering, Chinese University of Hong Kong, Hong Kong, Hong Kong; ^{2}Materials Science and Technology Research Center, Chinese University of Hong Kong, Hong Kong, Hong Kong; ^{3}Dept. of Phsyics, Chinese University of Hong Kong, Hong Kong, Hong Kong.

ZnO films have received considerable attention due to their potential applications in numerous 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 AlO$_x$ capped ZnO nano-patterns have been systimatically 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. Such optical intensity enhancement and conductivity decrease can be attributed to the recombination enhanced defect reaction. Since the recombination occurs in the proximity of defect sites, 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 upward 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 AlO$_x$ and ZnO, 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.

E4.12

RHEED Oscillation Study of GaAs(331)B Surface.
Vahid R. Yazdanpanah, Z H. M. Wang, S. H. Seydmohamadi and Greg Salamo; Physics, University of Arkansas, Fayetteville, Arkansas.

RHEED oscillations have been intensively studied for the control of growth rates and growth conditions. The oscillation is generally observed under growth conditions that lead to layer-by-layer two-dimensional (2D) growth. During the 2D growth, the surface morphology 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). For the first time, a RHEED oscillation is reported on high index GaAs(331)B faceted surface with (110) and (111)B facets. The RHEED oscillation was observed only along the [-1-16] direction. Absence of any RHEED oscillations along [11-6], [-110], and [1-10] indicates a growth model for the GaAs (331)B in which the surface is growing only along (111)B facets although the (110) facets have the same chance to receive the Ga and As atoms. In another word, all deposited material on (110) facets move toward (111)B in order to form the new layer of atoms. These results help us to better understand the nature of RHEED oscillation on high index GaAs.

E4.13

Structural and Electrical Characterization of Fe Implanted GaInP: Interaction of Fe with Ion Induced Defects and Deep Trap Activation. Tiziana Cesca^1, Andrea Gasparotto^1, Adriano Verna^1, Beatrice Fraboni^2, Giuliana Impellizzeri^3, Francesco Priolo^3, Luciano Tarricone^4 and Massimo Longo^4; ^{1}Physics Department, INFM and University of Padova, Padova, PD, Italy; ^{2}Physics Department, INFM and University of Bologna, Bologna, BO, Italy; ^{3}Physics and Astronomy Department, INFM and University of Catania, Catania, CT, Italy; ^{4}Physics 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 midgap deep acceptor character it is widely employed to produce highly resistive layers for leakage current blocking and electrical insulation in optoelectronic devices. Moreover, Fe has peculiar optical properties, interesting from both a fundamental and an applicative point of view, related to luminescent emission in the mid-IR region of the electromagnetic spectrum; these can be potentially exploited to produce mid-IR emitter devices, LED or lasers. In order to display these properties, high concentrations of Fe atoms have to be introduced in substitutional sites in the semiconductor lattice. It has been shown recently that high densities of electrically and optically active Fe centers can be incorporated in InP by high temperature ion implantation and proper post-implantation annealing treatments: by this method both solubility limitations and damage-related undesired redistribution phenomena can be overcome and avoided, creating a supersaturation of substitutional Fe atoms in a slightly damaged crystal (1). Despite to the technological interest, the knowledege about the Fe related electrical and optical properties in ternary (and quaternary) InP related materials is at present very little. Aim of our work is to extend the results obtained for Fe implantation in InP to these compounds. The main goal is to understand the mechanisms leading to the final location of the Fe atoms and to correlate the structural information (with regard both to the local environment of the Fe atoms and possible interactions with implant-induced defects) to the Fe-related electrical properties. In this preliminary report we examined single GaInP layers, grown by MOVPE lattice matched to GaAs. The role of the implantation temperature and dose in determining the crystal damage, and the recovery of this damage by the following high temperature annealing treatments is investigated mainly by RBS-channeling measurements. Channeling is used again, in conjunction with ion-induced X-ray detection (PIXE), to study the local configuration around the implanted Fe atoms and its modification after the annealing treatments. SIMS depth profiling and HRXRD were also employed to complete the structural characterization. The electrical properties related to Fe implantation are studied by current-voltage measurements on mesa devices, and related to the different implantation and annealing conditions. The deep level properties of the Fe centers were studied by means of PhotoInduced Current Transient Spectroscopy (PICTS). The results allow a first analysis of the similarities and differences showed by the Fe implanted InGaP with respect to the InP case. (1) T. Cesca et al., Phys. Rev. B 68, 224113 (2003).

E4.14

Transmission Electron Microscopy Study of Nonpolar a-Plane GaN Grown by Pendeo-Epitaxy on $(11\underline{2}0)$ 4H-SiC. Dmitri N. Zakharov[1], Zuzanna Liliental-Weber[1], Brian Wagner[2], Zach Reitmeier[2], Edward Preble[2] and Robert Davis[2]; [1]Lawrence Berkeley National Laboratory, Berkeley, California; [2]North Carolina State University, Raleigh, North Carolina.

Recent studies have shown that $\{11\underline{2}0\}$ (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 separations of electron and holes wave functions in GaN-based quantum well structures. Our transmission electron microscopy investigations performed on a-plane GaN grown by organometallic vapor phase epitaxy at 1015°C on 4H-SiC substrate with AlN buffer layer revealed, however, the high density of defects (threading dislocations $4.0\times10^{10}\mathrm{cm}^{-2}$ and basal stacking faults (BSFs) $1.6\times10^{6}\mathrm{cm}^{-1}$). We applied pendeo-epitaxy (PE) growth on such substrates in order to see decrease of density of these defects. Uncoalesced and coalesced a-plane GaN layers with thicknesses 2μm and 12μm, respectively have been studied. Our results show decrease of threading dislocation density from $4.4\times10^{10}\mathrm{cm}^{-2}$ to $2.0\times10^{8}\mathrm{cm}^{-2}$, and BSFs from $1.0\times10^{6}\mathrm{cm}^{-1}$ to $2.3\times10^{4}\mathrm{cm}^{-1}$ in 'seed' and 'wing' areas, respectively. These dislocations are mainly partial dislocations which terminate BSFs. Prizmatic stacking faults are also observed. Cross-section images reveal cracks and voids at the areas where two coalesced wings meet each other. Formation mechanism of these defects will be discussed in conjunction with epitaxial growth process.

E4.15

TEM Analysis of Mechanical Polishing Related Damage in Silicon Carbide. Joshua Russell Grim[1], M. Benamara[1], V. D. Heydemann[2], W. J. Everson[2] and Marek Skowronski[1]; [1]Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, Pennsylvania; [2]Electro-Optics Center, Pennsylvania State University, Freeport, Pennsylvania.

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 * 1010 dislocations / cm2 is produced. TEM analysis of the Burgers vectors indicates that the initial perfect dislocations have a burgers vector of +/- a/3 <1 1 -2 0> type then dissociates into a stacking fault bounded by two partial dislocation with burgers vector of +/- a/3 <1 -1 0 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 substrates exhibit threading dislocation pairs along scratches on the surface of the epilayer. The linear dislocation density along the scratch is 8 dislocations / micron.

E4.16

The Influence of Stoichiometry on Grown-in Point Defects and Impurities in PVT Growth 6H-SiC Single Crystals. Qiang Li[1], Alexander Polyakov[1], Mark Fanton[2] and Marek Skowronski[1]; [1]Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, Pennsylvania; [2]Pennsylvania 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.

E4.17

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

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

E4.18

Defect Characterization on CdTe Bulk Crystals Doped with Heavy Elements. Svetlana Neretina[1], N. V. Sochinskii[2], P. Mascher[1] and E. Saucedo[3]; [1]Center for Electrophotonic Materials and Devices (CEMD), Department of Engineering Physics, McMaster University, Hamilton, Ontario, Canada; [2]Instituto de Microelectronica de Madrid-CNM-CSIC, Madrid, Spain; [3]Material Physic Department, Universidad Autonoma de Madrid, Madrid, Spain.

Cadmium Telluride (CdTe) has been successfully employed as room temperature X-ray and gamma-ray detector material in markets such as medical and industrial imaging, security and monitoring, nuclear safeguards, non-destructive testing, and astrophysics. In order to provide stronger absorption and higher detection efficiency, investigated CdTe samples have been doped with heavy elements such as Bi, Yb, Ge:Yb, Tl, and Hg of different concentrations. However, dopants often form defect complexes, for example vacancy-impurity complexes, which act as carrier trapping and recombination centers and deteriorate the device performance. For this work, defect structure and luminescence properties of a variety of doped samples have been studied by Positron Lifetime Spectroscopy (PLS) and low-temperature photoluminescence (PL). The possible correlation between the PLS results and PL will be discussed. Photoluminescence 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 doping. We have correlated the relative intensity of PL bands associated with recombination process involving defects with 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 Challenge Fund (ORDCF) 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 Hommerich[1], Althea G. Bluiett[1], Ivy K. Jones[1], EiEi Nyein[1], Sudhir Trivedi[2] and Ramesh T. Shah[3]; [1]Dept. of Physics, Hampton University, Hampton, Virginia; [2]Brimrose Corporation, Baltimore, Maryland; [3]Applied 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 doping or through a thermal diffusion process. All 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 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 (b) through Dq 1/b5. 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 CdTe and ZnTe. 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+ centers, most likely due to Cr2+ ions entering into substitutional Zn and Cd lattice sites. The obtained results will be discussed in terms of possible applications of Cr: CdZnTe in IR solid-state lasers and for passive optical Q-switches.

E4.20

Relaxation Mechanism of SiGe Thin Film on SOI Substrate. Zengfeng Di[1,2], Miao Zhang[2], Weili Liu[2], Ming Zhu[1,2], Chenglu Lin[2] and Paul K. Chu[1]; [1]Physics & Materials Science, City University of Hong Kong, Kowloon, Hong Kong; [2]The 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 Si layer exclusively, 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, SiO2 is not expected to be viscous, and so the strain ratio is reduced in a linear fashion between 600°C and 900°C. When the annealing temperature becomes higher (for instance, 1000oC that is 58.5% of its melting point of 1710°C), the oxide can reflow and the SiGe/Si bilayer behaves like a 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 Bouville[1], Dongzhi Chi[1], Shenyang Hu[2], Long-Qing Chen[2] and David J. Srolovitz[3]; [1]Institute of Materials Research and Engineering, Singapore, Singapore; [2]Department of Materials Science and Engineering, Pennsylvania State University, University Park, Pennsylvania; [3]Department 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 silicides) or germanium (germanides) is key to the performance in semiconductor devices. NiSi is a candidate for replacing CoSi$_2$ because of its lower resistivity and its lower Si consumption, but is less stable at high T. As the NiSi grains agglomerate into islands *via* grain boundary grooving the film may lose connectivity. At elevated temperature a higher resistivity disilicide phase, NiSi$_2$, will form. We use phase field simulations to predict the evolution of the microstructure and morphology of the silicide film to determine the controlling mechanisms and key physical parameters to aid in metal silicide optimization. Diffusion, phase transformation, elastic energy, and interfacial energy all play important roles in the evolution. Experimental observations suggest that alloying Ni with Pt or implanting BF$_2$ increases the resistance of NiSi to agglomeration and delays the transition from NiSi to NiSi$_2$ to higher temperature. The mechanisms by which these species modify the agglomeration and phase transformations remain unclear. We test two possible mechanisms: additive modification of the (i) interface energies (which changes the wetting angles and hence the driving force for boundary grooving) and (ii) the relative stability of the phases. We suggest approaches to control 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 Lau[1], Alfred T. S. Tan[1], Nathan P. Sandler[2] and Taejoon Han[2]; [1]School of EEE, Nanyang Technological University, Singapore, Singapore; [2]Lam Research Corpoartion, 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 (ZBTSC) spectrocopy 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 approaches to reduce defect states. 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 nitridation before deposition helps to suppress Si/O 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. We can see clearly that Si/O 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. Dente[1,2], Michael L. Tilton[2], Andrew Ongstad[2] and Ron Kaspi[2]; [1]GCD Associates, Albuquerque, New Mexico; [2]Air Force Research Laboratory, Kirtland AFB, New Mexico.

Over the last decade, lasers, detectors and other optoelectronic devices exploiting the unique electronic properties of heterostructures and superlattices have been developed. In many cases, these devices contain extremely thin layers composed of just a few atomic layers of semiconductor material. For this reason, pseudopotential approaches have often been implemented as more accurate alternatives to envelope function approaches for calculating the electronic and optical properties of these structures. [1,2,3] In our superlattice empirical pseudopotential method (SEPM), we make the critical assumption that the heterointerface charges redistribute, forming charge and dipole sheets near the interface in order that the constituent pseudopotentials remain as unperturbed as possible. This assumption allows us to form the potential of the superlattice using only the pseudopotential form factors for the constituent materials, as well as a band offset for each constituent pair. [2] These form factors are determined by fitting the band diagram of each material in the superlattice. This represents a considerable reduction in parameters when compared to other pseudopotenial methods for superlattices, and most importantly, the SEPM does not require an interpolation between the form factors of the constituent materials. [3] To date, all applications of the SEPM have been successful, accurately predicting the measured subband energies in a wide variety of Type-I and Type-II superlattice samples. [1,2,4] In this presentation, we will provide a self-consistent calculation that supports the SEPM construction, proving that SEPM accurately represents the lowest-energy configuration for the many-electron superlattice. We consider a two-component superlattice made up of a material A and a material B. First, we self-consistently solve for the valence electrons interacting with the bulk A-core lattice, arriving at a self-consistent potential for the material A. Next, using the identical method, we solve for the self-consistent many-electron potential for the material B. Finally, we solve for the self-consistent one-monolayer/one-monolayer superlattice potential by solving the many-electron problem on the superlattice ion-core lattice made up of alternating A and B cores; this result represents the true potential of the superlattice. We then use the SEPM prescription, as well as the calculated A potential and the B potential to form the SEPM approximation to the true superlattice potential. Upon comparing the SEPM result with the true potential of the superlattice, we find essentially perfect agreement. [1] G. C. Dente and M. L. Tilton, J.Appl. Phys., Vol. 86, no. 3, 1420-1429, (1999). [2] G. C. Dente and M. L. Tilton, Phys. Rev. B 66, 165307 (2002). [3] D. M. Wood, A. Zunger, Phys. Rev. B 53, 7949 (1995). [4] A. P. Ongstad, et. al., J. Appl. Phys., Vol. 89, no. 4, 2185-2188, (2001).

E4.24

Point Defects Interaction with Extended Defects and Impurities in the Si-SiO2 System during the Process of its Formation. Daniel Kropman, Uno Abru, Tiit Karner, Ylo Ugaste, Enn Mellikov, Marit Kauk, Ivo Heinmaa and Ago Samoson; Estonian Maritime Academy, Tallinn, Estonia.

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-monotonous. This indicates that interaction between point defects, extended defects and impurities occurs in the Si-SiO2 system during the process of its formation. The purpose of the present work is to investigate the dependence of point defects generation kinetics on the oxidation condition and its influence on some structural and electro-physical properties of the Si-SiO2 system by means of EPR, nuclear magnetic resonance (NMR), surface photovoltage spectra (SPV) and MOS capacitance technique. It has been established that EPR and SPV (0.49 eV) signal intensity dependencies on the oxide thickness reveal a minima or a maxima depending on the oxidation ambient (impurity content). Surface states Ec-0.49eV are identified as interstitial Si atoms. We suggest that simultaneous decrease of the EPR and SPV signals 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 prepared on n- and p-type wafers grown by CZ and FZ methods, respectively, coinside 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. The extent of this effect goes up with the extent 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 condition.

E4.25

Modelling the MOS Device Conductance Using an Extended Tunnelling Model and Subsequent Determination of Interface Traps. Nikolaos Konofaos, Computer Engineering and Informatics Dept., University of Patras, Patras, Achaia, Greece.

Admittance spectroscopy measurements on Metal-Oxide-Semiconductor (MOS) devices allow the determination of electronic states at the oxide/semiconductor interface. The contribution of the AC conductance on the measurements allows the calculation of the interface traps density and the relevant time constant. As shown in recent articles, two equivalent model approaches can be applied in order to explain the experimental results. One model is the classical statistical model based on the Shockley-Read-Hall (S-R-H) recombination statistics and the other one is a model based on the quantum tunneling effect. Recent evidence suggest that the tunneling model can be equivalent to the statistical one if a continuum of states 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 attenuation mechanisms are considered as parts 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 existence of a continuum of states distributed at 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 P_b Centers. Felice Friedrich, Christoph Boehme and Klaus Lips; Silizium-Photovoltaik, Hahn-Meitner-Institut, Berlin, Germany.

P_b defects at the (111) oriented crystalline silicon (c-Si) to silicon dioxide (SiO_2) interface are strongly localized, paramagnetic point defects whose energy level is distributed throughout the Si bandgap. Because of this, P_b defects are important trapping and recombination centers of the c-Si/SiO_2 interface. In this study, we present low temperature pulsed electrically detected magnetic resonance (pEDMR) measurements of charge trapping and recombination at paramagnetic P_b 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 P_b 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, they can be paramagnetic. The data reveals that the Landé factor difference of the two electrons within these pairs are almost vanishing in X Band ($< 50\ \mu$T) and that they are, within the measurement accuracy, identical to the Landé factor of the uncharged, singly occupied P_b center. We conclude that trapping and recombination at P_b 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 defects at the c-Si/SiO_2 interface can be explained by readjustment out of different spin configurations of P_b defects. What remains is the question of why different paramagnetic species such as uncharged P_b centers in the ground state ($S = 1/2$) exhibit identical Landé factors and an identical anisotropy as charged two electron ($S = 1$) P_b centers in triplet configurations.

E4.27

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

Strained and relaxed Si and SiGe thin films are expected to play an increasingly important role in CMOS in the near future due to the increased electron and hole mobility expected in strained channels. 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 and ion-implantation followed by annealing has shown the most promise. 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 mechanisms. 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 Phen and Kevin Jones; University of Florida, Gainesville, Florida.

Stress has become an increasingly important parameter in semiconducting 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 Cluster (BIC) formation. These dopant-defect clusters are inactive immobile species which decrease the active concentraiton of carriers in semiconducting devices. 300mm n-type CZ grown silicon wafers were implanted with bost at a dose of 1x10^{15} atoms/cm^2 and energy of 500eV. The wafers were cleaved into 13cm x 1cm sample strips and were subsequently subjected to a 4 point bend which induced 150-250 MPa of tensile or compressive forces in the implanted layer. The strained samples were then annealed in temperatures ranging from 500-700°Cfor times ranging from 10-60 minutes under a N_2 ambient. This temperature range is within the region where reverse annealing phenomenon occurs in boron and BIC formation is predominant. Hall Effect measurements will be used to support SIMS data. Also, plan-view Transmission Electron Microscopy willb eused to study how the interstitial population changes with applied stress.

