Monday Morning, November 15, 2004

Semiconductors
Room 304B - Session SC+MI-MoM

Dilute Magnetic and Ferromagnetic Semiconductors

Moderator: C.J. Palmström, University of Minnesota

8:20am **SC+MI-MoM1 Heterointerfaces and Magnetism in Ferromagnetic Semiconductor Heterostructures***, **N. Samarth,*** Pennsylvania State University **INVITED**

We discuss recent experiments that demonstrate how heterointerfaces impact the magnetic properties of heterostructures derived from the "canonical" ferromagnetic semiconductor (Ga,Mn)As. In this material, holes created by the Mn acceptors mediate a ferromagnetic interaction between the Mn ions themselves, and the Curie temperature is determined by a complex interplay between substitutional magnetic ions, interstitial defects and holes. Although as grown epilayers of (Ga,Mn)As typically have Curie temperatures lower than 110 K, post-growth annealing at low temperatures (180 C - 250 C) significantly enhances the ferromagnetic properties, leading to Curie temperatures above 150 K. The first set of experiments examines the effects of capping ferromagnetic Ga1-xMnxAs epilayers with a thin layer of undoped GaAs. We find that the overgrowth of even a few monolayers of GaAs significantly suppresses the enhancement of the ferromagnetism associated with low temperature annealing, suggesting that heterointerfaces have a direct impact on the migration of interstitial defects during post-growth annealing. In the next set of experiments, we demonstrate the first exchange biasing of (Ga,Mn)As by an overgrown antiferromagnet (MnO). Although the exchange bias effect is unambiguous when successful, we also find that the high reactivity between Mn and GaAs affects the ferromagnet/antiferromagnet heterointerface, presenting interesting experimental challenges for the routine achievement of exchange bias in this important spintronic material. This work was carried out in collaboration with K. C. Ku, M. B. Stone, K. F. Eid, P. Schiffer, T. Shih, and C. Palmstrom. Supported by ONR and DARPA.

9:00am **SC+MI-MoM3 Structural and Magnetic Properties of a Magnetic Semiconductor MnGeN@sub2@ Grown by MBE***, S.H. Cheung, M.L. Harland, V.K. Lazarov,* University of Wisconsin, Milwaukee*; Y. Zhang,* Peking University, China*; M. Weinert, M. Gajdardziska-Josifovska,* University of Wisconsin, Milwaukee*; Z. Gai,* Peking University, China*; **L. Li**,* University of Wisconsin, Milwaukee

A novel magnetic semiconductor MnGeN@sub2@ was synthesized on 6H-SiC(0001), Al@sub2@O@sub3@(0001), and MgO(111) substrates by plasma assisted molecular beam epitaxy. In situ reflection high-energy diffraction, ex situ atomic force microscopy and transmission electron microscopy (TEM) investigations indicate that the films grown are epitaxial on all three substrates, with the ones on MgO having the best overall quality. Detailed analysis of high-resolution TEM digital diffractograms and convergent beam electron diffraction patterns of the films show that the MnGeN@sub2@ is orthorhombic, and has the following crystallographic orientation relationships with the substrate: MnGeN@sub2@(001)//MgO(111), MnGeN@sub2@(100)//MgO(11-1), and MnGeN@sub2@(210)//MgO(01-1). Investigations by SQUID magnetometry indicate that the magnetic properties of the films can be controlled by the stoichiometry, i.e. Mn/Ge ratio, varying from paramagnetic to ferromagnetic, with the ferromagnetic samples exhibiting a Curie temperature above 300 K.

9:20am **SC+MI-MoM4 Thermal Stability of GaCrN Epitaxial Layers***, **G.T. Thaler**, R.M. Frazier, C.R. Abernathy, S.J. Pearton,* University of Florida

A number of recent studies have reported the observation of room temperature ferromagnetism in GaMnN. However, this material appears to be thermally unstable during processing at temperatures as low as 500°C unless co-doped with oxygen. For the development of spintronics devices based on GaN, thermal annealing at or above ~700°C is necessary to improve contact resistances and for p-dopant activation. An alternative material that has received some interest of late is GaCrN, which has also been reported to be ferromagnetic at room temperature. However, little is known as yet about the thermal stability of this material and its suitability for integration with GaN device processing technology. In this talk we will discuss the thermal stability of GaCrN and the effect of Cr concentration on both the as-grown magnetic behavior and the magnetic properties as a function of annealing. Epitaxial growth was performed using Gas Source Molecular Beam Epitaxy. Films with magnetic transition temperatures above room temperature were produced for a variety of Cr concentrations, though the signal appeared to maximize around 2-3% Cr, as is the case for GaMnN. Unlike GaMnN, the addition of Cr to GaN produced material that was thermally stable after annealing up to 700°C with little change observed in the magnetic behavior of the GaCrN films. The implications of this stability for device processing and performance will also be discussed. This work was supported by the Army Research office under: ARO-DAAD19-01-1-0701 and by NSF under: ECS-0224203.

9:40am **SC+MI-MoM5 Structural Characterization of GaMnN Thin Films Grown by Chemical Beam Epitaxy (CBE).***, **L.A. Carreno**, C. Boney, A. Bensaoula, Z. Zhang,* University of Houston

Diluted magnetic semiconductors (DMS) based on Mn doped GaN are intensively investigated for their potential spintronics applications. Ferromagnetism has been demonstrated in Mn-doped implanted p-type GaN, Mn-diffused GaN, and n-type films of GaMnN grown by MBE. Two approaches to understanding the magnetic properties of DMS materials are pursued: one considers these materials as more-or-less random alloys; the second one considers the magnetic atoms forming small clusters that produce the observed ferromagnetism. To clarify these issues we have performed structural analysis of GaMnN thin films grown by CBE using two in-situ time of flight (TOF) ion spectroscopy techniques combined with SARIC trajectory simulations. These were complemented with ex-situ XRD, PL, Raman spectroscopy, and Backscattering/ channeling combined with PIXE. GaMnN has been grown using TEG, NH@sub 3@, and solid Mn on sapphire/GaN templates prepared by CBE and MBE. Evolution of the stress for the as grown and annealed thin films has been studied by XRD and Raman. Samples grown on sapphire/GaN templates prepared by CBE show n-type conductivity, those grown on MBE GaN templates are highly resistive. The reactor is fitted with two in-situ TOF techniques, Direct Recoil Spectroscopy (DRS) and Mass Spectroscopy of Recoiled Ions. For structural characterization, azimuthal DRS scans are used to extract the surface periodicity and from that construct models of GaMnN surfaces. Simulations of scattering and recoiling scans for GaMnN surfaces have been performed for different possible lattice locations of Mn in GaN. Similar experiments were performed using Rutherford backscattering/channeling combined with particle induced X-ray emission. DRS confirmed retention of wurtzite crystal structure obtained by RHEED and XRD for Mn concentrations up to 2.5%. Although results have shown mainly substitutional incorporation of Mn atoms at Ga sites, DRS scans also show presence of Mn atoms at interstitial positions.

