Title	Microstructure of the deep level defect E1/E2 in 6H silicon carbide (Abstract)
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photo-induced EPR experiments used to determine defect levels will be discussed, with a particular focus on the carbon vacancy. The use of high frequency EPR to resolve the many different types of centers in SiC will also be covered. Finally, the presentation will review the thermal stability of the intrinsic defects detected in as-grown 4H SiC. 1. M. E. Zvanut and V. V. Konovalov, Appl. Phys. Lett. 80, 410 (2002). 2. N.T. Son, Z. Zolnai, and E. Janzen, Phys. Rev. B64, 2452xx (2003). 3. W.E. Carlos, E.R. Glaser, and B.V. Shanabrook, in Proceedings of the 22nd conference on Defects in Semiconductors, Aarhus, Denmark, July 2003.

*The work at UAB was completed with the assistance of Dr. V. Konovalov and Ms. Haiyan Wang. The UAB studies are supported by Dr. Colin Wood, Office of Naval Research.

Contributed Papers

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P10 2 Role of intrinsic defects in compensation of high purity semi-insulating SiC* MARY ELLEN ZVANUT, HAIYAN WANG, *University of Alabama at Birmingham* WILLIAM C. MITCHEL, WILLIAM D. MITCHELL, *Air Force Research Laboratory, WPAFB* We report the use of photo-induced electron paramagnetic resonance (EPR) to study the role of the intrinsic defects in high purity semi-insulating (HPSI) 4H SiC to be used as substrates for high power devices. EPR measurements were conducted at 4 K prior to illumination and during photo-excitation, and temperature-dependent Hall measurements were performed up to 1000 K. Hall measurements indicated carrier activation energies between 1.1 and 1.4 eV, and EPR spectra revealed the positively charged carbon vacancy. After annealing at 1600 ^{o}C in Ar, results differed among several pieces cut from the same wafer. Some samples showed an increase in the activation energy, and EPR indicated removal of the carbon vacancy and a dominance of the shallow boron acceptor. On the other hand, both photo-EPR and Hall results for other pieces were unchanged by the heat treatment. The variation in results suggests that several defects may be involved in compensation, some of which anneal at temperatures below 1600 ^{o}C.

*This work is support by Dr. Colin Wood, ONR

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P10 3 Spectral Ellipsometry and Micro-Raman Investigations of MBE Grown GaN on 4H SiC TODD HOLDEN, *Applications* ZHIXUN MA, LYUDMILA MALIKOVA, VLADIMIR CHALDYSHEV, FRED H. POLLAK, *Brooklyn College of CUNY and Center for Advanced Technology in Ultrafast Materials and Applications* BENJAMIN HEYING, RANDY SANDHU, MIKE WOJTOWICZ, *Northrup Grummand Space Technology* Spectral ellipsometry is a powerful tool to Study $Ga_xAl_{1-x}N$ based heterostructure properties, such as material quality, interface quality, surface roughness layer thicknesses, and dielectric functions. The dielectric function and sample structure of several molecular beam epitaxy (MBE) grown GaN films on 4H SiC substrates (c-axis perpendicular to the surface) were studied using spectral ellipsometry for the energy range 0.8-5.3 eV. SiC is a desirable substrate for $Ga_xAl_{1-x}N$ based devices because of its relatively small lattice mismatch (1-4high thermal conductivity. Several samples, consisting of the SiC substrate, a 15 nm AlN nucleation layer, and 500 nm GaN, were grown under varying conditions. For energies below the fundamental bandgap of GaN, complicated interference patterns were observed due to the (birefringent) SiC and GaN layers. The data was analyzed using a uniaxial anisotropic model to allow for the birefringence of the SiC substrate. The extracted dielectric function of GaN was fit using a model taking into account both discrete and continuum excitonic effects for both the A and B excitons. The exciton binding energy was found to be 25 meV. Information about the nucleation layer, the layer thicknesses, the strain state, and the material quality were extracted from the study. Micro-Raman was used to determine the strain state and uniformity in the films from the E_2(high) peak of GaN. The strain in the GaN films from the ellipsometry determined fundamental bandgap agreed well with the Raman data.