E4.29

Modeling of Germanium/Silicon Interdiffusion in Silicon/Silicon Germanium Heterostructures.
Mohammad 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 a Si/SiGe/Si single quantum well (SQW) structure can be detrimental to device performance. Thus it is important to develop predictive models for interdiffusion phenomena in heterostructures. In this work, the vacancy flux model [1] is implemented using the FLOOPS-ISE process simulator and used to simulate previously published data [2] on Si-Ge interdiffusion Si/$Si_{0.85}Ge_{0.15}$/Ge SQW structures grown by MBE and annealed at 900°C, 1000°C, and 1100°C for different anneal times in inert and oxidizing ambients. Our implementation of the model takes into account the conservation of lattice site density to relate the vacancy flux to the flux of the two diffusing species. We also account for the dependence of the vacancy equilibrium concentration and the intrinsic diffusivities of Si and Ge on the Ge fraction. Table 1 lists the values of intrinsic self diffusivities of Si ($D_{Si}{}^{int}$) and Ge ($D_{Ge}{}^{int}$) as functions of temperature and Ge fraction compared with published values [3]-[6]. In all cases, values of $D_{Ge}{}^{int}$ and $D_{Si}{}^{int}$ 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 $D_{Ge}{}^{int}$ and $D_{Si}{}^{int}$ 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 high temperatures (1100°C and above) other diffusion mechanisms (e.g. an interstitial mechanism) might play a major role for interdiffusion to occur. References [1] C.-Y. Tai, Ph.D Thesis, Stanford University, CA, 1997. [2] M. D. Griglione, Ph.D thesis, University of Florida, 1999. [3] N. R. Zangenberg et al., Phys. Rev. Lett. 87, 125901 (2001). [4] B. L. Sharma, Defect and Diffusion Forum, 70 & 71, 1 (1990). [5] R. J. Borg, and G. J. Dienes, An introduction to solid state diffusion, (Academic Press, Boston, 1998). [6] P. Laitinen et al., Phys. Rev. Lett. 89, 85902 (2002).

E4.30

Trisilane Based Epitaxy of Biaxially Stressed Silicon Films Doped with Carbon and Arsenic for CMOS Applications.
Matthias Bauer[1], Stefan Zollner[2], David Theodore[2], Michael Canonico[2], Pierre Tomasini[1], Bich-Yen Nguyen[2] and Chantal Arena[1]; [1]ASM America Inc., Phoenix, Arizona; [2]Freescale Semiconductor, Tempe, Arizona.

Arsenic doped Si:C films were grown epitaxially using RTCVD from trisilane, monomethylsilane and arsine as source gases with growth rates as high as 200, 90 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 5-6E20 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 5.334 $\AA$, 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 Kelires et. al. Films with a low thickness-stress product show pronounced interference fringes in x-ray or spectroscopic ellipsometry spectra, while these fringes are significantly broadened in films with larger thicknesses or higher carbon concentrations. Nevertheless, (224) grazing exit reciprocal space maps show the full tetragonal strain tilt expected from the C content, i.e., no relaxation of the films has occurred. The Si:C (004) and (224) Bragg peaks in reciprocal space show considerable broadening in the latter films, indicating the presence of periodicity-breaking defects, which do not relax the strain. Spectroscopic ellipsometry spectra were acquired in the 0.74 to 6.6 eV photon-energy range. For Si:C alloys without As, the E1 critical point shows the expected blueshift due to the doping of Si with C. For Si:C:As, there is a strong broadening of the E1 and E2 transitions due to the scattering of Bloch electrons in the crystal by As dopants. Additionally, free carrier effects lead to a decrease (increase) of the real (imaginary) part of the dielectric function in the near-infrared, consistent with a free carrier concentration in excess of 5E20 cm-3. UV Raman and FTIR transmission spectroscopy show a softening of the Si-Si vibration due to the addition of carbon, accompanied by a weak Si-C vibration at 605 cm-1, and a broad band at 480-490 cm-1 (a-Si mode) due to disorder and defects. TEM of 37 nm thick As doped Si0.977C0.023 showed single-crystal epitaxial growth. Occasional defects were present, consisting of microtwins nucleating partway up the layer. Such defects can arise as a consequence of increasing strain-energy as the film grows thicker.

E4.31

Transmission Electron Microscopic Studies of Strained Si CMOS. Qianghua Xie[1], Peter Fejes[1], Mike Kottke[1], Xiangdong Wang[1], Mike Canonico[1], David Theodore[1], Ted White[2], Mariam Sadaka[2], Victor Vartanian[2], Aaron Thean[2], Bich-Yen Nguyen[2], Shawn Thomas[4], Ran Liu[5] and Alex Barr[3]; [1]Physical Analysis 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]Embedded Systems 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. Thus, stress-related defect generation can great impact device reliability. In this paper, we present data on the correlation between defect density and leakage current for conventional strained Si CMOS devices on bulk substrates. Various types of defects (threading 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. Germanium upper-diffusion has been studied by scanning transmission electron microscopy (STEM). SGOI-devices processed using optimized thermal budget show minimal Ge diffusion and minimal process related defects. These SGOI devices show improved speed and drive current together with good device reliability (e.g. hot-carrier-leakage and negative-bias-temperature-instability).

E4.32

Device Parametric Shift Mechanism Caused by Boron Halo Redistribution Resulting from Dose Rate Dependence of SDE Implant. Ukyo Jeong, Jinning Liu, Baonian Guo, Kyuha Shim and Sandeep Mehta; Varian Semiconductor Equipment Associates, Gloucester, Massachusetts.

Change in sheet resistance was observed for Arsenic source drain extension (SDE) implants when they were performed at various dose rates. The high dose SDE implant amorphizes the surface of the silicon substrate and the thickness of the amorphous layer is strongly influenced by the rate of dopant bombardment. It is well known that the ion implantation process introduces excess interstitials. While the amorphous region is completely re-grown into single crystal during subsequent anneal without leaving behind extended defects, interstitials that are injected beyond the amorphous layer lead to formation of {311} defects or dislocation loops in the end of range region. During thermal processing, these extended defects dissolve, release interstitials, which in turn lead to transient 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; Physics, University of Wurzburg, Wurzburg, Germany.

The HgTe/HgCdTe superlattice (SL) is of fundamental interest as well as potentially a useful material for infrared opto-electronic devices[1]. The initial interest in these SLs was fueled by the possibility of a more accurate production of the desired cut-off 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 $\lambda = 17.0 \pm 1.0$ μm at 40 K as desired for some space applications, requires a Cd concentration given by $x = 0.206 \pm 0.002$. In other words it requires the Cd concentration to be maintained with a precision better than 1.0 %, a difficult task. The same wave length criterion can be satisfied with a HgTe/HgCdTe SL with a HgTe well width of 4.8 nm and a 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 HgTe and HgCdTe; the perpendicular electron effective mass, $m\_\perp\hat{*}$, can be increased by increasing the HgCdTe barrier layer thickness. However, the desired vertical transport provides a practical limit for $m\_\perp\hat{*}$. For example, a possible trade off given by $m\_\perp\hat{*} = 10\ m\_\|\hat{*} = 0.16\ m\_0$, can be chosen by selecting a HgCdTe barrier width of 5.0 nm. These SLs have recently been employed in very long wave length photovoltatic detectors[2,3]; even though more work on p-type doping questions concerning diffusion, etc. is required. [1] J. N. Schulman, and T. C. McGill, Appl. Phys. Lett. 34, 663 (1979). [2] Y. D. Zhou, C. R. Becker, Y. Selamet, Y. Chang, R. Ashokan, R. T. Boreiko, T. Aoki, D. J. Smith, A. L. Betz, S. Sivananthan, J. Electr. Mat. 32, 608 (2003). [3] Y. Selamet, Y. D. Zhou, J. Zhao, Y. Chang, C. R. Becker, R. Ashokan, C. H. Grein and S. Sivananthan, J. Electr. Mat. 33, 503 (2004).

E4.34

Impact of Small Miscuts of (0001) Sapphire on the Growth of AlxGa1-xN /AlN Superlattices with AlN Buffer Layer. Zheng Gong, Wenhong Sun, Jianping Zhang, Mikhail Erikovich Gaevski, Hongmei Wang, Jinwei Yang and Asif Khan; Electrical Engineering, University of South Carolina, Columbia, South Carolina.

Recently, several groups including ours have reported deep ultraviolet light-emitting diodes (UVLEDs) over sapphire substrates with emission wavelength from 300 to 250nm. For all the reported UVLEDs one key design is the use of defect-reduction, crack-elimination and strain-management AlN/AlGaN superlattice (SL) which was first proposed and employed by us to enable the growth of thick high-quality n+-AlGaN cladding layers and AlGaN/AlGaN multiple quantum wells (MQWs)[1,2]. To date, limited work has been completed to understand the relationships between the quality of AlGaN/AlN SLs and the miscuts of basal-plane sapphire substrates. In this paper, using chemical etching, atomic force microscope (AFM) and High- resolution X-ray diffraction (HRXRD), we report a study of the effect of various small miscuts of (0001) sapphire substrate (<1°) and the way to further improve the material quality. A set of AlN epilayers and AlN/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 7×106 cm-2 for normal-oriented (0°-off) from the starting value of 7×107 cm-2 for 0.5°-off. The dislocation densities exacted from XRD Williamson-Hall Plot are consistent with the chemical etching method. We found the surface morphologies can be easily controlled by the different substrate miscut angles. The 1-2 Monolayers (MLs) step flow morphology for normal- oriented 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 *Å* with a 5umX5um scan. Thermal dynamics and kinetics during the growth are the key factors that are responsible for the surface morphologies. This finding may help enhance the quality of full structure UVLED material and eventually improve the lifetime of the devices. [1] A. J. Fischer, A. A. Allerman, M. H. Crawford, K. H. A. Bogart, S. R. Lee, R. J. Kaplar, W. W. Chow, S. R. Kurtz, K. W. Fullmer, J. J. Figiel, Appl. Phys. Lett. 84 3394 (2004). [2] W. H. Sun, J. P. Zhang, V. Adivarahan, A. Chitnis, M. Shatalov, S. Wu, V. Mandavilli, J. W. Yang, M. A. Khan, Applied Physics Letters 85, 531(2004).

E4.35

Magnetic and Transport Properties of Ge: Mn Granular System. Wu Yihong[1,2], Li Hongliang[1,2], Liu Tie[1,2], Wang Shijie[3] and Guo Zaibing[2]; [1]Electrical and Computer Engineering, National University of Singapore, Singapore, Singapore; [2]Data Storage Institute (DSI), Singapore, Singapore; [3]Institute of Materials Research and Engineering (IMRE), Singapore, Singapore.

Among the different types of diluted magnetic semiconductors (DMSs) which are being intensively studied, the Ge-based group IV system has received much attention because of its simple structure and ease in fabrication. A Curie temperature of 285 K [1] has been reported for epitaxially grown samples. However, it is still not clear if the ferromagnetic properties originate from carrier-mediated ferromagnetism or are due to the clusters of GeMn phases. In this work, we fabricated thin films containing GeMn nanocrystallites in an amorphous host matrix, using MBE at a base pressure of 10^{-8} Torr. The typical substrate temperature, growth rate and film thickness are 573 K, 3nm/min and 35 nm, respectively. Both TEM and Raman observations show that the thin film is polycrystalline embedded in an amorphous host matrix. The ZFC and FC measurements showed a Curie temperature of about 285 K, suggesting that the nanocrystallites are either Ge_3Mn_5 or $Ge_{11}Ge_8$. The M-H curves show clear hysteresis up to 280 K. A typical semiconductor behavior has been observed in the temperature-dependent resistivity. The I-V curves measured by a 4 probe technique show a nonlinear behavior in temperature range from 10 K to 300 K, which might be caused by the formation either Schottky junctions at the nanocrystallite / amorphous interface or tunnel junctions between the nanocrystallies. A weak zero-bias anomaly was also observed in the dI/dV curve when the sample is cooled to below 30 K. We are now fabricating the thin films into nanowires with different widths so as to study their electrical transport properties and correlate them with magnetic counterparts. [1] Sunglae Cho et al., Phys. Rev. B 66, 033303 (2002)

E4.36

Radiative Versus Nonradiative Decay Processes in Germanium Nanocrystals Probed by Time-resolved Photoluminescence Spectroscopy. P. K. Giri[1], R. Kesavamoorthy[2], B. K. Panigrahi[2] and K. G. M. Nair[2]; [1]Department of Physics, Indian Institute of Technology Guwahati, Guwahati, Assam, India; [2]Materials Science Division, Indira Gandhi Center for Atomic Research, Kalpakkam, Tamil Nadu, India.

Si and Ge nanocrystals (NCs) have attracted much interest because of their potential application in Si-based optoelectronics, nanophotonics, and electronic/optical memory devices. In contrast to Si NCs, Ge NCs exhibit direct band gap nature and stronger confinement effects and has great potential for optoelectronic and memory device applications. However, 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 room temperature photoluminescence (PL) from ion-beam synthesized Ge NCs embedded in SiO_2 using steady state and time resolved PL measurements. Ge nanocrystals of diameter 4-13 nm were grown embedded in thermally grown SiO_2 layer by Ge ion implantation and subsequent annealing. X-ray diffraction and Raman (optical and low frequency) measurements were performed to study the evolution 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 SiO_2 matrix. Time-resolved PL studies reveal double exponential decay dynamics in the nanoseconds time scale. The faster component of the decay with time constant t1 3.1 ns is attributed to the nonradiative lifetime, since the time constant reduces with increasing defect density. The slower component with time constant t2 10 ns is attributed to the radiative recombination at the Ge nanocrystals. Our results are in close agreement with the theoretically predicted radiative lifetime for small Ge NCs. Thes results suggest that the defects at the surface of the Ge NCs primarily control the light emission and vibrational properties of the Ge NCs.

E4.37

Direct Measurement of Ion Beam Induced, Nanoscale Roughening. Bentao Cui[1,2], Phillip I. Cohen[2] and Amir M. Dabiran[3]; [1]Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, Minnesota; [2]Department of Electrical and Computer Engineering, University of Minnesota, Minneapolis, Minnesota; [3]SVT Associates, Inc, Eden Prairie, Minnesota.

Periodic nano-patterns, such as ripple, dots, or dimples, can be produced by ion bombardment of a surface. The driving forces for this ion induced nanopattern formation typically include the curvature dependence of the sputter yield in the Bradley-Harper (BH) mechanism, the asymmetrical attachment kinetics of mobile surface defects at steps (Ehrlich-Schwoebel barriers), and surface stress relaxation. The BH mechanism contributes the major driving force on the process of the nanopattern orientation. The asymmetrical attachment kinetics can be important in crystalline materials, determining the dimension of the nanopatterns. Surface stress is the major driving force to determine the shapes of the nanopatterns. The nanopatterns form round shapes in order to minimize the surface energy. For a specific materials system, such as Si or GaN, which of the three mechanisms will dominate during ion bombardment is still an open question. By studying the surface morphology change using real time in situ Reflection High Energy Electron Diffraction (RHEED), the dominant mechanism can be identified. GaN and patterned Si samples are used. A Kaufman ion source was used to supply sub-KeV ions from glancing incidence. AFM was used to examine the surface morphology post growth ex situ. The samples were rotated at 1.2 rpm to preclude ripple generation. Dimple structures with diameters ranging from 50 nm to 500 nm, have been produced using both argon ions and nitrogen ions with energies ranging from 100 -1200 eV at an ion flux of 3.6E14 ions/(sec*cm2). Using both RHEED and AFM we measure a minimum in the local roughness near 320 C. From the evolution of the dimple dimensions we obtain the first direct measurement of the curvature driven roughening. Rapid edge diffusion is required to explain the shapes of the observed roughening at low temperatures. This result suggests that the surface stress relaxation by annealing plays a key role during the ion-induced pattern formation. * Partially supported by the Air Force Office of Scientific Research.

E4.38

Elastic Stress Relaxation at Nanoscale: A Comprehensive Theoretical and Experimental Investigation of the Dislocation Loops Associated with As-Sb Nanoclusters in GaAs. Vladimir Chaldyshev[1], A. L. Kolesnikova[2], N. A. Bert[1] and A. E. Romanov[1]; [1]Ioffe Institute, Saint Petersburg, Russian Federation; [2]Institute 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 prismatic nanoscale dislocation loops nearby the nanoclusters. Our theoretical model explores the elastic properties of an inclusion with uniaxial dilatation. For such inclusions, the elastic stresses and stored energy are determined in a closed analytical form. The theoretical analysis predicts a specific non-linear dependence of the dislocation loop diameter on the cluster diameter, which fits well the experimentally observed one. It is demonstrated that both the change in the inclusion self energy 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.

E4.39

Defect-Induced Unoccupied Electronic States in Nanostructured SnO$_2$. Sergei O. Kucheyev, T. van Buuren, T. F. Baumann, Y. M. Wang, T. M. Willey, R. W. Meulenberg, J. H. Satcher, L. J. Terminello and A. V. Hamza; Lawrence Livermore National Laboratory, Livermore, California.

Tin dioxide is a wide band gap semiconductor whose technological applications largely depend on the electronic properties of both bulk and surface defects. In this presentation, we discuss the electronic properties of low-density monolithic nanocrystalline SnO$_2$ 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 O K as well as Sn $M_{2,3}$ and $M_{4,5}$ edges. In such measurements, we study the dependence of the element-specific partial 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 electron yield detection methods are used. Experimental results are also compared with PDOS calculations. Results show that both soft x-ray irradiation and the presence of undercoordinated surface atoms can induce Sn-related electronic states of f and d symmetry close to the conduction band minimum. These results demonstrate a successful application of XANES spectroscopy to study defect-related electronic states in wide band gap semiconductors. This work was performed under the auspices of the U.S. DOE by the University of California, LLNL under Contract No. W-7405-Eng-48.