10:00am **SC+MI-MoM6 Induced Host Moments and Mn Electronic Structure in Mn-Doped Iii-V Ferromagnetic Semiconductors***, **D.J. Keavney**,* Argonne National Laboratory*; D. Wu, J. Shi,* University of Utah*; E. Johnston-Halperin, D.D. Awschalom,* University of California, Santa Barbara*; Y. Cui, L. Li,* University of Wisconsin-Milwaukee **INVITED**

We have used soft x-ray magnetic circular dichroism (XMCD) and absorption spectroscopy (XAS) to examine induced host magnetic moments and the local Mn environment in Mn-doped GaAs and GaN. X-ray absorption probes unoccupied states via transitions from deep core levels, thus providing electronic structure information with element specificity. With circularly polarized radiation at the L edges, element specific moments can be detected via their projection onto the Mn 3d and host 4s states, providing a test of predictions made by the carrier-mediated model of ordering. In (Ga,Mn)As, we find small XMCD signals at the onset of the absorption edge for both Ga and As, which we attribute to induced 4s moments. The relative orientations of all three elements are as expected for carrier-mediated coupling, and we estimate that the As moment is larger than the Ga moment. In (Ga,Mn)N, we detect a weak Ga XMCD signal 2-3 eV above the absorption edge of opposite sign to that in (Ga,Mn)As, which may be attributable to Mn 3d tails at the Ga sites. The absence of a Ga 4s moment would suggest a weaker p-d hybridization consistent with the deeper position of the Mn acceptor level. In both systems, XAS shows that Mn is divalent, although with differing amounts of line broadening, suggesting that the Mn 3d localization varies significantly depending on the host. (Ga,Mn)N has a lineshape closer to atomic Mn 2+ than (Ga,Mn)As. These results show that the Mn 3d and valence band electronic structure in doped III-V systems is strongly dependent on the host, and have implications for the degree of p-d hybridization and the coupling mechanism responsible for ferromagnetism. Use of the Advanced Photon Source was supported by the U.S. DOE, Office of Science, Contract No. W-31-109-Eng-38. Work at the Univ. of Utah was supported by ONR/DARPA grant No. N00014-02-10595, at UCSB by ONR/DARPA grant No. N00014-99-1-1096 and AFOSR F49620-02-10036, and at Univ. of Wisconsin by NSF DMR-0094105.

10:40am **SC+MI-MoM8 Intrinsic Versus Extrinsic Nature of Co Doped TiO@sub 2@ Diluted Magnetic Semiconductor Thin Films***, **S.R. Shinde**, S.B. Ogale, J. Higgins, T. Zhao,* University of Maryland*; S.E. Lofland,* Rowan University*; V.N. Kulkarni,* University of Maryland*; A.J. Millis,* Columbia University*; S. Das Sarma, R.L. Greene, R. Ramesh, T. Venkatesan,* University of Maryland

The issue of Co distribution in TiO@sub 2@ (in anatase and rutile forms), a widely studied oxide based diluted magnetic semiconductor (DMS) system, is still controversial. Although all the reported studies have discovered room temperature ferromagnetism in this system, some of the researchers claim that the material is intrinsic, whereas others have found that cobalt forms small clusters and therefore the material has extrinsic origin of ferromagnetism. In our work we have grown (by pulsed laser deposition) and characterized epitaxial thin films of Co:TiO@sub 2@ at different growth conditions and Co doping concentrations. We noticed that Co distribution strongly depends on the growth parameters. At lower growth temperature (~700C) there is a limited solubility of Co (up to ~2%) above which nanometer sized Co clusters are formed. When the films are grown in ultrahigh vacuum (10-8 Torr), the films have low resistivity and show the anomalous Hall effect. Although this could be interpreted as a signature of carrier induced DMS nature of these particular films, our detailed magnetic and structural analysis shows the presence of Co nanoclusters in these films. In the magnetization data of these films we observe superparamagnetism with a blocking temperature of 250K. This temperature corresponds to Co particles of 7nm diameter, the presence of which was further confirmed by transmission electron microscopy (TEM). On the other hand, when the films grown at lower temperature are annealed at high temperature (~900C) the clusters dissolve in titanium dioxide matrix leading to an intrinsic DMS with a Curie temperature ~650C. Similar properties are observed for films directly grown at high temperature and no indication of any clustering of Co is observed in TEM. We have also observed electric field induced reversible modulations, in the magnetization of these films in PbZr@sub 0.2@Ti@sub 0.8@O@sub 3@/Co:TiO@sub 2@/SrRuO@sub 3@ field effect transistor structure.

11:00am **SC+MI-MoM9 Ferroelectric Field Effect on Ferromagnetism in Diluted Magnetic Insulator Anatase Co:TiO@sub2@***, **T. Zhao**, S.R. Shinde, S.B. Ogale, H. Zheng, T. Venkatesan,* University of Maryland*; R. Ramesh,* University of California, Berkeley*; S. Das Sarma,* University of Maryland*; J. Misewich,* Brookhaven National Laboratory

Recently considerable success is reported in making a non-magnetic semiconductor ferromagnetic by dilute doping of magnetic impurities. However, the possibilities of extrinsic effects such as dopant clustering, impurity magnetic phases etc., have not been completely ruled out in many systems. In this work we report the first successful implementation of an external electric field modulation of ferromagnetism in an oxide-based DMS anatase Co:TiO@sub2@. An anatase TiO2 layer with 7% Co doping and a ferroelectric PbZr@sub0.2@Ti@sub0.8@O@sub3@ layer were epitaxially grown on a conducting SrRuO@sub3@ buffered LaAlO@sub3@ substrate by pulsed laser deposition. The high-quality of epitaxy and uniform distribution of Co were confirmed by X-Ray diffraction and transmission electron microcopy. The Co:TiO@sub2@ channel grown in this case at a high temperature of 875°C is insulating in nature. The magnetic hysteresis loops of the Co:TiO@sub2@ were measured by superconducting quantum interference device after positive or negative electric poling on PZT. The room temperature saturated magnetic moment clearly shows two stable states which are reversible by switching the ferroelectric polarization. The observed effect, which is about 15% in strength can be modulated over several cycles. This first demonstration of electric field effect in an oxide based diluted ferromagnetic insulator system provides evidence of its intrinsic nature. Furthermore, the ability of electric field modulation of ferromagnetism is very promising for next-generation multi-functional electronic devices. Possible mechanisms for electric field induced modulation of insulating ferromagnetism are discussed. This work was supported by DARPA SpinS program (through US-ONR) and the NSF-MRSEC (DMR 00-80008) at Maryland. The PLD and RBS facilities used in this work are shared experimental facilities (SEF) supported in part under NSF-MRSEC.