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P10 4 Interface trap passivation for SiO_2/ (11$\bar{2}$0) 4H-SiC S. DHAR, *Interdisciplinary Materials Science, Vanderbilt University,Nashville, TN, U.S.A* Y.W. SONG, L.C. FELDMAN,* *Dept. of Physics and Astronomy, Vanderbilt University, Nashville, TN, U.S.A* J.R. WILLIAMS, T. ISAACS-SMITH, S. WANG, *Physics Dept. Auburn University, Auburn, AL, U.S.A* G. CHUNG, *Dow Corning Corporation,Midland, MI, U.S.A* High interface trap densities($> 10^{13}cm^{-2}eV^{-1}$) near band edges of 4H-SiC results in low inversion channel mobilities of 4H-SiC MOSFETs. Passivation of these traps and interface characterization has been a major challenge in the field of SiC MOS physics. Post-oxidation anneals (POA) in nitric oxide (NO) is an effective approach for significantly reducing the interface state density (D_{it}) on the (0001) 4H-SiC[1]. Another approach has been trying to find an alternate crystal face with improved interface properties. In particular, the (11$\bar{2}$0) face of 4H-SiC is a promising candidate[2]. We have reported recently that D_{it} of dry oxides grown on (0001) and (11$\bar{2}$0) are similar before and after the NO POA[3]. On both faces, the NO process lowers the D_{it} near the conduction band edge by an order of magnitude (from $\sim 10^{13}cm^{-2}eV^{-1}$ to $\sim 10^{12}cm^{-2}eV^{-1}$). In this paper, we report a further reduction of D_{it} on the (11-20) face by sequential anneals in NO and hydrogen from 1.5 x $10^{12}cm^{-2}eV^{-1}$ to 6 x $10^{11}cm^{-2}eV^{-1}$ at $\sim$ 0.1eV below the conduction band. Comparisons made with the (0001) Si-face and the (000$\bar{1}$) C face show a similar effect. Passivation of dangling bonds at the interface by hydrogen incorporation could be the dominant mechanism in this process. Current investigations of the hydrogen (deuterium) accumulation at the interface will also be described. References: 1. G.Y.Chung et. al., Appl. Surf. Sc. 184(2001) 399 2. H.Yano et.al., Jn. Appl. Phys. 78(2001) 374 3. S. Dhar et.al. submitted to Appl. Phys. Lett.

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P10 5 Microstructure of the deep level defect E1/E2 in 6H silicon carbide* C. C. LING, *Department of Physics, The University of Hong Kong* X. D. CHEN, *Department of Physics, The University of Hong Kong* M. GONG, *Department of Physics, Sichuan University* Deep level transient spectroscopy (DLTS) was used to study the deep level defects in low energy electron irradiated 6H-SiC materials. The electron energy was varied as 0.2MeV,

0.3MeV, 0.5MeV and 1.7MeV in order to study the threshold electron energy required to create the various deep levels. No deep level was observed after the 0.2MeV irradiation. Deep levels E1/E2 (EC-0.36/0.44eV) and Ei (EC-0.50eV) were observed after the 0.3MeV irradiation. By considering the minimum energy required to displace the carbon or the silicon atoms in the SiC lattice, it is concluded the creation of the E1/E2 and the Ei defects by the electron irradiation process involves the displacement of the carbon atom in the lattice. Our result suggests the deep levels E1/E2 and Ei should have a microstructure containing a carbon vacancy or a carbon interstitial.

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P10 6 Design of shallow donor levels in diamond by isovalent-donor coupling DAVID SEGEV, *National Renewable Energy Laboratory* SU-HUAI WEI, *National Renewable Energy Laboratory* Diamond can be doped p-type relatively easily by boron acceptors, but efficient shallow n-type doping is very difficult to achieve. Based on theorical considerations, we propose a new method to overcome the high ionization problem in n-type doping of diamond, by combining donor (e.g. N) with isovalent (e.g. Si) impurities. Using the first principles pseudopotential method, we show that Si induces fully occupied isovalent levels near the valence band maximum. The Si levels interact with N donor levels, making them much shallower. Moreover, the level repulsion decreases the energy of the fully occupied isovalent levels, and stabilizes the isovalent-donor complex. The donor transition energy level of the N+4Si defect complexes is found to be at 0.09 eV below the conduction band minimum, which is the shallowest level found so far for this system.