E4.40

Infrared Spectroscopy of Impurities in ZnO Nanoparticles. W. M. Hlaing 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 hydrogen carbonate. IR spectroscopy showed the presence of CO$_2$ 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} (^{12}CO$_2$) and 2277 cm^{-1} (^{13}CO$_2$) varied according to the ^{12}C and ^{13}C concentrations. These results demonstrate conclusively that the impurities originated from the precursors. Isochronal annealing results revealed that the CO$_2$ molecules are stable even at elevated temperatures. The stability of the impurities is markedly different from that of CO$_2$ adsorbed on bulk ZnO surfaces, where the molecules are unstable at room temperature. By comparing our observations with studies of CO$_2$ trapped in carbon nanotubes [J. Physics. Chem. B **107**, 12930 (2003)], we conclude that the molecules are located inside the ZnO nanoparticles. In addition to unintentional CO$_2$ impurities, experiments were performed to intentionally introduce hydrogen into ZnO nanoparticles. Our results show that post-growth annealing in hydrogen ambient dramatically changes the IR transmission properties of the nanoparticles. This change is presumably due to the increase in free carrier concentration brought about by the introduction of hydrogen donors. A comparison between hydrogen in bulk and nanoscale ZnO will be made. This work was supported by the National Science Foundation and the ACS Petroleum Research Fund.

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

Chairs: S.R. Schofield and M. Tabe
Wednesday Morning, March 30, 2005
Room 2006 (Moscone West)

8:30 AM *E5.1

Electrical Transient Based Defect Spectroscopy in Polymeric and Organic Semiconductors. Yashowanta N. Mohapatra[3,2,1], Vishal Varshney[1], Vineet Rao[1,3], Samarendra P. Singh[3,1] and Girija S. Samal[2,1]; [1]Samtel Centre for Display Technology, Indian Institute of Technology Kanpur, Kanpur, U.P., India; [2]Materials Science Programme, Indian Institute of Technology Kanpur, Kanpur, U.P., India; [3]Department of Physics, Indian Institute of Technology Kanpur, Kanpur, U.P., India.

Organic semiconductors are emerging as attractive material base for many display and electronic applications, specially as light emitting diodes and thin film transistors. Though there has been considerable progress in device structures and materials, there is a lack of studies on relation between electrically active defects in these materials and degradation, which is necessary to understand trapping and other charge processes in these devices. In this paper, we study defect related charge processes using electrical transients in polymeric and organic diodes. We use popular light emitting diode structures consisting of ITO/PPV/CN-PPV/Al, and similar structures wherein the active layers are based on small molecules. We monitor slow charging and discharge currents as a function of time for both virgin and electrically aged devices. The current and charge transients are analyzed spectroscopically in time domain using a technique called Time Analyzed Transient Spectroscopy, which is similar to DLTS in its implementation. We observe highly stretched exponentials over 3-4 orders of magnitude in time up to thousands of seconds indicating existence of large distribution in time constants. In addition we are able to separate out distinctly trap-like sources of charge emission corresponding to localized states. We demonstrate both the need, and our ability to distinguish between 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 Priolo[1], Domenico Pacifici[1], Giorgia Franzo[1] and Fabio Iacona[2]; [1]Dept. Physics & Astronomy, MATIS-INFM & Univ. Catania, Catania, Italy; [2]IMM, 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 nanostructures has been shown to be one of the most promising methods. Indeed, light emission two orders of magnitude more efficient than in pure silica 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 amorphous 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 sensitizing centers. Aim of this work is to understand the details of the interaction mechanisms occurring between Si nanoclusters and the rare earth ions, with a particular attention to the Er-doped Si nanoclusters system. A model based on an energy level scheme taking into account the coupling between each Si nanocluster and the neighboring Er ions will be reported. Through a comparison with photoluminescence data, a value of 3x10-15 cm3 s-1 for the coupling coefficient has been determined. Moreover, an energy transfer time of 1 ms has been estimated, confirming that Si nanoclusters can actually play a crucial role as efficient sensitizers for Er. However, a strong cooperative up-conversion mechanism, active between two excited Er ions and characterized by a coefficient of 7x10-17 cm3 s-1, is shown to limit the Er excitation rate at high pump powers. The role of Si nanoclusters and of strong gain limiting processes, such as cooperative up-conversion and confined carriers absorption from an excited nanocluster, in determining positive gain at 1.54 mm will be investigated in details, and the implications of the finite transfer time on the overall efficiency of the energy transfer mechanism will be discussed. In particular, due to the finite energy transfer time and to the sequential nature of the interaction mechanism, it is shown that pulsed excitation of the Er-doped Si nanoclusters system with time duration smaller than the tranfer time prevent all of the Er ions to be excited. On the other hand, under continuous wavelength excitation, as much as 30-40 Er ions can be excited by a single nanocluster, thus making it possible to obtain population inversion. The feasibility of efficient electrical pumping of both Si nanocrystals and rare earths doped Si nanoclusters embedded in light emitting diodes will be demonstrated. The impact of these findings on the future development of an all Si based microphotonics will be discuss

9:30 AM E5.3

Efficient Spin Injection from NiFe/CoFe into GaAs in Spin-LED Structures. Shin Kim[1], Jungho Choi[1], Donggi Choi[1], Eunsoon Oh[1], Yongju Park[2], Kyung Ho Shin[2], Kwang Yoon Kim[2] and Dong Geun Oh[3]; [1]Department of Physics, Chungnam National University, Daejeon, South Korea; [2]Korea Institute of Science and Technology, Seoul, South Korea; [3]Korea 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, transition due to bound exciton was dominant at lower temperatures and at higher temperatures free excitonic transition became dominant. The circular polarization of the free excitonic transition was about 15 % at 20 K, whereas that of the bound exciton was almost negligible. At relatively 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-elastic 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 *E5.4

Atomically-Precise Positioning of Phosphorus in Silicon using STM. Steven Richard Schofield[1,2], Neil J. Curson[2], Hugh F. Wilson[3], Nigel A. Marks[3], Oliver Warschkow[3], Frank J. Ruess[2], Toby Hallam[2], Phil V. Smith[1], Marian W. Radny[1], Michelle Y. Simmons[2], David R. McKenzie[3] and Robert G. Clark[2]; [1]School of Mathematical and Physical Sciences, University of Newcastle, Callaghan, New South Wales, Australia; [2]Centre for Quantum Computer Technology, School of Physics, University of New South Wales, Sydney, New South Wales, Australia; [3]Centre 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 result 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 (PH_3) molecules, which only adsorb to the regions of bare Si exposed by the STM tip [4], as proposed by Tucker et al. [5]. Finally, the individual P atoms from the adsorbed PH_3 molecules are incorporated into the top layer of the Si(001) surface using a thermally activated process where a P atom displaces a surface 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 PH_3 with Si(001). While this system has been studied using a variety of techniques over the past two decades, recent observations have revealed that this interaction is much more complex that previously thought [6]. We have combined atomic-resolution STM studies with detailed first-principles calculations to outline a mechanism for the dissociation of PH_3 and the substitutional incorporation of P to Si(001). Key results of this mechanism will be presented culminating with the demonstration of the incorporation of single P atoms into Si(001) with 1 nm precision. [1] S. R. Schofield, N. J. Curson, et al. Phys. Rev. Lett, 91, 136104, 2003. [2] B. E. Kane. Nature, 393, 133, 1998. [3] J. W. Lyding, et al. J. Vac. Sci. Technol. B, 12, 3735, 1994. [4] J. L. O'Brien, S. R. Schofield, et al. Phys. Rev. B, 64, 161401, 2001. [5] J. R. Tucker and T. -C. Shen. Solid-State Elec., 42, 1061, 1998. [6] H. F. Wilson, O. Warschkow, N. A. Marks, S. R. Schofield, et al. Accepted for publication in Phys. Rev. Lett. (2004)

10:45 AM *E5.5

Imaging Electrically Deactivating Defects in Si One Impurity at a Time. Paul Voyles[1], David Muller[2] and John Grazul[2]; [1]Materials Science and Engineering, University of Wisconsin, Madison, Madison, Wisconsin; [2]School 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 Sb-doped Si [1]. These images showed that the electrically deactivating defect in low-temperature MBE grown Sb-doped Si must contain only two Sb atoms. Further comparison of low-angle, strain sensitive ADF and high-angle Z-contrast images measured the off-site displacement of the Sb atoms due to the deactivating defects. These images lead to the proposal of a new deactivating defect, the donor-pair vacancy-interstitial complex [2]. Especially with new aberration-corrected STEMs, these techniques are generally applicable to imaging high-Z impurities in low-Z host crystals, one impurity at a time. [1] P. M. Voyles, D. A. Muller, J. Grazul, P. H. Citrin, and H.-J. L. Gossmann, Nature 416, 826 (2002). [2] P. M. Voyles, D. J. Chadi, P. H. Citrin, D. A. Muller, J. L. Grazul, P. A. Northrup, and H-J. L. Gossmann, Phys. Rev. Lett 91, 125505 (2003).

11:15 AM E5.6

Polysilicon Memory Switching: The Role of Crystalline Defects. Brad Herner, 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 biassing. The forward diode current at +2 V increases by 5 orders of magnitude after a +8 V pulse. A diode rectification ratio of 10^8 at ±2 V is achieved after high voltage pulse. When $TiSi_2$ is used to contact the p^+ cell diode terminal instead of TiN, and the silicon is crystallized after $TiSi_2$ formation, 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 (TiN contact) have a high density of silicon grain boundaries and twin defects, while diodes without memory switching ($TiSi_2$ contact) contain few grain boundaries or twin defects. The reduced defect density is consistent with C49 phase $TiSi_2$-seeded crystallization of silicon. 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 Raymund Taylor[1], Eric Stach[2], Ajay Malshe[4] and Gregory Salamo[3]; [1]Microelectronics-Photonics, University of Arkansas, Fayetteville, Arkansas; [2]Material Science, Purdue University, West Lafayette, Indiana; [3]Department of Physics, University of Arkansas, Fayetteville, Arkansas; [4]Department of Mechanical Engineering, University of Arkansas, Fayetteville, Arkansas.

It is widely known that the nucleation of epitaxial quantum dots is mediated by strain mechanisms. Nanoindentations are created in the GaAs(100) surface to act as strain centers for the controlled 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 mN) and low load (0.2-8 mN) indentation combined with transmission electron microscopy (TEM) characterization of the deformation mechanisms. The loads required to produce sub-150 nm width indentations in GaAs are in a lower regime of <0.2 mN. These loads approach incipient plasticity behavior of GaAs. At such low loads and small scale, the preparation of the sample for TEM becomes difficult and extremely so for cross-sectional TEM, as the indent is difficult to locate and image, and sample manipulation must be performed delicately to 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 nanoindents was studied by cross-sectional transmission electron microscopy. A focused ion beam system was 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, fracture, or phase 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 findings are being correlated to the growth of quantum dots on the indentation sites. The success of this work could lead to a relatively simple and inexpensive process for the development of various nanoelectronic-photonic devices, for example, on-chip optical communication using quantum dots.

11:45 AM E5.8

Hydrogen in GaMnAs: Engineering of Magnetism by Defects. Martin S. Brandt[1], Christoph Bihler[1], Hans Huebl[1], Sebastian T. B. Goennenwein[3] and Wladimir Schoch[2]; [1]Walter Schottky Institute, Garching, Germany; [2]Universitaet Ulm, Ulm, Germany; [3]TU 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, Bouanani-Rahbi, Lemaitre and coworkers as well as our group have shown that the hole concentration in this material can be adjusted independently from the concentration of Mn by post-growth incorporation of hydrogen. When hydrogen is introduced in concentrations similar to the Mn concentration, thin films of GaMnAs, which are ferromagnetic and metallic in their as-grown state, become semiconducting and paramagnetic in the hydrogenated state. FTIR experiments indicate that Mn-As-H complexes are formed, which lead to the observed passivation of the Mn acceptors. In this contribution, we address two important issues concerning H in GaMnAs: the lattice expansion upon hydrogen incorporation and the diffusion of hydrogen through GaMnAs. GaMnAs thin films grown 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 $\Delta a/a=0.6\mathrm{x}10^{24}\mathrm{cm}^3$[H]. This increase is markedly lower than the corresponding increase in hydrogenated Si:B of $2.4\mathrm{x}10^{24}\mathrm{cm}^3$[H], where H is incorporated in a bond-center position. This difference suggests that H is built into GaMnAs on a lattice site which leads to a small lattice dilatation only such as the antibonding site. The effective indiffusion of hydrogen is determined via measurements of the ferromagnetic resonance 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 mode upon hydrogenation and anneal and the comparison of these shifts to those found upon wet-chemical etching of the films show a critical balance between in- and out-diffusion at the temperatures used. Such brief hydrogenation treatments can be used to change the magnetic properties of the ferromagnetic thin films such as the magnetic anisotropy and therefore allow a magnetic device engineering via defects.

SESSION E6: Defects in Devices

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

1:30 PM *E6.1

Electronically Stimulated Degradation of Crystalline Silicon Solar Cells. Jan Schmidt[1], Karsten Bothe[1], Daniel Macdonald[2], James Adey[3], Robert Jones[3] and Derek Palmer[3]; [1]Institute of Solar Energy Research Hameln/Emmerthal (ISFH), Emmerthal, Germany; [2]Department of Engineering, Australian National University (ANU), Canberra, Australian Capital Territory, Australia; [3]School 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. 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, in silicon: (i) the dissociation of interstitial iron-substitutional boron ($\mathrm{Fe}_i\mathrm{B}_s$) pairs and (ii) the formation of recombination-active boron-oxygen complexes. In solar-grade multicrystalline silicon (mc-Si), the first mechanism is most relevant. This well-known process, which is linked to the degree of iron contamination in the material, can also be observed in single-crystalline iron-contaminated B-doped float-zone (FZ) and Czochralski (Cz) silicon and is not restricted to mc-Si. The second carrier lifetime degradation effect can be observed in metal-impurity-free B-doped Cz-Si rich in oxygen. This effect is attributed to the simultaneous presence of B_s and interstitial oxygen (O_i). Interestingly, as for the $\mathrm{Fe}_i\mathrm{B}_s$ dissociation, this degradation effect also occurs in the dark when minority-carriers are injected (e.g., by a forward-biased pn junction), leading to the conclusion that the degradation is caused by the presence of minority-carriers and that photons are not directly involved. However, in contrast to the $\mathrm{Fe}_i\mathrm{B}_s$-related lifetime degradation, which also occurs during annealing above 100°C, the latter degradation effect is fully reversible by annealing above 200°C, i.e., the degraded lifetime recovers during low-temperature annealing, making it relatively easy to distinguish between the two effects. 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 proposed defect reaction model [J. Schmidt and K. Bothe, Phys. Rev. B 69, 024107 (2004)] of the boron-oxygen degradation, in which a fast-diffusing oxygen dimer (O_{2i}) is trapped by B_s to form a $\mathrm{B}_s\mathrm{O}_{2i}$ complex, acting as a highly effective recombination center. Results of theoretical calculations using density functional theory show that $\mathrm{B}_s\mathrm{O}_{2i}$ is a bistable defect with a donor level in the upper half of the silicon band gap, in good agreement with the results of temperature- and injection-dependent lifetime measurements. Calculated activation energies for the dissociation and association of the $\mathrm{B}_s\mathrm{O}_{2i}$ 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 Sopori[1], Chuan Li[1], S. Narayanan[2] and Dave Carlson[2]; [1]National Renewable Energy Laboratory, Golden, Colorado; [2]National Renewable Energy Laboratory, Golden, Colorado; [3]BP Solar, Fredrick, Maryland; [4]BP 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 clustering 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 defected regions, which can be several millimeters in dimension and cover many grains. 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 photoresponse maps (LBIC) were generated to correlate local photoresponse/recombination properties with the cell performance. The theoretical modeling was done using a Network Model, which synthesizes a large-cell from a large number (1600) 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 dislocation density. The output of the model consists of terminal I-V characteristics of the total cell and spatial distribution of cell voltages and currents for any terminal voltage. Excellent agreement between calculated and the measured cell parameters was obtained. The salient results of our analysis are: (i) Defect clusters are the primary sites of impurity precipitation, and hence are not gettered 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 dissolved impurities only), and cell processing technology. (vi) Defect clusters 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 E6.3

Silicon Wafer Defect Self-Characterization with CCD Image Sensors. William C. McColgin, Alexa Perry, Dean J. Seidler and James P. Lavine; Image Sensor Solutions, Eastman Kodak Company, Rochester, New York.

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 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 upward along crystalline axes 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 show that working pixels can be made atop such defects, but that high dark 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 inwards from the wafer edge with reduced dark current along the slip line, but with a small cluster of brighter pixels at the ending dislocation. Faint arc patterns can sometimes be observed in the imager dark current. If images are taken from each imager on the wafer, the arcs 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 rings in n epi on n wafers and p epi on p+ wafers, including silicon from different wafer vendors. Striations in imagers have been previously reported,[1] but the explanations do not seem to apply in our case. We will show the extent to which these dark-current rings can be correlated with substrate properties. [1] L. Jastrzebski, P.A. Levine, A.D. Cope, W.N. Henry, and D.F. Battson, "Material Limitations Which Cause Striations in CCD Imagers," IEEE J. of Solid-State Circuits **SC − 15**, 759 (1980).

2:30 PM E6.4

Silicon Light Emissions from Boron Implant-Induced Extended Defects. Grant Z. Pan[1], Roman P. Ostroumov[2], Yaguang Lian[1], Liping P. Ren[3] and Kang L. Wang[2]; [1]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]Nanoelectronics and Nanophotonics Laboratory, Global Nanosystems, Inc., Los Angeles, California.

Efficient silicon light-emitting diodes (Si LEDs) can allow integration of optics with electronics in high-density Si nanoelectronic integrated circuits [1]. It was reported that a planar p-n junction Si LED integrated with boron implant-induced extended dislocation defects could have quantum efficiency as high as 10^{-3} [2]. There are types of extended defects that evolve during the post implant anneal [3]. Depending on implant parameters and annealing conditions such as the ion spices, energy, dosage, and annealing temperature and time, the defects may be interstitial clusters, {113} 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 electroluminescence (EL) and photoluminescence (PL) of boron-implanted p-n junction silicon light-emitting diodes in correlation with the implant-induced defects of different types. By varying the post implant annealing conditions to tune the extended defects of different types and by using plan-view transmission electron microscopy (PTEM) to identify them, we found that {113} defects along <110>Si are the ones that result in strong silicon light emission of the p-n junction Si LEDs other than {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 finding, for the first time, is highly significant in the development of high efficient defect-engineered Si 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 edge radiative recombination. The high emissions resulting from the extended {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 by localizing them in the damage-repaired defect-free regions. 1. L.C. Kimerling, The Electrochemical Society Interface **9**, 28 (2000). 2. W.L. Ng, M.A. Lourenco, R. M. Gwilliam, S. Ledain, G. Shao and K.P. Homewood, Nature **410**,192 (2001). 3. G.Z. Pan and K.N. Tu, J. Appl. Phys. **82**, 601 (1997).