11:20am **SC+MI-MoM10 Applications of a Dilute Magnetic Semiconductor Based on AlN***, **R.M. Frazier**, G.T. Thaler, J.Y. Leifer, C.R. Abernathy, S.J. Pearton,* University of Florida

With the increasing interest in spintronics, many attempts have been made at incorporating spin-based functionality into existing semiconductor technology. One approach, utilizing dilute magnetic semiconductors (DMS) formed via introduction of transition metal ions into III-Nitride hosts, would allow for integration of spin based phenomena into current wide bandgap technology. Further, the use of AlN broadens III-V DMS applications to tunneling devices and UV light emitters. The most evident application of ferromagnetic AlN is as a ferromagnetic tunnel barrier, similar to EuS, but unlike EuS should allow for operation at room temperature. Ion implantation has been shown to be an effective survey method for introduction of various transition metals into AlN. However, it is not a technique which will allow for the development of advanced spin based devices. Such devices will require epitaxial methods of the sort currently used for synthesis of III-Nitride optoelectronics. In this study, one such technique, Gas Source Molecular Beam Epitaxy (GSMBE) has been used to synthesize AlN films doped with Cr and Mn. In the Mn doped films, increasing the V/III ratio corresponded to an increased magnetic signal, indicating an increase in active Mn sites. In the case of both Mn and Cr doped AlN, the magnetic signal was found to depend on the flux of the dopant, and the optimal growth conditions were found. Growth of tunnel devices using AlTMN as a barrier will also be discussed. This work is supported by the Army Research Office under ARO-DAAD19-01-0-0701 and NSF under ECS-0224203.

11:40am **SC+MI-MoM11 Ferromagnetism and Polaron Percolation in Mn@sub x@Ge@sub 1-x@ Dilute Magnetic Semiconductor***, **A.P. Li**, J.F. Wendelken, J. Shen,* Oak Ridge National Laboratory*; J.R. Thompson, H.H. Weitering,* Oak Ridge National Laboratory, University of Tennessee

In dilute magnetic semiconductors (DMS), ferromagnetic ordering is carrier mediated. This picture seems to be accepted more or less universally, but the detailed nature of the ferromagnetism varies greatly from system to system. We have studied ferromagnetism and the correlation between transport and ferromagnetism in Mn@sub x@Ge@sub 1-x@ DMS for Mn concentrations up to 9%. By carefully controlling the growth conditions, we obtained precipitate-free Mn@sub x@Ge@sub 1-x@ that exhibits magnetic phase transitions at Tc = 20 K and Tc* = 112 K. The magnetic response to temperature and doping concentration is indicative of a magnetic-polaron percolation transition at Tc [1], which coincides with a metal-insulator transition and Hall-effect sign anomaly. Tc* is the ferromagnetic ordering temperature within isolated polarons which can be determined from a Curie-Weiss plot of the high-temperature magnetic susceptibility. Ferromagnetism in Mn@sub x@Ge@sub 1-x@ DMS reveals a striking analogy with the magnetism of so-called "clustered states" in manganite compounds [2]. [1] A. Kaminski and S. Das Sarma, Phys. Rev. B 68, 235210 (2003) [2] G. Alvarez and E. Dagotto, Phys. Rev. B 68, 045202 (2003).

Semiconductors
Room 304C - Session SC-TuA
Semiconductor Heteroepitaxy and Nanostructures

Moderator: R.S. Goldman, University of Michigan

1:20pm **SC-TuA1 Lattice Mismatched Heteroepitaxy: Evolution and Revolution***, **E.A. Fitzgerald**,* Massachusetts Institute of Technology **INVITED**

The scientific understanding of lattice-mismatched epitaxy has lead to a third era in the applications of epitaxy. Epitaxy was applied in applications benefiting from lattice-matched materials, and has migrated to applications with mild lattice-mismatch, such as the SiGe HBT and the InGaAs pHEMT. Today, we are able to create relaxed lattice constants that have significant lattice-mismatch with respect to bulk substrate, and in turn use those lattice constants to create extremely high levels of strain in new and conventional materials. In this talk, we will review the general principles of strain-relaxed epitaxy and show how new SiGe templates on Si have extended the electron and hole mobility in SiGe materials to unforeseen enhancements. Such enhancements promise to increase the current drive in MOSFET transistors at a time when smaller transistors are losing their driving efficacy as scaling continues. We show that strained SiGe nanochannels are most likely shaping the vertical wavefunction of carriers, leading to the very high enhancements in mobility despite very high vertical fields. New structures that not only add strain but are further engineered for robust processing will be presented.

2:00pm **SC-TuA3 Strain Relaxation of MBE-grown Step-Graded Metamorphic InAsP Buffers on InP Substrates***, **M.K. Hudait**, Y. Lin, S.A. Ringel,* The Ohio State University

Step-graded metamorphic InAsP buffers grown on InP substrates to increase the substrate lattice constant are of interest to support a range of high-speed electronic and infrared optoelectronic devices. Recent work by our group has shown that grading the composition of the anion sublattice using InAsP buffers as opposed to the group-III cation sublattice using InAlAs buffers is advantageous for MBE growth for such applications since decoupling the growth rate from the composition control results in superior morphological and thermophotovoltaic device properties. Here, we discuss the strain relaxation properties of step-graded InAs@sub y@P@sub 1-y@ (y=0.32-0.4) buffers, representing a total misfit of ~1.1-1.2% with respect to InP. For this study, InAsP buffers were grown on both (100) and 2° off-cut (100) InP substrates under identical MBE growth conditions with an average grading rate of 20% As/µm. The relaxation of each layer within each buffer was measured along [1-10] and [110] directions using TAXRD to evaluate asymmetric relaxation and tilt relative to the initial substrate orientation. For both substrate types, the strain relaxation was found to be symmetric and greater than 90% for the top InAs@sub 0.4@P@sub 0.6@ layer. This indicates that @alpha@ ([1-10] direction) and @beta@ ([110] direction) slip systems have similar activation energies for dislocation nucleation. Moreover, a small epilayer tilt of ~20-190 arcsec was observed for both substrate orientations, which indicates that tilt generated by @alpha@ and @beta@ dislocations will be in proportion to the substrate offcut resolved in [110] and [1-10] directions, respectively. The relation between these observations and properties of group-V and group-III core dislocations will be made to optimize the growth of these buffers. Correlations with the strain relaxation properties, surface morphology and cross-sectional interface properties will also be made as a function of substrate misorientation.