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P10 7 Electronic structure of thin heterocrystalline supperlattices in SiC and AlN M. S. MIAO, WALTER R. L. LAMBRECHT, *Department of Physics, Case Western Reserve University* We carefully examine the spontaneous polarization, the valence band offset and the confinement effect for this SiC and AlN cubic/hexagonal heterocrystalline superlattices(HCSL) by performing full potential linear muffin-tin orbital (FP-LMTO) calculations on a series of HCSL with growing number of cubic inclusion layers in the hexagonal region. We find that the polarization is significantly screened and reduced while the length of the cubic region grows. The band offsets do not change with layer thickness. For thin superlattices, the quantum confinement effects dominate and the gap stays always larger than the gap of the bulk cubic structure, which is in contrast to early studies in HCSL but consistent with the recent studies for stacking fault bands in 4H and 6H SiC. The energy levels of the bound states in the quantum well resemble the pattern of the energy levels of conventional III-V based quantum wells and superlattices but at a much smaller length scale, which is due to the higher quantum well depth and the larger effective masses in SiC and AlN systems.

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P10 8 Electronic structures of the quaternary wide band gap semiconductors (SiC)1-x(AlN)x TANG YU-HUI, *Department of Physics, National Sun Yat-Sen University, Kaohsiung, 804 Taiwan* TSAI MIN-HSIUNG, *Department of Physics, National Sun Yat-Sen University, Kaohsiung, 804 Taiwan* AlN and SiC have band gaps of 6.28 and 2.86eV, respectively. The quaternary semiconductors formed by SiC and AlN will have a wide range of band gaps. If these semiconductors have direct band gaps, the wavelength of the light emitted can be turned over a wide range. In this study, the first-principles molecular-dynamics (MD) calculation method has been first used to obtain atomic structures of these semiconductors. The first-principles pseudofunction calculation method has then been used to obtain the electronic structures based on the atomic structures determined by MD calculations. The lowest unoccupied energy levels at high symmetry k points, corresponding to F, K, L, and M, in the hexagonal Brillouin zone of a wurtzite structure have been calculated to find out the threshold of x for direct band gap. For the binary SiC, i.e. x=0, the lowest unoccupied energy levels at the K, L, and M points are lower than that at the F point while the valance band maximum is located at the F point, so the band gap is indirect. For the binary AlN, i.e. x=1, the conduction band minimum is at the F point and the band gap is direct. Our calculations show that at the lowest unoccupied energy level at the F point drops below those of K, L, and M points and the band gap becomes direct. Between and 1.00, the direct band gap varies from about 2.1 to 6.28eV, i.e. the wavelengths of the optoelectronic devices fabricated from (SiC)1-x(AlN)x can be turned over a wide range. This work was supported by the National Science Council of ROC (contract number NSC 91-2112-M-110-013).

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P10 9 Thermal effects in the size distribution of C induced roughness of Si(111) PATRICIO HBERLE, *Universidad T. Federico Santa Maria, Valparaiso, Chile* MARCOS FLORES, *Universidad T. Federico Santa Maria, Valparaiso, Chile* The strain-driven formation of three-dimensional coherent islands is a method for self-assembly of semiconductor nanostructures with potential applications in the architecture of novel semiconductor devices. In many of these applications the control of the surface roughness both in size and spatial distributions are essential. Frequently, the self-ordering of a single layer of islands is limited and therefore methods for enhancing island ordering are being vigorously studied by several techniques. We have studied the distribution of pyramid-shape islands on a Si(111) substrate using a UHV-STM. These nanostructures appear after annealing of a Si wafer with a high C bulk concentration. The thermal annealing, controlled by DC ohmic current was performed in steps. The first step, annealing at low temperatures, was different for each sample. Each one of them was subject to a different temperature between 500C and 800C for 12[h]. This procedure was followed, for all the samples, by a high temperature flash at 1100C (1min), and a subsequent gradual cooling. A typical STM image is shown. The flat surface is decorated by a distribution of pyramid-shape islands, which we assume are mostly Carbon Silicide (Si1-xCx), based in our in situ AES measurements. A series of volume and height distribution plots is shown. There are clear changes in the size distribution of the islands depending on the initial annealing temperature. Both volume and height distributions are narrower in