3:15 PM E6.5

Conductivity Enhancement in Thin Silicon-on-Insulator Layer Embedding Artificial Dislocation Network. Yasuhiko Ishikawa[1], Kazuaki Yamauchi[1], Ratno Nuryadi[1], Hiroya Ikeda[1], Michiharu Tabe[1], Yukinori Ono[2], Masao Nagase[2], Masashi Arita[3] and Yasuo Takahashi[3]; [1]Research Institute of Electronics, Shizuoka University, Hamamatsu, Japan; [2]NTT Basic Research Laboratories, Atsugi, Japan; [3]Graduate School of Information Science and Technology, Hokkaido University, Sapporo, Japan.

Formation of nanometer-scale potential-arrayed structures is important for ultrasmall 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 effect of the periodic structure, or perhaps the periodic potential, on the conduction property is examined. The dislocation network sandwiched by thin Si layers was artificially formed using a wafer bonding of a pair of (001) Si-on-insulator (SOI) wafers, which had the top p-Si layer (10 ohm cm) of 25 - 180 nm on the buried SiO_2 (BOX) layer of 400 nm. Since no SiO_2 layer was inserted at the bonding interface, a periodic array of screw dislocations was induced at the Si-Si bonding interface due to 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 SOI structure was formed with the thin top Si layer (50 - 200 nm) embedding the dislocation network. The transmission electron microscopy clearly revealed the formation of dislocation network at the bonding interface in the top Si layer. Furthermore, the dislocation network was found to increase the conductivity of top Si layer 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 current path around the dislocations, although the effect of *periodic* structure has not yet clarified. The MOSFETs using the Si layer embedding the dislocation network will be also presented. [1] J. L. Rouviere, K. Rousseau, F. Fournel and H. Moriceau, Appl. Phys. Lett. 77 (2000) 1135; Appl. Phys. Lett. 80 (2002) 4121.

3:30 PM E6.6

Physical Mechanisms of Negative-Bias Temperature Instability. Leonidas Tsetseris[1], X. J. Zhou[2], D. M. Fleetwood[2], R. D. Schrimpf[2] and S. T. Pantelides[1]; [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 underlying atomic-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 depassivate dangling bonds. Hydrogen release from dopants is greatly enhanced in the depletion region, when the substrate is driven into inversion, as happens under typical NBTI stress. The released hydrogen atoms can 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 effect of the drift of protons in the direction of the gate 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 address the effect of the polarity of the substrate (n-type or p-type), the polarity of the applied bias, and the possible role of water or hydrogen molecules, on the overall degradation.

3:45 PM *E6.7

Silicon Single-Electron Pump and Turnstile: Interplay with Crystalline Imperfections. Yukinori Ono[1], Yasuo Takahashi[2] and Hiroshi Inokawa[1]; [1]NTT Basic Research Laboratories, NTT, Atsugi, Kanagawa, Japan; [2]Graduate School of Information Science and Technology, Hokkaido University, Sapporo, Hokkaido, Japan.

The single-electron-tunneling device (SED), which has quantum dot(s) in its core, enables the control of electron motion on the level of an elementary charge. The single-electron pump and turnstile are members of the SED family and enable single-electron transfer syncronized with the gate clock. They have the potential for extremely low error rates of electron 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-K 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 charge pumping. We will then discuss the possibility of single-electron manipulation by single dopant levels in silicon. This work was supported by a Grant-in-Aid for Science Research from the 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[1], Mingqiang Bao[1], Kang L. Wang[1], XiaoLei Liu[2], Chao Li[2] and Chongwu Zhou[2]; [1]EE, UCLA, LA, California; [2]EE, USC, LA, California.

Self-assembled carbon nanotube (CNT) and nanowire field effect transistors (FETs) have been fabricated. However, atomic level interface imperfection and single defect can dramatically affect device performance in these nanoscale devices. In this work, giant random telegraph signals (RTSs) are studied in p-type semiconducting single wall carbon nanotube field effect transistors at various temperatures as a sensitive probe for characterizing the defects. CNT FETs were fabricated on silicon substrate covered with a 500 nm thermal oxide as the gate dielectric layer. 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 um. After the synthesis, photolithography was applied to define the source and drain electrodes on top of the nanotube, followed by Ti/Au deposition as the contacts. The following measurements were carried without electrically stressing on the gate of the device. Giant random telegraph signals are observed in p-type semiconducting SWNT field effect transistors. The characteristics of the RTSs are further analyzed under different gate (Vg) and source-drain (Vds) biases. The amplitude of the RTSs is up to 60% of the total current at 4.2K. 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 3nm). At certain gate biases, the observed RTSs show 4 levels of switching, and this effect is attribute 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 shown to relate to large low frequency (1/f) 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 for probing single defects with an excellent 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)

4:30 PM E6.9

A Comparison of Lattice-Matched GaInNAs And Metamorphic InGaAs Photodetector Devices. David Bryan Jackrel, Homan Yuen, Seth Bank, Mark Wistey, Junxian Fu, Xiaojun Yu, Zhilong Rao and James S. Harris; Solid State and Photonics Laboratory, Stanford University, Stanford, California.

The dilute-nitride GaInNAs shows great promise in becoming the next choice for 1 eV photodetector and multi-junction photovoltaic applications due to the ability for it to be grown lattice-matched on GaAs substrates. GaAs-based devices have several advantages over InP-based devices, such as substrate cost, convenience of processing, and optoelectronic band parameters. Metamorphic InGaAs is the current choice for 1 eV materials grown on GaAs substrates. However, rough interfaces and large numbers of point defects plague these devices due to the large concentration of misfit dislocations inherent to metamorphic structures. This talk will present results from high-power rear-illuminated photodetector devices fabricated from high-quality thick GaInNAs and metamorphic InGaAs materials grown by MBE. The absorbing layers of the rear-illuminated devices are directly adjacent to the heat sink thereby enhancing the thermal conductivity by orders of magnitude over conventional front-illuminated detectors. This results in devices with excellent linearity and potentially very high damage thresholds. The internal quantum efficiency of PIN photodiodes with thick GaInNAs films as the intrinsic region (roughly 50% at 1064 nm) is somewhat lower than comparable metamorphic InGaAs devices (roughly 90% at 1064 nm). However, the dark current density of the GaInNAs devices is also somewhat lower (roughly 10 μA/cm^2 at 5e4 V/cm bias) than the InGaAs devices (roughly 100 μA/cm^2 at 5e4 V/cm bias), while the breakdown voltages (beyond -20 V) are comparable. Materials characterization of each structure including photoluminescence studies, x-ray diffraction, deep-level transient spectroscopy, transmission electron microscopy, and surface roughness measurements will be presented in order to explain the characteristics observed in the devices composed of the two different material systems. It appears that increased compositional inhomogeneity in the GaInNAs material causes lower carrier mobilities, which leads to the lower device efficiencies as well as the lower dark current densities. However, the lower defect densities and cleaner interfaces present in the GaInNAs material could result in an overall improvement in device performance if the compositional inhomogeneity were reduced.

4:45 PM E6.10

A Novel Method to Synthesize Blue-luminescent Doped GaN Powders. Rafael Garcia[1], Abigail Bell[1], Fernando A. Ponce[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 electroluminescent lighting industry. Currently electroluminescent (EL) powders are based on ZnS:Cu,Cl and can be found in many applications including keypad lighting in cellular phones, automobile instrument cluster lighting, and as LCD backlights in small electronic devices. Current ZnS EL device efficiencies are not improving as fast as technology requires and so it is necessary to look at other semiconductors as possible alternatives. GaN is a very robust material with similar structural and electronic properties to ZnS. We have recently produced high quality undoped GaN powders with exceptional luminescent properties and also we have achieved Mg and Si doped GaN powders. The highly luminescent GaN powders have been grown by direct reaction between Ga and ammonia in a horizontal quartz tube reactor at 1100 °C. Si doped powders were prepared by reaction between a homogeneous 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 those 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 donor-acceptor pair band at 3.25 eV (380 nm). 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.

SESSION E7: Ion Implantation and Irradiation Effects
Chairs: S. Ashok and Y.N. Mohapatra
Thursday Morning, March 31, 2005
Room 2006 (Moscone West)

8:30 AM E7.1

Vacancy Engineering in Bulk and SOI Substrates for Ultra-Shallow Boron Junctions. Andy James Smith, Benjamin Colombeau, Russell Gwilliam, Nick Cowern and Brian Sealy; ATI, Surrey University, Surrey, United Kingdom.

In CMOS device generations beyond the 65 nm node the ultrashallow PMOS source-drain region will need to be activated to unprecedented levels, with boron concentrations well above the solubility values for conventional processing temperatures (<1100°C). This may be achieved either by ultrashort time processing at very high temperature, or by low-temperature nonequilibrium processing. Under normal circumstances implantation damage, whether in crystalline or preamorphised silicon, hinders boron activation and increases its diffusion, because boron clustering and diffusion processes are accelerated by the excess interstitials introduced by the implantation step. High-energy co-implantation, for example by silicon ions, can however reverse this trend by generating excess vacancies in the depth range of interest for ultrashallow junctions. This 'vacancy engineering' approach holds considerable promise for enhancing boron deactivation and junction steepness in boron ultrashallow junctions. In previous work we have shown that vacancy engineering in Silicon On Insulator may be even more effective in SOI than in bulk silicon wafers, because the buried oxide can separate the vacancyri−ch and interstitial-rich regions of the high-energy implant, ensuring maximum impact of the vacancy-rich region on boron implanted at lower energies. In this paper we will report a novel vacancy-engineering approach which can be applied to high-dose ultrashallow boron implants (1e15/cm2, 0.5−2keV). Results using this approach are characterised in terms of total atomic (SIMS) and electrical (high-resolution differential Hall) profiles, studied in both bulk and SOI material. The Hall measurements provide pairs of carrier concentration and mobility values as a function of depth, indicating the impact of the co-implant on boron substitutionality and material quality. RBS analysis is also performed to quantify the damage created. Our new approach enables diffusion to be suppressed and electrical activation to be increased by a factor of 30 or more at low temperature, leading to Rs / Xj values approaching those obtained by preamorphisation, without the presence of end-of-range defects. The new approach is compatible with process integration based on fully-depleted SOI, thus offering a clear perspective to meet the ITRS requirements for future CMOS technology generations.

8:45 AM E7.2

Diffusion and Clustering of Boron at High and Room Temperature. Enrico Napolitani[1], Davide De Salvador[1], Gabriele Bisognin[1], Alberto Carnera[1], Elena Bruno[2], Salvo Mirabella[2], Giuliana Impellizzeri[2] and Francesco Priolo[2]; [1]MATIS-INFM and Dipartimento di Fisica, Universita di Padova, Padova, Italy; [2]MATIS-INFM and Dipartimento di Fisica ed Astronomia, Universita di Catania, Catania, Italy.

The knowledge and control of dopants diffusion and electrical activation are crucial issues for the aggressive scaling down required by the future Si-based microelectronic devices. A key role is played by the interaction of dopants with point defects and impurities, as all the dopants diffuse in Si via a native defect mediated mechanism. In particular, the ion implantation process in crystalline silicon (c-Si) (which is widely used for several device production processes such as the doping itself) and post implantation annealing induce a huge injection of Si self-interstitial defects (I's). This promotes the well known Transient Enhanced Diffusion (TED) and clustering of boron, which are the most limiting phenomena for the junction scaling (and therefore also the most studied ones). Here we report on our recent experimental investigations on the formation and dissolution of B clusters generated by ion implantation in c-Si [1]. The I's were injected by Si ion implantation and annealing on B-delta- doped boron superlattices, grown by molecular beam epitaxy. We have investigated in details the migration of the I's and their interaction with B. I's are shown to diffuse, to interact with intrinsic traps (such as C), and to promote diffusion and/or clustering in intentionally grown Si layers with high concentrations of B. The mechanisms of the point defect diffusion, and of the formation and dissolution of boron clusters are quantitatively described in details and discussed comparing with the most recent theoretical calculations. Furthermore, we demonstrate that substitutional boron can migrate significantly even at room temperature (RT) and below, if stimulated by a high I flux [2]. We show that such effect occurs also during the analyses with the Secondary Ion Mass Spectrometry (SIMS) technique producing artifacts in the profiling of B deltas. Critically depending on the sample temperature, I's are injected by the sputtering beam, migrate for long distances, interact with B by producing mobile B species and eventually the mobile B migrates for long distances even at RT and below, producing significant tails in the B profiles. We have estimated, for the first time, the lower bound for the diffusivity of mobile B of 5x10^{-13}cm^2/sec at RT. Our data have a twofold implication. On one hand, they give significant insights on the migration and interaction of B and point defects at RT and below. On the other hand, this phenomenon, if not properly considered, induces an experimental artifact in the determination of B concentration profile by SIMS and therefore many of the observations obtained in the past might be revised. [1] S. Mirabella, E. Bruno, F. Priolo, D. De Salvador, E. Napolitani, A. V. Drigo, and A. Carnera, Appl. Phys. Lett. 83, 680 (2003). [2] E. Napolitani, D. De Salvador, R. Storti, A. Carnera, S. Mirabella, F. Priolo, Phys. Rev. Lett. 93, 055901 (2004).

9:00 AM *E7.3

Bubbles and Cavities Induced by Rare Gas Implantation in Silicon Oxide. Esidor Ntsoenzok[1], Hanan Assaf[1] and Marie Odile Ruault[2]; [1]CNRS-CERI, Orleans, France; [2]CSNSM, CNRS-IN2P3, Orsay, France.

Bubbles and cavities induced by light ions (mainly hydrogen and helium) have been widely studied in metals and semiconductors. Their applications to semiconductor technology include development of novel techniques such as the Smart-cut for semiconductor-on-insulator substrates and gettering of metallic impurities. However, thus far there have been no reports of bubble/cavity formation in spite of a large potential interest from both fundamental and applied perspectives. For instance, both low-k dielectrics and light emission technologies could benefit from the generation of nm-size cavities and gas-filled bubbles in SiO2 and other insulators. In this paper we will present the recent results obtained by our groups on rare gas implantation in SiO2. Characterization of implanted samples includes XTEM (cross section microscopy), RBS (Rutherford BackScattering) and PAS (positron annihilation spectroscopy). Some potential applications of these bubbles/cavities will also be discussed.

9:30 AM E7.4

Defects Induced by Helium Implantation: Impact on Boron Diffusivity. Frederic Cayrel[1], Daniel Alquier[1], Laurent Ventura[1], Christiane Dubois[2] and Robert Jerisian[1]; [1]LMP, University Francois Rabelais, Tours, France; [2]LPM, INSA, Lyon, France.

High dose helium implantation followed by a suitable thermal treatment induced defects such as cavities and dislocations. This technique is often used for the gettering of metallic impurities [1,2]. The interaction with dopants has also been evidenced within this defect layer. Evolution of the quantity of gettered dopant with regard to the defects involved has been investigated as a function of time, temperature, type and doping level [3,4]. Moreover, the presence of He-induced defects, both interstitial and vacancy type, influences dopant diffusion. Among the dopants, boron is of particular interest for realization of p-doped zones. Boron diffusion is known to be driven by interstitial mechanism. The presence of all these defects will inevitably affect the boron profile. In this work, we used N-type <111> Si wafers, uniformly doped at 1x10^{14} P.cm^{-3}. Helium implantations were performed at room temperature at [40-160]keV for doses of [1-5]x10^{16} He^{+}/cm^2. Wafers have been then implanted with boron (2x10^{13} B.cm^{-2} and 5keV). He implantation energy allows to localize the cavity band with regard to boron. Two set of experiments have been done: (i) helium and boron implantations at the same time (ii) helium implantation and annealing, to primarily form the defects, followed by the boron implantation. Classical thermal treatments are then applied under nitrogen in the temperature range of [500-1000]°C. A sample only implanted with boron is used as reference. Boron profiles were followed by Secondary Ion Mass Spectroscopy (SIMS) while the distribution and evolution of defects were studied by Transmission Electron Microscopy (TEM). Moreover, boron diffusion was evaluated by simulation using PROMIS 1.5 code. Our results enlighten the major impact of the defect layer on dopant diffusion. TED of boron, evidenced on reference samples, can be suppressed in presence of the defect band depending on implantation and anneal parameters. These results clarify the interaction of boron with He-induced extended defects. References: [1] S.M. Myers and D.M. Follstaedt, J. Appl. Phys 79 (1996), p. 1337. [2] V. Raineri, P.G. Fallica, G. Percolla, A. Battaglia, M. Barbagallo and S.U. Campisano, J. Appl. Phys. 78, (1995), p. 3727. [3] F. Cayrel, D. Alquier, D. Mathiot, L. Ventura, F. Roqueta, G. Gaudin and R. Jerisian, Nucl. Instr. and Meth. B 216 (2004) pp.291-296. [4] F. Cayrel, L. Vincent, D. Alquier, F. Cristiano, F. Roqueta, L. Ventura, C. Dubois and R. Jerisian, Solid State Phenom. Vol. 95-96 (2004) pp.599-604.

9:45 AM E7.5

Roles of Impurities and Implantation Depth on He+-Cavity Equilibrium Shape in Silicon. Gabrielle Regula[1], Marc Desvignes[3], Rachid El Bouayadi[1], Maryse Lancin[1], Esidor Ntsoenzok[2] and Bernard Pichaud[1]; [1]Laboratoire TECSEN, Marseille, France;

[2]CERI - CNRS, Orleans, France; [3]MECASURF, ENSAM, Aix-en-Provence, France.