2:20pm **SC-TuA4 Molecular Beam Epitaxy of High-quality Ge on Si by Self-directed "Touchdown" of Nanoscale Seed Pads Through a Thin SiO2 Layer***, Q. Li, D. Leonhardt, Y.B. Jiang, H. Xu, S.R.J. Brueck, S. Hersee, **S.M. Han**,* University of New Mexico

Growing a lattice-mismatched, dislocation-free epitaxial film on Si has been a challenge for many years. Herein, we exploit nanoheteroepitaxy to grow high-quality Ge epilayer on Si. A 1.2-nm-thick chemical SiO@sub 2@ film is produced on Si in a H@sub 2@O@sub 2@ and H@sub 2@SO@sub 4@ solution. When the chemically oxidized Si substrate is exposed to Ge molecular beam, relatively uniform-size nanoscale seed pads form in the oxide layer and "touch down" on the underlying Si substrate. Although the "touchdown" location is random, the seed pad growth is self-limiting to 7 nm in size. Upon continued exposure, Ge selectively grows on the seed pads rather than on SiO@sub 2@, and the seeds coalesce to form an epitaxial lateral overgrowth (ELO) layer. The Ge ELO layer is characterized by high-resolution, cross-sectional transmission electron microscopy (XTEM), Raman spectroscopy, and etch-pit density (EPD). The XTEM images reveal that the Ge ELO layer is free of dislocation network and that the epilayer is fully relaxed at 2 nm from the heterojunction. The Raman shift of Ge optical phonon mode exactly matches that of relaxed bulk Ge, further supporting that the ELO layer is fully relaxed. The XTEM images, however, show that stacking faults exist near the Ge-SiO@sub 2@ interface. A small fraction (~4x10@super -3@%) of these stacking faults propagate to the epilayer surface and form etch pits, when immersed in a solution containing HF, HNO@sub 3@, glacial acetic acid, and I@sub 2@. The resulting EPD is consistently less than 2x10@super 6@ cm@super -2@. The reduction of strain density near the Ge-Si heterojunction, leading to high quality Ge ELO layer, is mainly attributed to a high density (~10@super 11@ cm@super -2@) of nanoscale Ge seed pads interspaced by 2- to 12-nm-wide SiO@sub 2@ patches. This "touchdown" technique may potentially enable growing other highly lattice-mismatched epilayers on Si, such as GaN and SiC.

2:40pm **SC-TuA5 Tuning of the Emission Wavelength of Self-assembled InAs/InP (001) Quantum Dots using Grown-in Defects and Ion Implantation***, **C. Dion**, N. Shtinkov,* École Polytechnique de Montréal, Canada*; S. Raymond,* Conseil National de Recherche du Canada, Canada*; M. Chicoine, F. Schiettekatte,* Université de Montréal, Canada*; P.J. Poole,* Conseil National de Recherche du Canada, Canada*; R.A. Masut, P. Desjardins,* École Polytechnique de Montréal, Canada

We have investigated the effect of post-growth rapid thermal annealing (RTA), grown-in defects, and ion implantation on the low temperature photoluminescence (PL) spectra of self-assembled InAs/InP(001) quantum dots (QD) grown by chemical beam epitaxy (CBE) and metal-organic vapor phase epitaxy (MOVPE) in order to develop a detailed understanding of the key diffusion mechanisms involved in such defect-mediated intermixing techniques. In untreated samples, blueshifts of up to 90 meV in the PL spectra are observed after RTA at 800 °C for 210s with no broadening of the emission peak. We attribute this thermally induced shift to the diffusion of group V atoms between the QD and the surrounding material. In order to promote interdiffusion and to obtain larger blueshifts, we have studied the effect of introducing point defects into an InP capping layer, far from the QD region, either by growing InP at low temperature or by implanting P atoms at doses ranging from 10@super11@ to 10@super 14@ ion/cm@super 2@. The introduction of grown-in defects results in a marked increased in PL shifts, which can reach up to 250 meV following RTA at 765 °C for 90 s, revealing that the excess of points defects in that layer promote interdiffusion in the QD region. Even more dramatic effects are measured in ion implanted sample for which significant blueshifts of 300 meV can be observed following anneals at temperatures as low as 400 °C. In order to quantify these effects, we carried out tight-binding calculations of the transition energies in thin diffused quantum wells. Experimental results for the emission of the wetting layer and our simulations indicate that ion implantation leads to an important reduction of the activation energy for As/P interdiffusion to values as small as 0.4 ± 0.2 eV.

3:00pm **SC-TuA6 Gated Si/SiGe Quantum Dots with Low Charge Noise***, **L.J. Klein**, S. Goswami, K.A. Slinker, K.L.M. Lewis, S.N. Coppersmith, D.W. van der Weide, M.A. Eriksson,* University of Wisconsin, Madison*; J.O. Chu, J.A. Ott, P.M. Mooney,* IBM, TJ Watson Research Center

The stability and noise affecting single electron charging in quantum dots fabricated in a Si/SiGe heterostructure are investigated. Electron beam lithography and subsequent reactive ion etching are used to define the quantum dot. The dot potential and electron density are modified by laterally defined side gates in the plane of the dot. Low temperature measurements (0.2 K) show Coulomb blockade with a single electron charging energy of 4 meV. The long term stability of the Coulomb blockade oscillations is determined in part by the number and stability of electrons captured in trap states in the vicinity of the quantum dot. Motion of this trapped charge modifies the dot potential and is detected as discrete shifts in the Coulomb blockade peak positions. Thermally annealing the sample (400C in Ar) after reactive ion etching reduces the charge noise from such trap states, allowing the acquisition of stable Coulomb diamond data over several hours. Tunnel-coupled double quantum dots have been fabricated and measured using similar techniques. The potential application of such Si/SiGe quantum dots for spin based quantum computation is discussed.

3:20pm **SC-TuA7 Blue Photoluminescence of Si Nano-crystallites Embedded in Silicon Oxide*, G.-J. Kim,*** *J.H. Kim, K.A. Jeon, S.Y. Lee,* Yonsei University, Korea

Synthesis and luminescent characteristics of Si nano-crystallites are reported depending on deposition condition. Si nanocrystalline thin films on p-type (100) silicon substrate have been prepared by a pulsed laser deposition (PLD) technique using a Nd:YAG laser. The Si nano-crystallites with the average size of 2 nm are observed in the SiO@sub 2@ matrix. Strong blue photoluminescence has been observed at room temperature. The optical and structural properties of thin films have been investigated as a function of laser energy density, ambient gas pressure, annealing, and oxidation process. These results indicate that the blue photoluminescence of Si nano-crystallites is related to the quantum size effect of Si nanocrystallites.

3:40pm **SC-TuA8 Silicon Nanocrystal Formation in an Oxide Matrix: Chemical and Strain Effects*, D. Yu,*** *G.S. Hwang,* The University of Texas at Austin

Nanocrystalline Si (nc-Si) embedded in an oxide matrix has received great attention due to its promising applications for advanced electronic and optical devices. The unique electrical and optical properties of oxide-embedded nc-Si appear to be strongly influenced by the crystallite size, shape, density, and oxide composition. It is therefore necessary to develop a detailed understanding of the nc-Si growth. We have developed a multiscale computational model for nc-Si synthesis in an oxide matrix by phase separation of silicon suboxide. This multiscale approach combines i) first principles quantum mechanics calculations of fundamental processes and ii) kinetic Monte Carlo simulations of long-time scale phase separation. Using the computational approach, we have identified formation mechanism of Si clusters in silicon suboxide. In this talk, first we will present fundamental processes involved in the phase separation including: i) Si interstitial behavior in an oxide and ii) O diffusion energetics which depends on strain and chemical environment. Based on these results, we will discuss the relative contribution of strain and suboxide penalty to the phase separation. Finally, we will present the process of Si particle formation, together with a comparison to experimental observations.

Semiconductors
Room Exhibit Hall B - Session SC-TuP
Poster Session

SC-TuP1 Epitaxial Growth of GaN on Sapphire by RF-MOMBE*, S.Y. Kuo,* National Science Council, Taiwan, R.O.C.*; C.C. Kei,* National Science Council, Taiwan, Taiwan, R.O.C.*; C.K. Chao,* National Central University, Taiwan*; J.S. Chen,* National Science Council, Taiwan*; S.Y. Huang,* National Taiwan University, Taiwan*;* ***C.N. Hsiao,*** National Science Council, Taiwan, R.O.C.

A self-designed radio-frequency plasma metal organic molecular beam epitaxy (RF-MOMBE) system is developed to study III-nitride semiconductors. The surface morphologies and crystal structures were monitored by in-situ reflection high energy electron diffraction (RHEED). Up to 4 inches substrates of sapphire, silicon and other materials were available. Followed by substrate nitridation, a low temperature buffer layer was deposited to facilitate growth of III-nitride films on large lattice mismatched substrates. The III-nitride films were characterized by photoluminescence spectrometry, x-ray diffraction, scanning electron microscopy and transmission electron microscopy. The effect of growth temperature and III-V ratio on crystallinity and surface morphologies of III-nitride films was prominent. High quality III-nitride films were achieved by well optimized condition.

SC-TuP2 Comparison of Ga- and N-polar GaN Surfaces*,* ***R.P. Bhatta,*** *B.D. Thoms,* Georgia State University*; C.R. Eddy, Jr., R.T. Holm, R.L. Henry,* Naval Research Laboratory

Growth of wurtzite GaN(0001) thin films by metalorganic chemical vapor deposition (MOCVD) may produce either Ga- or N-polar surfaces resulting in differences in surface termination, electronic structure, and chemical reactivity. GaN surfaces of both polarities have been characterized, in particular by their reaction with atomic hydrogen and deuterium. Auger Electron Spectroscopy (AES) and Low Energy Electron Diffraction (LEED) showed that the surfaces were clean and ordered. Electron Energy Loss Spectroscopy (EELS) and High Resolution Electron Energy loss Spectroscopy (HREELS) were used to characterize the electronic and vibrational properties of the surfaces. After cleaning the N-polar surface by sputtering with 1 keV nitrogen ions and annealing to 900 @degree@C, HREELS showed Fuchs-Kliewer phonons, N-H stretching vibrations, and combination losses, which indicate that hydrogen is present on the surface after annealing. HREELS following exposure to atomic hydrogen (deuterium) confirmed the assignment of surface N-H (N-D) and showed no sign of surface Ga-H (Ga-D) species. In addition, heating to temperatures from 400 to 900 @degree@C was not sufficient to remove the surface N-H species. In contrast, HREELS of the Ga-polar surface after sputtering and annealing showed Fuchs-Kliewer phonons but not any adsorbate loss peaks, which indicates a hydrogen-free surface. HREELS following exposure to atomic hydrogen (deuterium) reveals Ga-H (Ga-D) stretching vibrations along with combination modes, but no N-H (N-D) vibrational modes are observed. Hydrogen is desorbed completely from this surface below 400 @degree@C. In addition to differences in surface termination and chemical reactivity, EELS was used to characterize differences in the electronic structure of the hydrogenated Ga- and N- polar surfaces.

SC-TuP3 Ohmic Contacts to AlGaN*, S.E. Mohney, H.J. Wang,* ***M.A. Horsey,*** The Pennsylvania State University*; B.A. Hull,* Cree, Inc.

Research on ohmic contacts to Al@sub x@Ga@sub 1-x@N of high Al fraction (x) is presented. The work was motivated by the requirements for low resistance ohmic contacts for short-wavelength devices. In the work on ohmic contacts to n-Al@sub x@Ga@sub 1-x@N with x = 0.6, we have achieved reproducible contact resistivities of 4 x 10@sup -6@ Ohm-cm@sup 2@ with V/Al/V/Au contacts, even without reactive ion etching prior to metallization. These contacts exhibit relatively smooth surface morphologies. We have also investigated the interfacial reactions in these contacts using transmission electron microscopy and Auger electron spectroscopy to provide more information on the mechanism for forming a low resistance ohmic contact. For contacts to p-Al@sub x@Ga@sub 1-x@N (x = 0.45), we have identified annealing conditions required to achieve ohmic contacts, and we discuss the need for passivation of the p-Al@sub x@Ga@sub 1-x@N surface in order to avoid degradation from exposure to light, due we believe to traps at the semiconductor surface. We also describe the relationship between the resistance of the contacts and the interfacial reactions between the contacts and p-Al@sub x@Ga@sub 1-x@N.