Either spherical or facetted-cube-octahedric 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 getter metallic impurities and, thus, improve the electrical properties of microelectronic devices. Nevertheless, no one is actually able to predict the final cavity shape after a given experimental treatment. Our goal is to determine the eventual impact of both the surface proximity and the impurity chemisorption on the cavity morphology. For such a purpose, we implanted both as-grown and metal-diffused (Pt, Au, Ni) silicon with He+. The He+ projection range (Rp), derived by transport range of ions in matter (TRIM) simulations, was thus tuned from 90 nm to 5.6 microns by using 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 tunned-Rp. Consequently, the cavity nucleation and growth parameters are 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 673K to 1323K. Cross section transmission electron microscopy (XTEM) observations show that implantations in as grown silicon at Rp beyond 350 nm give facetted cavities, whatever the annealing temperature. On the contrary, cavities created at 90 nm close to the silicon surface exhibit rounded-shape for all He+ doses and annealing temperature studied. Besides, in metal-diffused silicon, the shape of the cavities is found to drastically depend on both the nature and the amount of the contaminant trapped at cavities. The latter was measured by secondary ion mass spectrometry (SIMS). A simple model based on the surface energy associated to a cavity [1,2] and a finite element method simulation of the von Mises stresses around a cavity 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, D. M Follsttaedt, Nucl. Inst. and Meth. B 127/128, 301 (1997)

10:30 AM E7.6

Theory of Fluorine-Induced Suppression of Transient Impurity Diffusion in Silicon. Vincenzo Fiorentini[1,2], Giorgia Lopez[1,2], Giuliana Impellizzeri[3], Salvatore Mirabella[3] and Enrico Napolitani[3]; [1]Dept. of Physics, University of Cagliari, Monserrato, Italy; [2]INFM-SLACS, Cagliari, Italy; [3]INFM-Matis, Catania, Italy.

The transient enhanced diffusion of acceptor impurities affects severely the realization of ultra-high doping regions in miniaturized Si-based devices. Fluorine co-doping has been found to suppress this transient diffusion, but the mechanism underlying this effect is not understood. It has been proposed that fluorine-impurity, or fluorine–native-defect interactions may be responsible. Here we clarify this mechanism by first-principles theoretical studies of fluorine in Si in connection with purposely-designed experiments on boron- and fluorine-containing Si structures. The central interaction mechanism is the preferential binding of fluorine to Si-vacancy 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 interstitial-assisted transient diffusion: however, in view of the efficient fluorine-vacancy mutual trapping, we suggest that fluorine will also suppress vacancy-assisted diffusion, which is most relevant for donors.

10:45 AM E7.7

Fluorine Behavior in Preamorphized Si: Segregation and Point Defect Interaction. Giuliana Impellizzeri[1], Salvatore Mirabella[1], Lucia Romano[1], Maria Grazia Grimaldi[1], Francesco Priolo[1], Enrico Napolitani[2] and Alberto Carnera[2]; [1]MATIS-INFM-University of Catania, Department of Physics and Astronomy, Catania, Italy; [2]MATIS-INFM-University of Padova, Department of Physics, Padova, Italy.

In recent years, there has been considerable interest in the effect of F on B diffusion in Si. In particular, F implanted in preamorphized Si is able both to suppress the B transient enhanced diffusion (TED) [1,2] and to improve the thermal stability of activated junctions [3]. The origin of these effects is a matter of current debate. To shed light upon these phenomena we undertook a detailed study about the F incorporation and diffusion in preamorphized Si. We investigated the F incorporation during the regrowth process by solid phase epitaxy (SPE) at different temperatures (580, 700 or 800 °C) and for several implanted F energies (65-150 keV) and fluences (0.07-5x10^{14} F/cm^2). We always observed a strong F segregation towards the surface, promoted by the relatively high F diffusivity in amorphous Si compared to the SPE rate. We measured a diffusion coefficient of (0.9±0.1)x10^{-14} cm^2/s at 580 °C. The above phenomenon is accompanied by a SPE rate retardation and to a consistent F loss through the surface. Moreover, the concentration of F incorporated in our samples increased by increasing the SPE temperature. In samples doped with B atoms (1x10^{14} B/cm^2, 10 keV), we observed also an anomalous F accumulation at the B implantation peak during the SPE process. As we demonstrated, with a custom-designed experiment, the absence of any B-F chemical bonding during SPE and post-SPE annealings [4], we believe that the above increased F incorporation is due to the increase of the SPE velocity induced by B. We investigated also the diffusion of F during a post-SPE thermal treatment. As already known, the amorphizing implant induces at the end of the implant range a defect-rich region, called end-of-range region (EOR), which acts as a source of self-interstitials (Is) during the post-SPE annealing. We evidenced a Fickian-deviated F diffusion mechanism 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 able also 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 boron 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. Mokhberi, R. Kasnavi, P. B. Griffin and J. D. Plummer, Appl. Phys. Lett. 80, 3530 (2002). [3] B. J. Pawlak, R. Surdeanu, B. Colombeau, A. J. Smith, N. E. B. Cowern, R. Lindsay, W. Vandervorst, B. Brijs, O. Richard and F. Cristiano, Appl. Phys. Lett. 84, 2055 (2004). [4] G. Impellizzeri, J. H. R. dos Santos, S. Mirabella, F. Priolo, E. Napolitani and A. Carnera, Appl. Phys. Lett. 84, 2055 (2004).

11:00 AM E7.8

Clustering Analysis in Boron and Phosphorus Implanted (100) Germanium by X-Ray Absorption Spectroscopy. Mehmet Alper Sahiner[1], Parviz Ansari[1], Malcolm S. Carroll[2], Yong S. Suh[3], Roland A. Levy[3], Temel H. Buyuklimanli[4] and Mark C. Croft[5]; [1]Physics, Seton Hall University, South Orange, New Jersey; [2]Sandia National Laboratories, Albuquerque, New Mexico; [3]New Jersey Institute of Technology, Newark, New Jersey; [4]Evans East, East Windsor, New Jersey; [5]Rutgers University, New Brunswick, New Jersey.

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 local structural 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 anneals. The (100) Ge wafers were implanted and with B or P using energies ranging from 20 keV to 320 keV and doses of 5x10^{13} to 5x10^{16}/cm2. Pieces of the implanted wafers were subjected to thermal annealing at 400^{o}C or 600^{o}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.

11:15 AM E7.9

X-ray Spectroscopy of InN Heavily Irradiated with He. Jonathan Denlinger[1], S. X. Li[2,3], R. E. Jones[2,3], K.-M. Yu[2], J. Wu[2,3], J. W. Ager III[2], W. Walukiewicz[2], E. E. Haller[2,3], Hai Lu[4] and William J. Schaff[4]; [1]Advanced Light Source, Lawrence Berkeley National Lab, Berkeley, California; [2]Materials Science Division, Lawrence Berkeley National Lab, Berkeley, California; [3]Materials Science and Engineering, University of California, Berkeley, California; [4]Dept. of Electrical and Computer Engineering, Cornell University, Ithaca, New York.

We show that irradiation of InN with 2 MeV He ions produces a highly conducting n-type material. Electron concentration saturates at about 4x10^{20} 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 band (VB) electronic structure of InN containing these very high concentrations of free electrons and defects. XAS, a probe of unoccupied CB states, shows a depletion of states near threshold absorption corresponding to free-carrier filling of the CB, and the creation of two new peaks for irradiated InN that correspond to (i) the N-vacancy defect level, and (ii) the formation of N-pairs. XES, a probe of occupied states, shows additional emission above the VB maximum, not present in non-irradiated InN, resulting from filled CB states and from elastic scattering. The elastic scattering intensity shows an enhancement for photon excitation at the localized defect level and the non-elastic CB emission is consistent with a band gap narrowing of ≈0.4 eV arising from free-carrier electron-electron and electron-ionized defect interactions. The results provide additional support for previously reported low energy gap and large Burstein-Moss shift in heavily doped InN [1]. [1] J. Wu *etal.*, Phys. Rev. B 66, 201403 (2002).

11:30 AM E7.10

Electronic and Optical Properties of High Energy Particle-Irradiated In-rich InGaN Alloys. Sonny X. Li[1,2], Kin Man Yu[1], Rebecca E. Jones[1,2], Junqiao Wu[1], Wladek Walukiewicz[1], Joel W. Ager[1], Wei Shan[1], Eugene E. Haller[1,2], Hai Lu[3], William J. Schaff[3] and William Kemp[4]; [1]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California; [2]Department of Materials Science and Engineering, University of California, Berkeley, Berkeley, California; [3]Department of Electrical and Computer Engineering, Cornell University, Ithaca, New York; [4]Air Force Research Laboratory, Kirtland Air Force Base, Kirtland AFB, New Mexico.

InGaN alloys, whose fundamental bandgaps span almost perfectly the solar spectrum, are potential materials for high-efficiency tandem solar cells [1]. An important consideration for high-efficiency solar cell in space applications is the radiation resistance of the materials. We have carried out a systematic study on the effect of irradiation on the electronic and optical properties of InGaN alloys over the entire composition range. Three different types of energetic particles (1 MeV electrons, 2 MeV protons, and 2 MeV alpha particle) were used to produce displacement damage doses (D_d) spanning over five orders of magnitude. The electron concentrations in InN and In-rich InGaN increase with D_d and finally saturate after a sufficiently high dose of irradiation (typically over 10^{15} MeV/g). The saturation of carrier density is attributed to the Fermi level pinning at the Fermi Stabilization Energy (E_{FS}), as predicted by the amphoteric native defect model [2]. Electrochemical capacitance-voltage (ECV) measurements reveal a surface electron accumulation whose concentration is determined by pinning at E_{FS}. Using the room temperature photoluminescence intensity as a indirect measure of minority carrier lifetime, it is shown that $In_{1-x}Ga_xN$ 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, *PhysicaB* **302 − 303**, 123 (2001).

11:45 AM E7.11

Intrinsic and N-related Defects in Hydrogen-Free ZnO Films Fabricated by Plasma Immersion Ion Implantation. Y. F. Mei[1], Ricky K. Y. Fu[1], G. G. Siu[1], Paul K. Chu[1], C. L. Yang[2] and W. K. Ge[2]; [1]Physics & Materials Science, City University of Hong Kong, Kowloon, Hong Kong; [2]Physics, Hong Kong University of Science & Technology, Clear Water Bay, Kowloon, Hong Kong.

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

SESSION E8: Defect Properties, Activation, Passivation and Reaction

Chairs: N.M. Johnson and P.M. Voyles
Thursday Afternoon, March 31, 2005
Room 2006 (Moscone West)

1:30 PM *E8.1

Mutual Passivation in Dilute GaN_xAs_{1-x} Alloys. Kin Man Yu[1], Wladek Walukiewicz[1], Junqiao Wu[2], D. E. Mars[3], Michael A. Scarpulla[4,1] and Oscar D. Dubon[4,1]; [1]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California; [2]Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts; [3]Agilent Laboratories, Palo Alto, California; [4]Department of Materials Science and Engineering, University of California, Berkeley, California.

The dilute GaN_xAs_{1-x} alloys exhibit many unusual properties as compared to the conventional binary and ternary group III-V semiconductor alloys. We report on a new effect in the GaN_xAs_{1-x} 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 IV_{Ga}-N_{As} pairs. The passivation of the shallow donors and the N_{As} 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 $GaN_{0.017}As_{0.983}$ (with Si concentration of $9x10^{19}cm^{-3}$) starts to decrease rapidly at an annealing temperature of 700°C from $3x10^{19}cm^{-3}$ in the as-grown state to a n< $10^{16}cm^{-3}$ after an annealing schedule of 900°C for 10 sec. At the same time annealing of this sample at 950°C increases the gap by about 35 meV. This increase in band gap corresponds to a reduction of the concentration of the active N atoms by $8x10^{19}cm^{-3}$, very close to the total Si concentration. Calculations show that the passivation process can be well quantitatively explained by Ga vacancies mediated diffusion of randomly distributed donor species to the nearest N sites. The general nature of this mutual passivation effect is confirmed by our study of Ge doped GaN_xAs_{1-x} layers formed by N and Ge co-implantation in GaAs followed by pulsed laser melting. Consequently, GaN_xAs_{1-x} alloys doped with group IV donors result in a highly resistive GaN_xAs_{1-x} layer with fundamental band gap governed by a net "active" N equal to the total N content minus the donor concentration. The mutual passivation effect described here may therefore be exploited for electrical isolation, band gap engineering, and quantum confinement.

2:00 PM E8.2

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.

2:15 PM E8.3

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

Deactivation of donors in heavily doped silicon is one of the predominant problems that CMOS technology has to deal with in connection with the down-scaling of semiconductor devices. In the near future, source, drain, and channel regions of transistors need to feature doping concentrations in excess of the respective solid solubility limits. At the same time, every donor atom should release one of its electrons to the bulk, thereby contributing to a raise in electrical conductivity in the corresponding region. Unfortunately, a large percentage of up to 90 % of the donors introduced are compensated during the wafer manufacturing process. Co-doping is considered to be one method that could potentially forestall donor deactivation. Prerequisite for its investigation is a deep understanding of the deactivation mechanisms in silicon on an atomistic 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 (d$\hat{3}$ for short), 2. donor-vacancy clustering, 3. and ultimately precipitation. Based on ab initio calculations, 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. At the same time, the co-dopant should reduce the number of acceptor states of such a complex. Moreover, the co-dopant should be rather small in order not to increase the strain in the silicon lattice and to exhibit a high diffusivity in the silicon crystal. We find that the isovalent impurities C and Ge are unsuited for the intended purpose of clustering inhibition. Lithium and Magnesium, on the other hand, both bind strongly to vacancies while reducing the number of deep acceptor levels of compensating complexes in the band gap. Our ab initio results clearly favor the double donor Magnesium as a co-dopant of both P and As, possibly also for Sb.

3:00 PM *E8.4

Determination of Diffusivities of Si Self-Diffusion and Si Self-Interstitials using Isotopically Enriched Single- or Multi-30Si Epitaxial Layers.

Satoru Matsumoto[1], S. Seto[1], S. Aid[1], T. Sakaguchi[1], Y. Nakabayashi[1], K. Toyonaga[1], Y. Shimamune[2], Y. Hashiba[2], M. Sakuraba[2], J. Murota[2], K. Wada[3] and T. Abe[4]; [1]Electrical Engineering, Keio University, Yokohama, Japan; [2]Tohoku University, Sendai, Japan; [3]MIT, Cambridge, Massachusetts; [4]Shin-Etsu Handoutai, Isobe, Japan.

In order to understand the properties of point defects (vacancy, Si self-interstitial) in Si, it is important to clarify diffusivity of Si self-diffusion over a wide temperature range. We used highly isotopically enriched 30Si epitaxial layers as a diffusion source. 30Si epitaxial layers were grown on CZ-Si substrates by gas-source MBE or low-pressure chemical vapor deposition (LCVD) systems, using 30SiH4 source purchased from Kurchakov Laboratory. Diffusion was performed under very pure Ar(99.999%) atomosphere at 867-1300C. The concentrations of the respective Si isotopes were obtained with SIMS analysis. Diffusivity of 30Si (called Si self-diffusivity, Dsd) was determined using numerical fitting process with SIMS profiles. In this process, the as-grown profile of 30Si was used as an initial condition. The best fit was determined by minimizing the root-mean-square error. Dsd can be described by an Arrhenius equation with one single activation enthalpy, Dsd=14exo(-4.37eV/kT). The present result is in good agreement with that of Bracht et al. The fractional component of Si self-interstitials, fI, in self-diffusion was also determined from the experiments of Si self-diffusion under heavy doping condition. Its values were relatively similar to those of Ural et al. Using the fI values, we separated the component of vacancy and Si self-interstitial mechanisms, CV*DV and CI*DI. CV and CI are the thermal equilibrium concentrations normalized by the number of lattice site of silicon. DV and DI are the diffusivity of vacancy and Si self-interstitial, respectively. Then we have CV*DV =17.4exp(-4.49eV/kT),and CI*DI=4.0exp(-4.29eV/kT). Next, we determined one of the most basic parameters, i.e., diffusivity of Si self-interstitial, using multi-layer structures consisting of alternative layers with isotopically enriched 30 Si and natural Si under oxygen ambient annealing. Spreading of 30Si spikes of each layer, which was caused by the diffusion of Si self-interstitials generated at the surface, was measured with SIMS analysis. The diffusivity of Si self-interstitials, DI, was obtained from the fitting with experimental results. In the temperature range between 820 and 920C, DI and CI(thermal equilibrium concentration of Si self-interstitials) are described by the Arrhenius equation, DI=3.48e4 exp(-3.82eV/kT) and CI=9.62e18 exp(-o.475eV/kT), respectively.

3:30 PM E8.5

Diffusion of Arsenic-Silicon Interstitial Complexes.

Scott A. Harrison, Thomas F. Edgar and Gyeong S. Hwang; Chemical Engineering, University of Texas at Austin, Austin, Texas.

Arsenic doping is an essential ingredient in the fabrication of silicon devices. As device dimensions scale down in nanometer structures, atomic-level control of doping profiles becomes necessary. Low-energy ion beams are currently most widely used to introduce dopants into the Si substrate, followed by high-temperature thermal annealing to eliminate substrate damage generated by energetic ion bombardment and to electrically activate the injected dopants. During the annealing, the arsenic atoms exhibit transient enhanced diffusion (TED). While the underlying TED mechanism is still unclear, recent theoretical studies have suggested that arsenic-vacancy complexes, such as AsV and As_2V, may be primarily responsible for the TED. However, recent experimental observations have suggested interstitials promote As TED. In addition, mono- and di-vacancy arsenic complexes appear to easily be annihilated in the presence of interstitials. In this talk, we will present the interaction of interstitials with arsenic and arsenic-vacancy complexes based on density functional theory calculations within the generalized gradient approximation. We have identified the structure and diffusion of arsenic-interstitial and di-arsenic pairs. For arsenic-interstitial pair diffusion, our DFT calculations predict two pathways, with overall barriers of 0.28 (0.40) eV and 0.46 (0.13) eV in the neutral (+1 charge) 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-arsenic pair diffusion is predicted to occur by overcoming an overall barrier of 1.33 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 important role of interstitials in arsenic TED. The increased understanding our study provides will greatly assist in improving current models for arsenic junction formation.

3:45 PM E8.6

Effects of Silicon Nitride Passivation Layer on Mean Dark Current and Quantum Efficiency of CMOS Active Pixel Sensors.

D. Benoit[1], P. Morin[2], M. Cohen[1] and J. L. Regolini[1]; [1]STMicroelectronics Crolles1, Crolles, France; [2]STMicroelectronics Crolles2 Alliance, Crolles, France.