SC-TuP4 Fabrication and Properties of Thin Film Photon Sieve Diffractive Lens*,* ***N. Bradman****, H. Chung, M. Davidson, P.H. Holloway, K. Woo, D. Tanner, S. Selcuk, A. Hebard,* University of Florida*; O. Shenderova, A. Shenderova, G.E. McGuire,* International Technology Center

Photon sieves are diffractive lens that offer better focusing than Fresnel zone plates and are lighter weight and lower volume than refractive lens. The photon sieve lens in this study consists of a transparent substrate coated with an opaque metal thin film with a pattern of holes in a circular array. The size of the holes range from above to below the wavelength of light being focused. Fabrication of the photon sieve lens will be described, which consists of a thin electron beam metallization, pattern writing by electron beam lithography, and pattern development by reactive ion etching. In addition to significant reductions in weight and volume, photon sieves offer a larger field of view than refractive optics, but they suffer from poor transmission. Surface plasmon resonant coupling will be reported to improve the transmission by factors of two to five at the resonant wavelength. The coupling of the surface plasmon resonant structure with the photon sieve pattern will be discussed. Transmission data for traditional and modified photon sieves will be presented and compared.

SC-TuP5 Etch Characteristics of Sapphire using Inductively Coupled Plasmas*,* ***Y.J. Sung****, T. Jang, K.K. Choi, S.H. Chae, Y.H. Kim, J.S. Kwak, O.H. Nam, Y. Park,* Samsung Advanced Institute of Technology, South Korea

Sapphire has been widely used as a substrate for epitaxial growth of GaN-based optoelectronic devices due to its high chemical and thermal stability. Therefore it is essential to understand the dry etching technique in order to fabricate advanced optoelectronic devices. Recently, researches on the various etching of sapphire such as inductively coupled plasma etching, ion beam etching, chemical wet etching after ion implantation, reactive ion etching, etc. have been carried out and have focused on achievement of high etch rates and high selectivity over etch mask. In case of GaN-based laser diodes and light emitting diodes, various sapphire etching methods have been applied to techniques such as epitaxial lateral overgrowth(ELO) and lateral epitaxial patterned sapphire substrates(LEPS) to reduce dislocation density in GaN layer. However, until now there have been only a few works on the etching of sapphire and its properties. In this study, inductively coupled plasmas were used to etch sapphire. The effects of etch parameters such as gas combination of BCl@sub3@/ Cl@sub2@ and BCl@sub3@/Cl@sub2@/Ar, inductive power (400- 800Watts), bias voltage (-100--300Volts), and operational pressure (3-30mTorr) on the etch characteristics such as etch selectivity and etch properties of sapphire were investigated. To investigate the etch mechanism of sapphire, optical emissions from the plasmas during the etch process were monitored in situ and the sapphire surface composition after the etching was observed by X-ray photoelectron spectroscopy.

SC-TuP6 Exact-Exchange-Based Quasiparticle Calculations of II-VI Compounds and Group III Nitrides*,* ***P. Rinke,*** Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany*; A. Qteish,* Yarmouk University, Jordan*; J. Neugebauer,* University of Paderborn, Germany*; M. Scheffler,* Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany

We present a systematic ab initio study of the electronic structure for a wide range of II-VI compounds and group III nitrides in the zinc-blende structure. The challenge from a computational point of view is to capture the exchange-correlation effects arising from the shallow semicore d-electrons of the cation, which we explicitly treat as valence states in our pseudopotential approach. In order to correctly describe the dominant exchange interaction we apply density-functional theory (DFT) in the exact-exchange (EXX) approximation. Although the EXX Kohn-Sham bandstructure compares well with experiment for standard semiconductors@footnote 1@ the bandstructure as measured by photoemission is a property of the excited system. We therefore apply many-body perturbation theory in the GW approximation to the EXX groundstate. The hirarchy of our approach allows us to systematically investigate the role of exchange and correlation in these materials from first principles. Our results show that it is crucial to treat exchange and correlation on the same footing at every stage. To achieve this in our EXX calculations we employ the newly developed EXX-pseudopotentials@footnote 2@. Furthermore we obtain GW bandstructures in very good agreement with existing all-electron GW calculations. Our results indicate that, in contrast to common believe, a pseudopotential approach including only the d-electrons of the semicore shell in question, is sufficient to accurately describe the electronic structure if treated in the EXX+GW formalism. @FootnoteText@ @footnote 1@ W.

G. Aulbur et al, Phys. Rev. B 62, 7121 (2000)@footnote 2@ M. Moukara et al, J. Phys.: Condens. Matter 12, 6783 (2000) .

SC-TuP7 Transparent Conducting Oxides Based on ZnO by Reactive Sputtering, ***M.A. Santana-Aranda,*** Instituto Mexicano del Petroleo, México; *M. Meléndez-Lira,* Centro de Investigación y Estudios Avanzados, México, Mexico; *M. Becerril-Silva, S.J. Jiménez-Sandoval,* Centro de Investigación y Estudios Avanzados, México

Transparent conducting oxides have a broad variety of applications in the electric and optoelectronic industries. Applications like conducting window material for solar cells as well as active layers of LEDs and laser diodes emitting in the UV. We have employed reactive sputtering to deposit ZnO and Al:ZnO thin films on glass substrates. The target was formed with zinc and aluminum circular plates; we controlled the aluminum content changing the ratio of Al/Zn areas. Surface morphology and aluminum content were monitored with a scanning electron microscope. X ray diffraction and Raman spectroscopy measurements were performed to monitor the crystalline structure of the films. The energy of the absorption edge was monitored by optical transmission measurements. The changes observed in the absorption edge are related with the changes in the aluminum content of the films. Resistivity of the films was determined by electrical measurements, these results are also well correlated with the aluminum content.

SC-TuP8 XPS and UPS Study of ZnO:N Thin Films, ***C.L. Perkins,*** National Renewable Energy Laboratory; *X. Li,* University of Texas at Arlington; *S. Asher, T.J. Coutts, S.-H. Lee,* National Renewable Energy Laboratory

There are strong motivations for obtaining nitrogen-doped p-type ZnO, including the possibilities of air-stable, high quality UV lasers, detectors, and efficient photocatalytic water splitting. Problems remain with the growth of this material however. Reproducibility of conductivity type is difficult, and the distributions and identities of nitrogen species in N-containing ZnO films are not well known. Although theory predicts that N can be incorporated in at least two different states, one of which, N@sub 2@ occupying a position on the oxygen sublattice (N@sub 2O@) should be a double shallow donor, and the other, NO, being the desired acceptor, there have been few determinations of the chemical states of nitrogen in ZnO:N materials. In order to gain a better understanding of their chemical and electronic properties, we have examined via XPS and UPS thin films of ZnO:N produced by two different methods. MOCVD films were grown using diethylzinc and nitric oxide. Sputtered films were produced with a Zn target and a mixture of O@sub 2@ and N@sub 2@. Core level photoemission shows that the films contain 0.5-2.5 % nitrogen, and that the nitrogen occupies at least four different chemical environments. With UPS the relative positions of the films' valence bands are determined with respect to the Fermi level. Results from the thin polycrystalline films are compared to initial results obtained on ZnO(0001) single crystals reacted in UHV with nitric oxide, and with data obtained from N-implanted Zn foil. Definitive XPS peak assignments are made for N@sub 2O@, N@sub O@, and two other nitrogen chemical states that have not previously been identified in ZnO:N.

SC-TuP9 Electrical Characteristics of Al-doped ZnO (Al-ZnO) Films and their Application to Al-ZnO/p-Si Solar Cells, ***T. Ichinohe,*** *S. Masaki,* Tokyo National College of Technology, Japan; *K. Kawasaki,* TDY Co., Ltd., Japan

We fabricated aluminum doped zinc oxide (Al-ZnO) films by DC-magnetron sputter-deposition. The films showed n-type semiconductor characteristics: they were electron carriers with a negative coefficient of resistivity. We attempted to fabricate a p-n junction structure using Al-ZnO films formed on a p/p@super +@-Si epitaxial substrate. The Al-ZnO/p-Si structure showed rectified I-V characteristics, indicating a p-n junction has been fabricated. The photocurrent for reverse bias increased to several hundred times higher than dark current when a halogen lamp irradiated its surface. The open circuit voltage (V@sub oc@) increased when the halogen lamp power was increased, and the value saturated at about 0.2 V. We infer that the value of V@sub oc@ is appropriate for built-in potential (0.3 eV) in the interface of Al-ZnO/p-Si, as estimated by the Kelvin-probe work function measurement system. Energy efficiency of the Al-ZnO/p-Si structure was about 1.2%, as estimated by the standard quasi-solar light exposure system. Reducing the resistivity of Al-ZnO films and the contact resistance of the cell structure can further increase the energy efficiency.

SC-TuP10 Supermagnetron Plasma CVD of Amorphous CNx:H Films Using Rf Power-Ratio Control, ***H. Kinoshita,*** *R. Ikuta, K. Sakurai,* Shizuoka University, Japan

Amorphous CNx:H films were deposited on lower electrode using i-C4H10/N2 supermagnetron plasma CVD. @footnote 1@ By a control of rf power-ratio, hard and soft CNx:H films were deposited at upper electrode rf power of 800W. Above the lower electrode rf power (LORF) of 40W, CNx:H films became hard and opaque. Below LORF of 20W, however, CNx:H films became soft and transparent. The optical band gap of hard film was below 0.8eV and that of soft film was above 1.9eV. Hardness of hard film was above 19GPa and that of soft film was about 7GPa. Electrical resistivity of hard film was low and that of soft film was high. Soft films showed white photoluminescence. @FootnoteText@ @footnote 1@H.Kinoshita and T.Murakami, J.Vac.Sci.Tecnol.A 20, (2002) 403.

Semiconductors
Room 304C - Session SC-WeA

Narrow Gap Semiconductors

Moderator: J. Zinck, Hughes Research Laboratories

2:00pm **SC-WeA1 Growth and Properties of Dilute Nitride Semiconductors with a Bismuth Surfactant***, **T. Tiedje**, D,A, Beaton, S. Tixier, M.B. Whitwick, E.C. Young, N.R. Zangenberg,* University of British Columbia, Canada*; S. Francoeur,* National Renewable Energy Laboratory **INVITED**

The dilute nitride semiconductor In@suby@Ga@sub1-y@As@sub1-x@N@subx@ is a promising new III-V alloy for solar cells and lasers in which low concentrations of N cause an anomalous reduction in the bandgap. N alloying degrades the electronic properties, possibly through formation of localized N cluster states. We show that the electronic properties of GaAs@sub1-x@N@subx@ can be improved with the use of a Bi surfactant during plasma assisted MBE growth. The effect of modifying the active nitrogen species (ratio of atoms to excited state molecules) in plasma-assisted MBE growth has also been explored. The Bi surfactant reduces the surface roughness by a factor of ten and produces step flow growth at temperatures as low as 460°C. The surfactant also improves the room temperature photoluminescence (PL) efficiency in as-grown and annealed samples, and reduces the density of shallow gap states, as determined from the shape of the PL spectra. The N incorporation increases with the Bi coverage by up to 50% when the surface is saturated with Bi. In-situ mass spectroscopy experiments show that NAs (but not NBi) is present in the gas phase, during growth and that the partial pressure of NAs increases slightly with Bi flux, suggesting that the Bi surface layer enhances the reaction of active nitrogen with GaAs. The Bi covers the surface but does not incorporate (@450°C. If the As:Ga flux ratio is reduced to approximately 1:1, Bi will incorporate at low substrate temperatures (380°C). The dilute Bi alloys show room temperature photoluminescence @footnote1@ and similar to the dilute nitrides the bandgap has an anomalously large concentration dependence. @FootnoteText@ @footnote1@S. Tixier et al, Appl. Phys. Lett. 82, 2245 (2003).

2:40pm **SC-WeA3 Nitrogen Incorporation in GaAsN Films and GaAsN/GaAs Superlattices***, **H.A. McKay**, M. Reason, X. Weng, N. Rudawski, W. Ye, V. Rotberg, R.S. Goldman,* University of Michigan

GaAsN and InGaAsN alloys with a few percent N have potential applications in infrared laser diodes, high efficiency solar cells, and other electronic devices. However, as-grown materials often exhibit poor photoluminescence efficiencies and lower than expected carrier concentrations and mobilities. A few studies have suggested that control of N incorporation via ex-situ annealing or superlattice (SL) growth may lead to improved optical and electronic properties. In this work, we are exploring in-situ approaches to controlling N incorporation during the growth of GaAsN films and GaAsN/GaAs SLs. In the case of GaAsN films, we have investigated N incorporation in GaAsN films grown by solid-source molecular beam epitaxy (MBE) using a 10% N@sub 2@/90%Ar or pure N@sub 2@ RF plasma source, with As@sub 2@ or As@sub 4@, and a variety of growth temperatures, Si-doping, and V/III ratios. Nuclear Reaction Analysis and Rutherford Backscattering Spectrometry in channeling and non-channeling conditions reveal significant composition-dependent non-substitutional incorporation of N, presumably as N-N or N-As split interstitials. We find that non-substitutional N incorporation is minimized for films grown at 400@super o@C with pure N@sub 2@, apparently independent of As species, Si-doping, and V/III ratio. In the case of GaAsN/GaAs SLs, we have developed an in-situ approach to prevent incorporation of N into the GaAs barriers of the superlattice, using an independently-pumped plasma source chamber, separated from the MBE via a gate valve. High-resolution x-ray diffraction studies reveal significant improvements in the interface quality for superlattices prepared with the active N flux controlled via the gate valve in comparison with a conventional shuttering approach. The effects of N incorporation on the electrical and optical properties of GaAsN films and GaAsN/GaAs SLs will also be presented. @FootnoteText@ This work is supported by DOE, AFOSR-MURI, NSF-NER, NASA-Lewis, and TRW.