Dark current reduction and quantum efficiency (QE) improvement in CMOS Active Pixel Sensor (CMOS APS) are fundamental in image sensors performance. In the present study, we have analyzed the influence of the silicon nitride (SiN) passivation layer properties on the mean dark current and the quantum efficiency of CMOS APS through electrical characterization of lot wafer processed with three different SiN passivation films. The SiN layers were characterized by Spectroscopic Ellipsometry (SE) and Fourier Transform Infra Red (FTIR) spectroscopy to 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 300 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 concentrations and therefore the Si/N ratio of the films. 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 light transmission is also presented. Requirements to minimize the mean dark current and to maximize quantum efficiency are somewhat in opposition. Actually, high [Si-H] and low [Si-N] bonds concentrations (for good passivation) are generally observed in silicon-rich SiN films, which contain high amount of [Si-Si] bonds (inducing high absorption, thus low QE). Increase simultaneously the [Si-H] and [N-H] bonds concentrations in the passivation layer can be a way to have high hydrogen desorption during passivation anneal just preserving a transparent layer. [1] D. E. Aspnes and J. B. Theeten, J. Appl. Phys. 50 (1979) 4928 [2] Z. Yin and F. W. Smith, Physical review B 42 (1990) 3658 [3] A. W. Weeber, H. C. Rieffe, W. C. Sinke and W. J. Soppe, 19th European Photovoltaic Solar Energy Conference and Exhibition (2004)

SESSION E9: Poster Session II

Chairs: J. Chevallier and M. Tabe
Thursday Evening, March 31, 2005
8:00 PM
Salons 8-15 (Marriott)

E9.1

Origin of Vacancy and Interstitial Stabilization at the Amorphous-Crystalline Silicon Interface. Scott A. Harrison[1], Taras A. Kirichenko[2], Decai Yu[1], Thomas F. Edgar[1], Sanjay K. Banerjee[2] and Gyeong S. Hwang[1]; [1]Chemical Engineering, University of Texas at Austin, Austin, Texas; [2]Electrical 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 junctions. Currently, ultra-low-energy ion implantation followed by high-temperature thermal annealing is most widely used to fabricate such ultrashallow junctions. In this process, a great challenge lies in achieving precise control of redistribution and electrical activation of dopant impurities. 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 greatly 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 vary with the phase. Since single vacancies and interstitials are highly mobile even at room temperature, their clustering and annihilation behaviors can be greatly affected by substrate amorphization (during implantation and 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 effect of the 'sponge-like' behavior of the amorphous phase toward native defects on ultrashallow junction formation in the fabrication of electronic devices. The fundamental understanding and data provided by this study will be very useful in developing a comprehensive kinetic model for ultrashallow *pn* junction formation.

E9.2

A New Post Annealing Method for AlGaN/GaN Heterostructure Field-Effect Transistors Employing XeCl Excimer Laser Pulses. Min-Woo Ha, Seung-Chul Lee, Joong-Hyun Park, Young-Hwan Choi, Kwang-Seok Seo and Min-Koo Han; School of Electrical Engineering #50, Seoul National University, Seoul, South Korea.

The wideband gap material of GaN has attracted for the high power and the high temperature applications due to a high two-dimensional electron gas (2DEG) concentration and a high critical electric field. The high voltage switching AlGaN/GaN heterostructure field-effect transistors (HFETs) should decrease on-state voltage drops and a leakage current for suppressing a power loss. Recently, post thermal annealing effects on device performances of AlGaN/GaN HFETs are reported to decrease a leakage current. But, the drain current of a thermal annealed AlGaN/GaN HFET decreases and the threshold voltage of that shifts positively due to the decrease of the two-dimensional electron gas concentration and the Schottky gate metal diffusion into a GaN layer. The purpose of our work is to propose a new post annealing method employing the excimer laser pulses, which increases a drain current and suppresses a leakage current without degrading the Schottky gate metal and a threshold voltage shift. The fabricated AlGaN/GaN HFET is post annealed by XeCl excimer laser pulses operating at 308 nm. The 3 μm unintentionally doped GaN layer can only absorb the excimer laser due to its lower energy band gap (3.4 eV) than excimer laser photon energy (4.025 eV) and the absorption coefficient of GaN (α=1.3$\times$10^5 cm^{-1}). During laser pulses, the generated heat in the unintentionally doped GaN can diffuse the region between the Schottky gate and the GaN layer. The interface defects under the Schottky gate decreases. In the proposed method, the Schottky gate metal does not diffuse into a GaN layer due to the Schottky gate metal reflection to the laser and the instant heat diffusion. After a single laser pulse with the energy of 100 mJ/cm^2, the drain current and the peak extrinsic transconductance (g$_m$) of the AlGaN/GaN HFET are 405.3 mA/mm and 102.8 mS/mm. Those of the virgin device are 363.7 mA/mm and 89.9 mS/mm. When a single laser pulse with the energy of 50 mJ/cm^2, the g$_m$ is increased from 88.9 mS/mm to 98.9 mS/mm. The laser pulse energy determines the surface temperature of the device and the laser pulse with the energy of 250 mJ/cm^2 damages the Schottky gate. The proposed post annealing method decreases the leakage current from 1.95 mA/mm to 1.53 mA/mm.

E9.3

Fabrication of Silicon Carbide PIN Diodes by Laser Doping and Planar Edge Termination by Laser Metallization. Z. Tian[1], N. R. Quick[2] and A. Kar[1]; [1]College of Optics and Photonics/CREOL, Mechanical, Materials, and Aerospace Engineering Department, University of Central Florida, Orlando, Florida; [2]Applicote Associates, LLC, Orlando, Florida.

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

E9.4

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

A2B6 semiconductors and their solid solutions (ZnSe, ZnTe, CdTe, ZnCdHgTe) are matter of choise for near- and far-infrared optoelectronics. The importance of maximally reduced degree of defectness 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 nanoindentation 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 nanoindentation effect on electric characteristics (in particular, current-voltage and capacitance-voltage) of ZnCdHgTe thin films and ZnCdHgTe/Cd(Zn)Te heterostructures at the room temperature. It is shown that nanoindentation leads to appearance of double-barrier structures. Experimental data reported in the work show sufficient effect of mechanical impact on room-temperature current-voltage and low-frequency (f = 1 kHz) capacitance-voltage characteristics of heterostructure p-ZnCdHgTe/p-CdTe grown by modified 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 epilayer ZnCdHgTe and may be governed technologically (variations of the growth conditions, doping levels, etc.). At the same time, influence of indentation on the current-voltage characteristics of the substrate (p-CdTe) is also significant. Changes of the carrier transport modes at room temperature can be used for previous barrier construction before growth of the film.

E9.5

Annealing of the Deformation-Induced Damage in Silicon Detected by Oxygen Agglomeration. Nikolai Yarykin[1] and Ellen Hieckmann[2]; [1]Institute of Microelectronics Technology RAS, Chernogolovka, Moscow Region, Russian Federation; [2]Dresden 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 1000°C. It is shown that the decay is determined by the oxygen diffusion to and agglomeration at the deformation-induced defects; rate of the process serves as a measure of the remained defects. The overall defect 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 of the implantation-induced damage. [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[1] and George A. Rozgonyi[2]; [1]Institute of Microelectronics Technology RAS, Chernogolovka, Moscow Region, Russian Federation; [2]Department of Materials Science & Engineering, North Carolina State University, Raleigh, North Carolina.

The spectrum of defects produced in silicon due to bombardment with energetic particles - and consequently the deep-level spectrum - are known to depend on the mass of incident particles. For instance, the second acceptor level of divacancy is suppressed in silicon implanted with heavier ions [1]. In p-type silicon the K2 center was recently observed [2]. Although the center is dominant in silicon implanted with Si and Ge ions, its nature is still unknown. The K2 center introduction rate decreases essentially for lighter ions, and the center was not unambiguously reported in electron-irradiated samples until now. At the same time, such observation could shed light 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 impurity contents, the comparison is done on the same set of crystals of different purity. It is observed that the K2 center can be created by irradiation with 5 MeV electrons. Its introduction rate in electron-irradiated samples is found to be is more sensitive to the crystal purity than in case of ion implantation. A notable concentration of the K2 centers is detected after electron irradiation only in epitaxial wafers. A possible nature of the K2 center and details of its near-surface distribution are discussed. [1] B. G. Svensson et al., Phys. Rev. B 43, 2292 (1991). [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. Esidor Ntsoenzok[1], Rachid El Bouayadi[2], Gabrielle Regula[2], Bernard Pichaud[2] and S. Ashok[3]; [1]CNRS-CERI, Orleans, France; [2]TECSEN, Case 151, Faculte des Sciences St-Jerome, Marseille, France; [3]Department of Engineering Science and Mechanics, the Pennsylvania State University, University Park, Pennsylvania.

Although bubbles/cavities induced by helium in silicon have been studied for decades, it is still a big controversy concerning the thermal growth of these nano-objects. The goal of this work is the study of bubbles/cavities thermal growth by a new approach. Float Zone (FZ) silicon samples have been implanted with helium ions at energies ranging from 0.8 MeV to 1.9 MeV in increments of 0.1 MeV, with the ion flux maintained between 5 x 1012 and 1 x 1013 He cm-2s-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. The dose was kept at 5x1016 He cm-2 for all the energies except 0.8 MeV for which a lower dose of 3x1016 He cm-2 was used. After thermal annealing, the samples were evaluated by cross sectional transmission electron microscopy (XTEM) using a Field Emission Gun Microscope (Jeol 2010F). The results were then compared with those obtained when only 1.55 MeV He is used at various doses. Our results clearly demonstrate that these cavities mainly grow by the Ostwald ripening mechanism that involves exchange of He and vacancies from smaller to bigger cavities. Multi-implantation provides the biggest cavities reported yet. The results of this study should help shed some light in resolving the controversy on the exact growth mechanism governing He-induced cavities in Si.

E9.8

Blistering and Splitting in Hydrogen-Implanted Silicon. Esidor Ntsoenzok[1], Hanan Assaf[1] and S. Ashok[2]; [1]CNRS-CERI, Orleans, France; [2]Department of Engineering Science and Mechanics, Pennsylvania State University, University Park, Pennsylvania.

Production of ultra-thin silicon top layers by means of hydrogen implantation, as established by the Smart Cut process, is now well known. The thickness of the top-Si layer realized in such a scheme currently ranges from 70 nm to 1 micron. In this technique, the resulting material is a combination of a thin silicon layer bonded to a handle wafer (usually oxidized Si). The goal of this study is determination of the threshold thickness above which lift-off of a free-standing silicon layer is possible in the absence of any handle wafer; in other words, the thickness above which layer-splitting is dominant over blistering. This will allow determination of the limit for obtaining free-standing films lifted off Si by the hydrogen-implantation-induced defect layer. We implanted H into Si over the energy range 500 keV - 2 MeV, corresponding to a peak implanted depth varying from 6.1 to 48.4 microns, according to TRIM2003 (TRansport of Ions in Matter) simulation. After implantation, a thermal anneal was applied to all the samples. For implant depths below 9 microns no clean lift-off of a silicon layer is obtainable; only rough blistering is seen. Increasing the implanted dose or thermal budget did not improve the situation significantly. However, for depths ? 9 microns (from 9 to 50 microns in this study) thermal annealing results in a clean lift-off of layers with thickness equal to the hydrogen implant depth. Blistering and transfer/lift-off of thin silicon layer are the consequence of thermal growth of platelets by Ostwald ripening where the efficiency of hydrogen collection is the limiting factor. The dose required for layer lift-off has been found to depend slightly on the implanted depth of hydrogen.

E9.9

Variation of Surface Sink Possibility for Point Defects Removing in Annealing. Min Yu[1], Xiao Zhang[1], Kai Zhan[1], Ru Huang[1], Xing Zhang[1], Yangyuan Wang[1], Jinyu Zhang[2] and Hideki Oka[3]; [1]Institute of Microelectronics, Peking University, Beijing, China; [2]Fujitsu R&D Center Co. Ltd., Beijing, China; [3]Fujitsu Laboratories Ltd., Atsugi, Japan.

Behavior of point defects in annealing is focused in order to suppress the Transient Enhanced Diffusion (TED) of boron urged by the development of integrated circuits. Surface sink possibility for point defects is very important in the case of ultra-shallow doping, however it is still ambiguous considering the inconsistent results. In this paper the variation of surface sink possibility is studied. By explaining experimental results with Kinetic Monte Carlo simulation, we proposed that surface sink possibility varies in different cases. Specially, the comparison results of different treatment on surface are reproduced by simulation with variation of surface sink. This will not only improve the understanding of surface sink but also indicate the new way to improve shallow junction technology. Kinetic Monte Carlo model is applied to simulate diffusion in high temperature annealing. The annealing on low energy (0.5kev   10kev) implantation of B is simulated and verified by SIMS data. TED of boron is reproduced by simulation and agreement to SIMS data is achieved. The simulation studies show that with complete sink surface model, TED for very low energy implantation, is obviously underestimated and only with very small surface sink possibility can it be well described. Similar conclusion is also achieved by Edmund G. Seebauer (IEEE ICSICT 2004). 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 model can well describe the phenomenon. And surface annihilation speed is discussed. Thirdly, in order to understand the surface sink possibility, comparison experiments 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. To understand and suppress enhanced diffusion, surface sink possibility must be considered.

E9.10

Abstract Withdrawn

E9.11

Optical Properties of Hydrogen Implanted ZnO. Jung-Kun Lee[1], Michael Nastasi[1], David Hamby[2] and Don Lucca[2]; [1]Materials Science and Technology, Los Alamos National Laboratory, Los Alamos, New Mexico; [2]School of Mechanical and Aerospace Engineering, Oklahoma State University, Stillwater, Oklahoma.

The optical and structural properties of 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 ZnO have shown that the increase in the relative ratio of the 3.361 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.

E9.12

Defect Structure in ZnO Studied by ab-initio Calculation. Naoki Ohashi 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 compensation mechanism. We used CASTEP code for calculation of defect structures. Local structure around the defects was evaluated by using super-lattice model and the formation energy of defects was calculated. For the calculation of charge compensation, complex defects, such as aluminum at zinc site with vacancy 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 on surface 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 Im[1], Won-ju Cho[1], Chang-Geun Ahn[1], Jong-Heon Yang[1], In-Bok Baek[1], Seongjae Lee[1], Sungkweon Baek[1] and Hyunsang Hwang[2]; [1]Nano Electronics Devices Team, ETRI, Daejeon, South Korea; [2]Material 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 effect. To meet this requirement, the ion implantation energy of the junction formation must be decreased. In addition, the thermal budget of post-implantation annealing must be reduced to minimize implanted dopant diffusion. However, lowering the beam energy in conventional ion implantation equipment inherently decreases the beam current, prolonging the implantation time which results in low throughput. Accordingly, plasma doping is receiving more and more attention for its very high ion current and dose rate capability at very low implantation energies, equipment of smaller size, simple 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.

E9.14

Germanium Ultra-Shallow n+/p Junction Formed by Low-Energy Plasma Doping and Laser Annealing. Sungho Heo[1], Sungkweon Baek[1], Dongkyu Lee[1], Hyungsuk Jung[2] and Hyunsang Hwang[1]; [1]Materials Science and Engineering, Gist, Gwangju, South Korea; [2]Samsung Electronics Co., Suwon, South Korea.

Silicon substrate has low hall electron mobility due to the intrinsic material property, which is enhanced in case of high-k oxide deposition due to the high defect density. To overcome this problem, germanium(Ge) substrate has regained considerable attention, recently. Due to the small band gap, the junction formed on Ge showed high leakage current. Therefore, most of research used high energy ion implantation with furnace annealing and rapid thermal annealing. For the application of Ge wafer on the submicron 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 Ωcm was used as a substrate. Prior to plasma doping, the substrate wafer was cleaned. The plasma doping system was performed using PH3(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 rapid thermal annealing(RTA) was performed in a vacuum ambient at temperature of 500°C for 10min. The laser annealing was conducted by a KrF eximer laser with 248nm wavelength in the energy 300 500mJ/cm2 at 1 pulse. The fabricated samples were analyzed by hall measurement, SIMS analysis and diode leakage current evaluation. Hall measurement was conducted in the liquid nitrogen atmosphere at 77K due to the small Ge band gap, which was resulted to the leaky characteristics. The laser-annealed sample in the energy of 300mJ/cm2 at 1 pulse showed the sheet resistance of 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.

E9.15

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

Near future a semiconductor technology will be faced to another red brick wall of quantum mechanical phenomena and a device-level scaling will be too difficult to carry on Moore's law. Therefore present integration technology using two-dimensional design with planar devices should be replaced by three-dimensional integration scheme with novel structure devices and together with new doping process for these devices. The non-planar SOI-MOSFET devices like FinFET, Tri-Gate, 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 wafers are exposed to high density plasma directly. Novel plasma doping process shows similar doping efficiency on narrow 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 doping show good current drivability and low subthreshold slope. However without post thermal annealing, this process generates many defects and traps as well as hydrogen ions on the interface and inside silicon, and these degrade device reliability. On the other hand, results of our ultra-small MOSFET research show possibility of new memory devices with these traps and ions in devices.

E9.16

Theoretical Investigation of Formation of (n-n+)-Junction in the Ion-implanted Crystalline Matrix. Halyna M. Khlyap[1] and Roman M. Peleshchak[2]; [1]Physics, Universsity of Technology, Kaiserslautern, Germany; [2]Physics, 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 good instrument for defect engineering in order to form isotype or anisotype junctions in the subsurface region of the substrate (the depth of this region depends on the energy and the mass of the ions in the beam). For obtaining materials with in-advanced defined properties it is very important to predict the profile of implanted ions distribution in the crystalline matrix as well as to get information about the self-consistent distribution of charge carriers and electrostatic potential in the implanted lattice. The abstract reports results of theoretical calculations performed for clarifying redistribution of electrons and electrostatic potential in the implanted crystalline matrix (100)-GaAs+Si(Ar) due to electron-deformation effects. The model requires self-consistent solution of the following set of equations: 1) time-independent Schroedinger equation; 2) equation of mechanical equilibrium: 3) Poisson equation to determine the distibution 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 Zhang[1], Yoshio Ashizawa[2] and Hideki Oka[2]; [1]Fujitsu R&D Center Co. Ltd, Beijing, China; [2]Fujitsu Laboratories Ltd., Akiruno, 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 CATSP using the GGA functional and ultra-soft pseudo-potentials. All the calculations were performed in a 64-atom supercell with periodic boundary conditions and 2*2*2 Monkhorst-Park k-point sampling with an energy cut-off 160eV. 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 -1 charge state, (110)-split is the most stable. In positive charge states, the H site becomes unstable. It spontaneously changes its form to T site. (110)-split is stable in +1 charge state but also changes to T site in +2 charge state. The T site becomes the most stable in positive charge state. We found +2 charge state of T site to be most stable at midgap. Different diffusion paths in 0, +1, +2 charge state are investigated. The migration barriers in 0, +1 and +2 charge states are 0.23eV, 0.44eV and 1.2eV respectively. Next the structure and formation energy of vacancy in different charge state are studied. The ionization levels for vacancy are in agreement with experimental results and previous studies. The migration barriers are 0.1eV, 0.38eV, 0.59eV 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 formation energy of FFCD is 0.5eV and 0.8eV 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 1.23eV given by previous tight-binding calculation. Our calculation shows that FFCD is the I-V complex proposed by previous tight-binding calculation. Its migration barrier can be considered as I-V recombination barrier in agreement with the values used in many analytical models of I-V recombination. 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 1.64eV. The migration barriers of divacancy in -1, 0 and +1 state all 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 Wang[1], Manmohan Daggubati[1], Hossein Paravi[1], Rong Yu[2] and Xiaofeng Zhang[2]; [1]Fairchild Semiconductor, West Jordan, Utah; [2]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California.

The precipitation and diffusion of oxygen in heavily arsenic doped Czochralski (CZ) silicon wafers (with resistivity at 3mΩ-cm and interstitial oxygen concentration of 7x10^{17}/cm^3) have been studied for different thermal budgets and different back surface treatments. After annealed at 1200°C for 45 minutes and 900°C for 15hrs sequentially, the wafers with damaged back surface show rodlike and platelike SiO_x 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 polyhedral oxygen precipitates were observed at the interface between the polysilicon film and the silicon substrate. They have a habit plane of {100}. These results differ significantly from the previous observations in heavily boron and antimony doped silicon wafers which show drastically enhanced oxygen precipitation when the back surface is sealed with polysilicon film. The kinetics of this oxygen precipitation behavior is discussed in detail. The SIMS and EDS analysis indicate that the diffusion of oxygen from the substrate to the epitaxial layer has been significantly reduced in the wafers with damaged back surface, compared with those with polysilicon sealed back surface. This diffusion difference shows significant impact to the performance of the devices built on these substrates.

E9.19

Influence of Oxygen Vacancies and Strain on Electronic Reliability of SiO_{2-x} Films. Ken Suzuki, Hideo Miura and Tetsuo Shoji; Fracture and Reliability Research Institute, Tohoku University, Sendai, Miyagi, Japan.

Local defects in thin gate oxide films used for sub 100-nm devices play a very important role on both the electronic performance and reliability of the devices. One of the most important local defects in the gate oxide is the compositional fluctuation caused by oxygen or Si vacancies. They are mainly introduced near the interface between the thermally oxidized Si-dioxide and the 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 and intrinsic defects on both electronic and structural characteristic of SiO_2, we performed a quantum chemical molecular dynamics analysis for SiO_{2-x} structure under strain by using the colors code [1]. The formalization of this program is based on the 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 present a clear view of the change in the structure of SiO_2 with oxygen vacancies on the atomic level. We found that oxygen vacancies in SiO_2 make silicon monoxide molecules and that the plural monoxide molecules start to cluster in the crystal. These structural changes seriously decrease the band gap of SiO_2. The calculated band gap of SiO_2 determined from energy difference between HOMO and LUMO was 8.5 eV. On the other hand, the band gap value was 7.2 eV on average for SiO_2 with an oxygen vacancy. This result indicates that the insulating property decreases in the SiO_2 film with oxygen vacancies. In addition, the band gap decreases further under high tensile strain. We found that the serious decrease of the band gap occurs when both the number of oxygen vacancies and tensile strain increase in the SiO_2 film. [1] K. Suzuki, Y. Kuroiwa, S. Takami, M. Kubo, A. Miyamoto and A. Imamura, Solid State Ionics, 152-153 (2002) 273-277.

E9.20

General Model of Diffusion of Interstitial Oxygen in Silicon and Germanium Crystals. Vasilii Gusakov, Institute of Slid 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, semiempirical and ab initio methods. It was established that the diffusion process of an interstitial oxygen atom (Oi) is controlled by the optimum configuration of three silicon (germanium) atoms nearest to Oi. The calculated values of the activation energy ΔE (Si) = 2.59 eV, ΔE (Ge) = 2.05 eV and pre-exponential factor D_0 (Si)= 0.28 cm^2 s^{-1}, D_0 (Ge)= 0.39 cm^2 s^{-1} are in a excellent agreement with experimental ones and for the first time describe perfectly an experimental temperature dependence of the Oi diffusion constant in Si crystals (T=350 - 1200 C). Hydrostatic pressure (P) results in a linear decrease of the diffusion barrier (δ_P ΔE = -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.

E9.21

Contact Free Defect Investigation in As-Grown Fe Doped SI-InP. Sabrina Hahn[1], Torsten Hahn[1], Bianca Gruendig-Wendrock[1], Kay Dornich[1], G. Mueller[2], P. Schwesig[2] and J. Niklas[1]; [1]Institut f. Experimental Physics, TU Freiberg, Freiberg, Germany; [2]Dept. of Materials Science, University Erlangen, Nuernberg, Germany.

InP is a promising semiconductor with properties suitable for many applications, particularly for optoelectronics and high frequency devices. The new experimental methods of microwave detected photo induced current transient spectroscopy (MD-PICTS) and microwave detected photoconductivity (MDP), which we used already successfully e.g. for the investigation of defects in GaAs Wafers, where applied to semi insulating (SI) Fe doped InP samples. These methods allow for defect investigations somehow similar to 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 fermi level position. According to solutions of a rate equation system we developed to account for the properties of the EL2 in GaAs this provides strong evidence that the iron center in InP:Fe must have properties of a recombination center. The associated activation energies to the conduction band and to the valence band, respectively, were determined. Beside this major defect we discovered a wide range of shallow defects. The new experimental methods MD-PICTS and MDP allow not only for a non-destructive defect investigation but also for the measurement of spatial distributions of these defects, which furnishes additional pieces of information like the homogeneity of the samples. This will be also demonstrated.

E9.22

Peculiarities of Defect Formation Processes in ZnSe Crystals

with Isovalent Te Impurity. Victor Makhniy[2], Peter Gorley[1], Irene Tkachenko[2], Paul Horley[1], Yuri Vorobiev[3] and Jesus Gonzalez Hernandez[3]; [1]Electronics and Energy Engineering, Chernivtsi National University, Chernivtsi, Chernivtsi, Ukraine; [2]Optoelectronics, Chernivtsi National University, Chernivtsi, Chernivtsi, Ukraine; [3]Unidad 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 two 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 zinc vacations V_{Zn}, together with selenium and zinc atoms occupying interstitial positions in crystalline lattice (Se_i and Zn_i). Single-charged defects create associates of V_{Zn}^- Zn_i^+, causing intensive radiation band at the energies of about 1.7eV. Annealing of the sample in saturated zinc vapors resulted in the shift of the band to 1.9eV. Recombination processes taking place in the system for this case involve Zn_i impurity levels. Doping of ZnSe with tellurium from the vapor phase lead to another shift of the effective radiation band to 2.3eV, caused by transitions with participation of single-charged zinc vacancies. Intrinsic 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[*].

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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 theory of s- and p-bonded substitutional impurities in PbTe, a classic narrow band gap semiconductor used for infrared detection and thermoelectric application. This theory explained the origin of resonant defect levels near the fundamental band gap and also predicted resonant 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 how these deep defect states get modified when different types of impurity microstructures are present. In particular we will discuss about a class of novel narrow band gap semiconductors and semimetals MSbPb_(2n-2)Te_(2n), where M is Ag, Na, K. We will discuss the modification in the electronic structure near the band gap region of PbTe caused by replacing divalent Pb atoms by monovalent M and trivalent Sb atoms preserving the overall charge neutrality. Possible reasonss behind the superior thermoelectric properties observed in these quaternary systems [3] will be discussed. [*] Work supported by an ONR-MURI grant [1] C. S. Lent et al., Solid State Communications 61, 83 (1987). [2] Daniel Bilc et al., Phys. Rev. Lett. 93, 146403 (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[1], Yue Ma[1], Yuelong Huang[1], Wolfgang R. Fahrner[1], Lars O. Keller[2], Achim Wiggershaus[2] and John T. Horstmann[2]; [1]Electrical Engineering and Information Technology, University of Hagen, Hagen, Germany; [2]Electrical Engineering and Information Technology, University of Dortmund, Dortmund, Germany.

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

E9.26
P-N Junction Diodes Fabricated on the Basis of Hydrogen Enhanced Thermal Donor Formation in P-Type Czochralski Silicon.

Yuelong Huang, Katrina Meusinger, Yue Ma, Wolfgang Duengen, Reinhart Job and Wolfgang R. Fahrner; Electrical Engineering and Information Technology, University of Hagen, Hagen, Germany.

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

E9.27
Hydrogen Diffusion and Crystallization Induced a Structural Change in Boron Doped Hydrogenated Amorphous Silicon Films.

Kail Fatiha[1,2], Hadjadj Aomar[2] and Roca i Cabarrocas Pere[1]; [1]Laboratoire de Physique des Interfaces et des Couches Minces, Ecole Polytechnique, 91128 Palaiseau, France; [2]Laboratoire d'Analyse des Solides, Surfaceset Interfaces, Universite de Reims, 51687 Reims Cedex 2, France.

We have studied the evolution of the structure of intrinsic and doped hydrogenated amorphous silicon films exposed to a hydrogen plasma. The substrate temperature was fixed at 230 C and the hydrogen plasma was obtained under an RF power of 30 W and a total pressure of 1 Torr. For this purpose we combine in-situ spectroscopic ellipsometry and secondary ion mass spectrometry measurements. We show that hydrogen diffuses faster in boron doped hydrogenated amorphous silicon, leading to a thick H-rich subsurface layer from the early stages of hydrogen plasma exposure. At longer times, hydrogen plasma leads to the formation of a microcrystalline layer via chemical transport where a silicon is etched by hydrogen from the reactor walls and deposited on the heated a-Si:H substrate. There is no evidence for crystallization of the a-Si:H substrate. Interestingly, we observe that hydrogen content decreases in the boron doped a-Si:H films exposed to deuterium plasma and once the microcrystalline layer is formed hydrogen diffuses out of the sample accompanied with decrease of boron content.

E9.28
Dopant Activation Enhancement by Hydrogen at Low Annealing Temperatures.

Aniruddha Vengurlekar[1], S. Ashok[1] and Christine E. Kalnas[2]; [1]Department of Engineering Science, Pennsylvania State University, State College, Pennsylvania; [2]Solid State Measurements Inc., Pittsburgh, Pennsylvania.

As silicon CMOS technology is scaled down to smaller dimensions, the ability to activate greater amounts of dopant atoms is a significant challenge for realization of shallow junctions. Dopant activation is more difficult to achieve in shallow junctions due to higher concentrations of dopants and possible formation of clusters. The high temperatures currently used to activate dopants result in increased junction depth, and problems with transient enhanced diffusion, however, lowering of annealing temperature results in lesser dopant activation. Our previous work reported on the enhancement of 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 prior to implantation. This effect was attributed to three factors. Firstly, lattice relaxation occurs due to the presence of hydrogen at a vacancy, which reduces the activation energy for boron to enter the site. Secondly, vacancies created by plasma hydrogenation and hydrogen out-diffusion during annealing lead to greater activation. It is known that the presence of a vacancy supersaturation in the crystal lattice enhances boron activation. Thirdly, it was postulated that the presence of a large concentration of hydrogen 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 antinomy, 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 Spreading Resistance Profiling (SRP). Effect of varying dopant concentration, and annealing time was also studied. Activation enhancement was observed even at lower boron implant concentration, where cluster formation is likely to be reduced. Activation enhancement with hydrogenation was also observed for both 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.

E9.29
Hydrogen Ion Implantation Caused Defect Structures in Heavily Doped Silicon Substrates. Minhua 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 2.5mΩ-cm) and phosphorous(P-doping level at 1.3mΩ-cm) doped (100) silicon substrates. At the implantation energy of 170keV and 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 1658nm 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^{16} ion/cm^{2}, 3x10^{16} ion/cm^{2}, through 5x10^{16} ion/cm^{2}, respectively. This is opposite to the trend in heavily boron doped substrates 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 dose and post-annealing conditions. A discussion is also given rise to the H^{+} ion straggling in the heavily boron, arsenic, and phosphorus doped silicon substrates.

E9.30
Dynamics of Hydrogenation-Induced Defects in Si during Solar Cell Processing. Bhushan Sopori[1], Kim Jones[1], Robert Reedy[1], Ajeet Rohatgi[2] and Vijay Yeludur[2]; [1]National Renewable Energy Laboratory, Golden, Colorado; [2]Georgia Institute of Technology, Atlanta, Georgia.

Hydrogenation is used extensively in solar cell fabrication as a technique to passivate residual impurities and defects. In the most common approach, hydrogen passivation is combined with deposition of AR coating and metallization. This consists of depositing a layer of hydrogenated silicon nitride (SiN:H) by a 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 it using an RTP-like process. Recent studies indicate that H transport from plasma to the bulk of the solar cell occurs as follows: H is "stored" at the surface of the Si wafer in the process-induced defects (PIDs) generated during the deposition of SiN:H. During the RTP step, H is released from the defects and diffuses into the bulk. One of the important requirements in making a good solar cell is that the PIDs must be annihilated during the RTP step. Residual defects due to incomplete annihilation or conversion into more stable defects can strongly degrade the device performance through two mechanisms: high surface recombination velocity and poor junction quality. Thus, a study of the dynamics of the PIDs and their effects on the surface recombination and junction properties is important to understand the transport of H and to minimize any residual defects or defect conversion. This paper will describe results of our studies in which samples were hydrogenated by two different PECVD techniques —low-frequency- and high-frequency-based plasmas. These techniques are known to produce different degrees of passivation, but the mechanisms are not known. The samples were processed under different RTP conditions and then analyzed to determine the residual defects and H diffusion profiles. These results verify our previous conclusions that a defect layer mediates H transport from PECVD plasma to the bulk of Si. H is stored in the damage produced by the plasma. Low damage levels are manifested as clusters of point defects. Higher damage appears as formation of stacking faults (SF) and platelets. RTA processing heals the damage to a large degree, but is also accompanied by formation of SF and platelets. We will discuss the differences in the defect dynamics in the two methods of hydrogenation.

E9.31
Effect of Deuterium Diffusion on the Electrical Properties of AlGaN/GaN Heterostructures. Jaime Mimila-Arroyo[1], Michel Barbe[1], Francois Jomard[1], Jacques Chevallier[1], Marie-Antoinette Poisson[2], Sylvain Delage[2], Christian Dua[2], Yvon Cordier[3], Maxime Hugues[3], Fabrice Semond[3], Franck Natali[3], Philippe Lorenzini[3] and Jean Massies[3]; [1]Laboratoire de Physique des Solides et de Cristallogenese, CNRS, Meudon, France; [2]Thales Research and Technology, Orsay, France; [3]Centre de Recherche sur l'Heteroepitaxie et Applications, CNRS, Valbonne, France.

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 carrier trapping by surface states and 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 provided 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 at 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 rf 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^{17} cm^{-3} 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 n_s decreases from 5.3x10^{12} cm^{-2} to 2.3x10^{12} cm^{-2}. From Hall effect and conductivity measurements, we find that, under deuterium diffusion, both the sheet carrier concentration n_s and the electron mobility μ decrease. After deuterium diffusion at 460 C, 30 W, 20 min, n_s decreases by a factor of 2 while μ decreases by a factor of 3. Under rapid thermal annealing at 800 C, 3 min, both the sheet carrier concentration and the electron mobility are mostly restored. This reversibility effet 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 at the AlGaN/GaN interface. The resulting H^{-} species act 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 stretch-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 atomic 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 modes for this defect complex will be discussed in comparison with the experiments.

E9.33
Effect of Substrate Orientation on the Growth Rate, Surface

Morphology and Silicon Incorporation on GaSb Grown by Metal-organic Vapor Phase Epitaxy. Jian Yu and Ishwara B. Bhat; Rensselaer Polytechnic Institute, Troy, New York.

The growth and dopant incorporation during metal-organic vapor phase epitaxy (MOVPE) strongly depends on the orientation of the starting substrates. MOVPE of Si-doped GaSb layers on (100), (111)B and (111)A substrates were used to investigate the effect of orientation on the growth rate, the surface morphology and the silicon incorporation. Orientation dependence of growth rates was studied as a function of temperature and V/III ratio. As the V/III ratio increases, the growth rate on the (111)B oriented substrate decreases, whereas that on the (111)A oriented substrate increases. The surface morphology on different substrates was studied by scanning electron microscopy (SEM) and atomic force microscopy (AFM). Flat-top hexagonal hillocks were observed on (111)B surface, and the growth was by step-flow on these facets. A surface kinetic growth model has been proposed to describe the growth features observed on (111)B surfaces. Finally, the orientation dependence of silicon incorporation was studied by secondary ion mass spectrometry (SIMS) and Hall measurements. It was found that the silicon incorporation rate was four times higher on (100) oriented surface than on (111)B oriented substrate. Although no conduction type switch was found on (111)B oriented substrate, throughout the Si doping range studied, a Ga slightly rich growth condition might be one of the factors accounting for the discrepancy between theoretical prediction and experimental results.

E9.34

Photoelectron Emission Technique for the Surface Analysis of Semiconductors. Takao Sakurai[1], Yoshihiro Momose[2], Masanori Kudou[2] and Keiji Nakayama[3]; [1]Division of General Education, Ashikaga Institute of technology, Ashikaga, Japan; [2]Department of Material Science, Ibaraki University, Hitachi, Japan; [3]National Institute of Advanced Industrial Science and Technology, Tukuba, Japan.

To characterize the state of real surfaces of semiconductor in ambient environments, we have developed an extremely sensitive technique for surface analysis using photoelectron emission. The emitted electrons are detected by a gas-flow Geiger counter with Q gas. This measurement is performed by scanning the wavelength from 300 to 200 nm of incident UV light from D2 lamp at different temperatures between 25 and 340 °C. The dependence of the intensity of photoelectron emission I_{ph} on the photon energy of incident light (yield spectrum of photoelectron) is obtained at each temperature. Using this technique, the photoelectron emission characteristics of commercial Si wafer (100) surface are investigated. The thickness of the Si wafer is 0.52 mm and the electric resistance is larger than 1000 Ω. In general, the theory of photoelectric emission from semiconductors predicts a power law from the yield near threshold [1] by the following equation: $I_{ph}=C_n(hv-E_n)^n$. The value of the exponent n and the threshold E_n depend on the excitation and escape mechanisms involved; and n is 2.5 for indirect transitions in the bulk. However, it was reported that experimental yield spectra of clean (111) Si surface prepared by cleavage in high vacuum showed that n = 3.0 and E_3 = 5.15 eV, likely due to indirect transitions from the top of the valence band to the vacuum level [2]. Photoelectric 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 through Ministry of Education, Culture, Sports, Science, and Technology. [1] E. O. Kane, Phys. Rev. 127, 131 (1962) [2] G. W. Gobeli and F. G. Allen, Phys. Rev. 127, 141 (1962) —

E9.35

Identification and Characterization of Submicron Defects for Semiconductor Processing. Wei Liu[1], Aime Fausz[2], John Svoboda[2], Brian Butcher[3], Rick Williams[3] and Steve Schauer[1]; [1]Physical Analytical Laboratory, Freescale Semiconductor, Chandler, Arizona; [2]MOS12 Die Fab, Freescale Semiconductor Inc., Chandler, Arizona; [3]MRAM, Technology Solutions Organization, Freescale Semiconductor Inc., Chandler, Arizona.

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 integration of defect inspection at only a few process steps during device fabrication results in the detection of many buried defects. In order to identify these defects, it is necessary to determine their composition. Combined with Focused Ion Beam (FIB) technique to expose 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 the use of 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. One CMOS product lot failed for 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 they were made of nitride or silicon and located beneath the nitride layer, which indicated that the defects were created before nitride film deposition. Based on the analytical and tool 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 a silica abrasive second step slurry. In this example, after copper CMP and two dielectric layers deposition, inline AIT inspection detected black spots on some of CMP wafers which are intermittent wafer to wafer. Auger and FIB analysis results revealed that the black spot defects were surface voids in the copper filled with Al, Si, O. This suggests that the defect could have been the product of copper corrosion caused by residual slurry from first-step polishing, and a possible incompatibility of the first- and second-step slurries as pad wear increases. As result of this finding, evaluation of different combinations of first- and second-step slurries has been initiated.

E9.36

Abstract Withdrawn

E9.37

Thermal Transformation of Hydrogen Bonds in a-SiC:H Films: Structural and Optical Properties. Andriy Vasin[1], S. P. Kolesnik[1], A. A. Konchits[1], V. S. Lysenko[1], A. N. Nazarov[1], A. V. Rusavsky[1] and S. Ashok[2]; [1]Institute of Semiconductor Physics, Kiev, Ukraine; [2]The Pennsylvania State University, University Park, Pennsylvania.

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, electron paramagnetic resonance (EPR), photoluminescence (PL) and Raman scattering. Thermal annealing was performed in vacuum (10^{-4} Pa) for 15 minutes over the temperature range 200 - 850 ^{0}C . As-deposited film showed weak room-temperature PL and a high concentration of paramagnetic centers N_s (3.2 x 10^{19} cm^{-3}). The PL band was centered at 2.3 eV and covered the entire visible range. After a 450 oC anneal, there was almost a decade change in the PL intensity, while Ns decreased by a similar order to 3.8 x 10^{18} cm^{-3}. For annealing temperatures above 450 ^{o}C, the PL intensity decreased and N_s increased monotonically. Analysis of the EPR line showed that in as-deposited films the spin was mostly related to carbon dangling bonds (g=2.0026), whereas silicon dangling bond signals (g=2.005) appeared after thermal annealing. The peak position and bandwidth (FWHM) of the PL band was almost unchanged after annealing while the optical band gap decreased significantly from the as-deposited value of 2.6 eV to 1.8 eV after annealing at 850 ^{o}C. We believe this to be evidence of inhomogeneity of the structure now composed of wide bandgap and low bandgap regions. Radiative recombination takes place in the wide gap regions while fundamental absorption edge is determined by low gap regions. Raman scattering measurements of the films annealed at high temperatures indicated formation of free amorphous carbon clusters. Chemical bonding of hydrogen in the films was analyzed by FTIR measurements in transmission geometry. As-deposited films showed three main absorption bands at about 800 cm^{-1}, 1100 cm^{-1} and 2100 cm^{-1}; we ascribe these to the Si-C stretching, C-H$_n$ wagging and Si-H$_n$ stretching modes respectively. The FTIR measurements also showed that the concentration of Si-H bonds steadily decreased with increasing anneal temperature. On the other hand the intensity of the C-H$_n$ absorption band changed in good correlation with the temperature dependence of PL intensity, N_s and optical band gap. We draw the following conclusion from our experimental data: At low annealing temperatures, the weak hydrogen bonds (including Si-H bonds) start to break. Released atomic hydrogen is trapped by carbon dangling bonds because the C-H bonds are still stable at such temperatures. Redistribution of hydrogen leads to a decrease of N_s and increase of PL intensity. At higher anneal 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 Photoelastic Stress Measurement Technique. X. H. Liu[1,3], H. J. Peng[1], N. Ke[1,3], S. P. Wong[1,3] and Shounan Zhao[2]; [1]Electronic Engineering, Chinese University of Hong Kong, Shatin, N.T., Hong Kong; [2]Applied Physics, South China University of Technology, Guangzhou, China; [3]Materials 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 infrared photoelastic method using a low level birefringence detection system [1]. This system has been applied to study the local stress distribution in Si under thin oxide layers. Because of the high sensitivity of this system, for the first time it was clearly showed that the local stress distribution under the thin oxide layer deviated from what predicted by bimetallic strip theory [2], and the deviation could be attributed to 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 stress measurement method to probe the defect distribution in the substrate. Details of the measurement system and quantitative analysis of the correlation between the process-induced defects and stresses will be presented and discussed. [1] H.J. Peng et al, Rev. Sci. Instr. 74 (2003) 4745. [2] X.H. Liu et al, Mat. Res. Soc. Symp. Proc. 821 (2004) P8.8.

E9.39

Defect Reduction in Si-based Metal-Semiconductor-Metal Photodetectors with Cryogenic Processed Schottky Contacts. 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 increased Schottky barrier height 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 substrate at 25 °C (RT) or -50 °C (LT). The devices fabricated using the LT process had better I-V characteristics compared to detectors fabricated using the standard room temperature (RT) metal deposition technique. The dark current for the LT film was found to be two orders lower in magnitude compared to the film deposited at RT. The dark current was significantly reduced from 4.06 to 0.089 nA. The active area for the device was determined to be 40 x 50 μm^2 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 0.73 eV. However, this 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 Photodetector Structure Treated with Hydrogen-Plasma. Hyoung Do Nam[1,2], Sung-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]; [1]Nano Devices Research center, KIST, Seoul, South Korea; [2]Dept. 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 5-stacked InAs dots in an InGaAs well structure. H-plasma treatment has been carried out at 150 oC for 10 min-40 min under 40 sccm of H2 gas flow rate and 10 W of RF power. After H-plasma treatment, photoluminescence (PL) intensities of 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 Warschkow[1], Hugh F Wilson[1], Nigel A Marks[1], Steven R Schofield[2,3], Neil J Curson[2], Phil V Smith[3], Marian W Radny[3], David R McKenzie[1] and Michelle Y Simmons[2]; [1]Centre for Quantum Computer Technology, School of Physics, The University of Sydney, Sydney, New South Wales, Australia; [2]Centre for Quantum Computer Technology, School of Physics, University of New South Wales, Sydney, New South Wales, Australia; [3]School 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. As reported elsewhere in this conference, extensive scanning tunneling microscopy (STM) experiments have identified a number of intermediate species of dissociation following low-dose PH3 exposure of the Si(001) surface at room-temperature. STM images sequences also show the conversion of these intermediates over time. On the basis of a comprehensive ab initio density functional survey of possible dissociation structures, their energetics and simulated STM images, we have been able to assign structures to the most prominent intermediate 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-by-step mechanisms for the two main paths 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
Chairs: Esidor Ntsoenzok and B.L. Sopori
Friday Morning, April 1, 2005
Room 2006 (Moscone West)

8:00 AM *E10.1

Hydrogen Interaction with Native Defects in Silicon. B. B. Nielsen, Physics and Astronomy, University of Aarhus, Aarhus, Denmark.

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

8:30 AM E10.2
Void Formation in Hydrogen Implanted and Subsequently Plasma Hydrogenated and Annealed Czochralski Silicon. Reinhart Job[1], Wolfgang Duengen[1], Yue Ma[1], Yuelong Huang[1], Lars O. Keller[2], Achim Wiggershaus[2] and John T. Horstmann[2]; [1]Electrical Engineering and Information Technology, University of Hagen, Hagen, Germany; [2]Electrical 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 (Cz) silicon wafers is studied by depth resolved micro-Raman spectroscopy. Standard (100)-oriented Cz Si wafers doping were used for the investigation. Hydrogen was implanted with an energy of 40 keV and a dose of 1E16 1/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 1/cm) and in voids (at 4150 1/cm) are analyzed to provide information about the evolution of vacancies and voids under our process conditions. During the hydrogen implantation vacancies are created serving as nuclei for voids, which are formed during the subsequent H-plasma treatments and annealing. After the plasma hydrogenation H-molecules trapped in vacancies can be observed by RS (3820 1/cm mode), if the substrate temperatures during the plasma exposure are not lower than 150 C. More insight can be obtained after post-hydrogenation annealing. The evolution of vacancies and voids is investigated in dependence on the annealing temperature. Transformations from vacancies to voids can be indirectly observed by RS. At lower annealing temperatures (T < 400 C) the 3820 1/cm mode (H-molecules in vacancies) is observed, while at higher temperatures the 3820 1/cm mode disappears and only the 4150 1/cm mode (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. Sungkweon Baek[1,2], Sungheo Heo[1], Dongkyu Lee[1], Won-Ju Cho[2], Kiju Im[2], Chang-Geun Ahn[2], Jong-Heon Yang[2], In-Bok Baek[2], Seongjae Lee[2] and Hyunsang Hwang[1]; [1]Material Science & Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea; [2]Future 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 the extreme limit of defect engineering. To obtain 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 resulted 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 regrowth rate for arsenic-implanted samples. Therefore, for the ultra-shallow junction less than 10nm, the control and understanding of hydrogen contained in the ambient and co-implanted during the plasma doping are necessary. In this study, the hydrogen was incorporated into the P, and As-implanted samples by hydrogen plasma doping. For the exact role of hydrogen, ion implantation energy and dose were divided into two regions. One is for containing the hydrogen profile(high energy & high dose), and the other is for overlapping the hydrogen profile with dopant profile(low energy & low dose/high dose). At the various annealing temperature of 600 900oC, 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 PH3 and B2H6, 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 stability of hydrogen donors in ZnO. To address these issues, we performed vibrational spectroscopy on bulk, single-crystal ZnO samples annealed in hydrogen (H_2) or deuterium (D_2) gas. Using infrared (IR) spectroscopy, we observed O-H and O-D stretch modes at 3326.3 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 hydrostatic 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 H_2 molecules, which have essentially no IR signature. Electrical measurements show a corresponding decrease in electron concentration, which is consistent with the formation of neutral H_2 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-0203832).

9:30 AM E10.5
Unusual Effects of Hydrogen in GaNP Alloys: A General Property of Dilute Nitrides. Irina A. Buyanova[1], M. Izadifard[1], I. G. Ivanov[1], J. Birch[1], Weimin M. Chen[1], M. Felici[2], A. Polimeni[2], M. Capizzi[2], Y. G. Hong[3], H. P. Xin[3] and C. W. Tu[3]; [1]Linkoping University, Linkoping, Sweden; [2]University of Rome "La Sapienza", Rome, Italy; [3]University 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, whereas the band structure of host lattices usually remains intact. In this work we report dramatic effects of hydrogen incorporation on the electronic structure and lattice properties of GaNxP1-x alloys with x< 0.008 grown by gas source molecular beam epitaxy. By employing photoluminescence (PL) excitation spectroscopy we show that post-growth hydrogenation not only leads to passivation of various N-related isoelectronic centers, starting from the ones which have the deepest energy levels in the bandgap, but also re-opens the band gap of the GaNP alloy and efficiently reduces the N-induced coupling between the Γ, X, and L conduction band states. By Raman spectroscopy, these effects are shown to be accompanied by hydrogen-induced breaking of the Ga-N bond in the alloy, evident from disappearance of the corresponding vibrational mode. According to the performed Raman and X-ray diffraction measurements, the hydrogenation is also found to cause strong expansion of the GaNP lattice which changes tensile strain in the as-grown GaNP epilayers to compressive strain in the post-hydrogenated structures.

SESSION E11: Defect Characterization
Chairs: Reinhart Job and Matthew D. McCluskey
Friday Morning, April 1, 2005
Room 2006 (Moscone West)

10:15 AM *E11.1
Three Dimensional Hydrogen Microscopy in Diamond.

Guenther Dollinger, Fakultat fur Luft - und Raumfahrttechnik, Institut fur Angewandte Physik und Messtechnik, Neubiberg, Germany.

We introduce proton-proton scattering at a microprobe of 17 MeV protons to quantitatively image three dimensional hydrogen distributions in polycrystalline diamond at a lateral resolution better 1 μm and high sensitivity. The images show that most of the hydrogen of a <110>-textured undoped polycrystalline diamond film is located at grain boundaries. The average amount of hydrogen is $(8.1\pm1.5)\cdot10^{14}$ atoms/cm$_2$ along the grain boundaries which corresponds to about a third of a monolayer. The content within the grain is below the detection limit of $1.4\cdot10^{16}$ at/cm^3 (0.08 at-ppm).

10:45 AM E11.2

Non Destructive Electrical Defect Characterisation and Topography of Silicon Wafers and Epitaxial Layers. Kay Dornich, T. Hahn and J. R. Niklas; Experimentelle Physik, Technical University Bergakademie, Freiberg, Germany.

Recent progress in the development of experimental technology made it possible to improve the sensitivity of microwave detected photoconductivity (MDP) by several orders of magnitude. This opens completely new possibilities for a contact less non-destructive electrical 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 down to 1 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 mappings 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 capture cross sections, however, again contact-less, non-destructive, and highly spatially resolved. Moreover, in contrast to DLTS, doping is not a critical parameter and the investigations are not restricted to just deep levels. We called this technique "microwave detected photo induced current transient spectroscopy (MD-PICTS)". MDP and 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.

11:00 AM E11.3

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

Variable-energy (beam-based) positron annihilation spectroscopy (VEPAS) has for two decades been applied successfully to the non-destructive study of open-volume point defects in thin films and in the first few microns beneath the surface of solids. Control of the energy of the implanted positrons, typically between 0.5 and 30 keV, allows one to gain some semi-quantitative information non-destructively on the depth profile of the defects. However, positron implantation profile broadening with increasing energy and pre-annihilation positron diffusion limit the detail one can obtain from these measurements. Here we demonstrate a significant enhancement in the depth profiling capabilities of VEPAS by combining conventional measurement with non-destructive chemical etching. Using this approach we have determined the depth distribution of open-volume point defects created by room-temperature implantation of Cz silicon by 100 keV B+ ions at a dose of 5 x1014 cm-2. The depth resolution of PAS is maintained at 50nm by using positrons implanted at energies below 2 keV to probe each layer as it is brought close to the surface by the etching process. The etch depths have been verified by using SIMS to profile the boron 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 50keV Si+ ion implantation at a dose of 5x1013cm-2 into Cz, FZ and epitaxially grown silicon.

11:15 AM E11.4

Electrical Characterization of MOS Structures and Wide Bandgap Semiconductors by Scanning Kelvin Probe Microscopy. Seong-Eun Park[1], Stoyan Jeliazkov[1], Joseph J. Kopanski[1], John Suehle[1], Eric Vogel[1], Albert Davydov[2] and Hyun-Keel Shin[3]; [1]Semiconductor Electronics Division, National Institute of Standards and Technology, Gaithersburg, Maryland; [2]Metallurgy Division, National Institute of Standards and Technology, Gaithersburg, Maryland; [3]Gwangju Techno Park, LED/LD Packaging Service Center, 958-3 Daechon-dong, Buk-gu, Gwangju 500-706, South Korea.

Electrical properties of Al (Ag, Cr)/SiO$_2$/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 (SHBs) were calculated. Measurements of metal work function and SiO$_2$ surface barrier height were sensitive to respective material surface condition. The oxidation or contamination of surfaces led to a decrease in the CPD. Furthermore, variations in work functions and SBHs were studied as a function of In or Al content in InGaN and AlGaN films. Variations in CPD at the interface of Al or B implanted SiC films were imaged to estimate doping levels.

11:30 AM E11.5

Comparison of Techniques for Measuring Recombination Lifetime in Semiconductors. Richard K. Ahrenkiel[1,2], Jamiyana Dashdorj[2,1], Steven Johnston[1] and Wyatt Metzger[1]; [1]Measurement and Characterization Division, National Renewable Energy Laboratory, Golden, Colorado; [2]Department 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 (QSSPC). Here we will present data and 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 photoconductance techniques (C and D) are especially sensitive to shallow (temporary) trapping effects. For the latter situation, the data must be properly massaged in order to extract real recombination lifetimes. Three of the techniques (A, C, and D) are suitable for measuring lifetime over a wide range of injection levels (injection-level spectroscopy, ILS. However, the photoconductance techniques (C and D) must include an algorithm to account for the variation of carrier mobility with injected carrier density. Although the TRPL technique provides the most unambiguous results for ILS studies, it is a functional lifetime-measurement technique only for the direct-bandgap semiconductors. Techniques A, B, and C are readily adaptable to the measurement of temperature-dependent lifetime. The latter has proven to be 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.

11:45 AM E11.6

Cavity Ring-Down Spectroscopy on Thin Films: Absolute and Highly-Sensitive Detection of Defect-Related Absorptions. I. M. P. Aarts, B. Hoex, W. M. M. Kessels and M. C. M. van de Sanden; Applied Physics, Eindhoven University of Technology, Eindhoven, Noord-Brabant, Netherlands.

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 direct and absolute detection 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 contribution, several key issues concerning 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 absorption coefficient with decreasing film thickness, indicating 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 measuring the absorption profile 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.