3:00pm **SC-WeA4 Optical Properties of GaAs@sub 1-x@N@sub x@: A Tight Binding and Variable Angle Spectroscopic Ellipsometry Study***, **S. Turcotte**, S. Larouche, J.-N. Beaudry, N. Shtinkov, L. Martinu, R.A. Masut,* École Polytechnique de Montréal, Canada*; R. Leonelli,* Université de Montréal, Canada*; P. Desjardins,* École Polytechnique de Montréal, Canada

We have carried out a series of tight-binding (TB) calculations and variable-angle spectroscopic ellipsometry (VASE) measurements in order to investigate the excited states above the band gap of GaAs@sub 1-x@N@sub x@ layers on GaAs(001). The calculations are carried out using an empirical TB model in the sp@super 3@d@super 5@s*s@sub N@ parameterization, which provides a band-anticrossing description of the GaAs@sub 1-x@N@sub x@ band structure over the entire Brillouin zone for energies up to 5 eV above the valence band maximum. A series of fully-coherent GaAs@sub 1-x@N@sub x@ layers with x up to 0.012 were grown on GaAs(001) by organometallic vapor phase epitaxy using trimethylgallium, tertiarybutylarsine, and dimethylhydrazine precursors. The GaAsN dielectric function was reliably determined from 0.76 to 4.4 eV through point by point fitting of the experimental data with a model which also takes into account the GaAs substrate and the oxide overlayer. In addition to the band edge transition E@sub -@, the L point related optical transition E@sub 1@ and their split-off replica, we also observe, for the first time in room temperature VASE measurements, the E@sub +@ level signature which appears as a well defined critical point contribution to the dielectric function. The comparison between experimental data and TB calculations provides information on the specific contributions of the different Brillouin zone points to the GaAsN dispersion curves.

3:20pm **SC-WeA5 Growth Modes of InN on Sapphire (0001) with GaN Buffer Layers***, S.R. Leone,* University of California*; **B. Liu**, D.X. Chen,* Lawrence Berkeley National Laboratory*; T. Kitajima,* National Defense Academy of Japan

InN is an important group-III nitride semiconductor. Use of InN can extend the working wavelength of the nitride-based optoelectronic devices from ultraviolet to infrared. However, heteroepitaxy of InN has encountered difficulties due to the thermal instability of InN and the large lattice mismatches between InN and the commonly used substrates (e.g., sapphire). During growth, the high equilibrium pressure of nitrogen requires a high V/III flux ratio to suppress InN decomposition, which often results in undesired three-dimensional (3D) rough surfaces. In this work, using atomic force microscopy (AFM) and scanning tunneling microscopy (STM), we study the growth modes and the surface morphologies of InN grown by plasma-assisted molecular beam epitaxy on sapphire (0001) substrates with intermediate GaN buffer layers. With smooth GaN buffer layers, 3D InN islands are observed to have mesa-like shapes with atomically flat tops. However, prolonged growth in this mode does not produce continuous two-dimensional (2D) InN films by coalescence of InN islands. With 3D rough GaN buffer layers, continuous 2D InN films are obtained showing the characteristics of step-flow growth. STM imaging reveals the defect-mediated surface morphology of the 2D InN films, including surface termination of screw (or mixed) dislocations and a high density of shallow surface pits with depths of about 0.1 nm. The mechanisms of the different growth modes and surface defect formation are also discussed.

3:40pm **SC-WeA6 Energy Gap and Stokes-like Shift in Cubic In@sub x@ Ga@sub 1-x@N Epitaxial Layers***, DG Pacheco-Salazar, J.R.L. Fernandez,* University of Sao Paulo, Brazil*; **J. Soares**,* University of Illinois at Urbana Champaign*; J.R. Leite,* University of Sao Paulo, Brazil*; F. Cerdeira, E.A. Meneses,* University of Campinas, Brazil*; S.F. Li, O. Husberg, D.J. As, K. Lischka,* University of Paderborn, Germany

Group-III nitrides have been intensively investigated due to their recent applications in optoelectronic and electronic devices. The light emission mechanism of efficient blue-green-ultraviolet LED and laser diodes based on these materials is still object of investigation, and several works have been carried out recently on the optical properties of the In@sub x@Ga@sub 1-x@N alloy, the active medium in these optoelectronic devices. In the present work photoluminescence (PL), photoluminescence excitation (PLE) and Cathodoluminescence (CL) are used to investigate emission and absorption mechanisms in cubic 100 nm thick In@sub x@Ga@sub 1-x@N epitaxial layers grown on thick GaN/GaAs(001) buffer layers by MBE. High resolution x-ray diffraction (HRXRD) revealed that the InGaN layers were pseudomorphic with the GaN buffer. The In fraction x was calculated from the strained lattice constants obtained from the HRXRD reciprocal space maps. Reflectivity was used to measure the thickness of our films. PL and PLE spectra were recorded at 7 K and 300 K.

CL spectra were performed at room temperature. The main features observed in the PL spectra are the characteristic emission from the band edge region of c-GaN and a lower energy peak which we ascribe to the InGaN layer. From the PLE spectra, we have determinated the alloy energy gap as a function of the In content. Comparing results from PL and PLE we observe a large Stokes-like shift for all samples. Another absorption band at lower energy than that of the alloy energy gap is observed on some of the PLE spectra. We tentatively ascribe this band to an absorption mechanism taking place in In-rich regions in the InGaN alloy. These findings are supported by a multi-peak structure obtained by PL and depth-resolved CL. In depht-resolved CL, the relative intensity of the peaks changes with increasing excitation depth, indicating a second InGaN fase close to the GaN/InGaN interface.

4:00pm **SC-WeA7 InAs-based Heterojunction Bipolar Transistors**, ***P.W. Deelman****, P.D. Brewer, D.H. Chow, K.R. Elliott, T. Hussain, R.D. Rajavel, S.S. Thomas, III,* HRL Laboratories **INVITED**

We have demonstrated the first InAs-based heterojunction bipolar transistors (HBTs) with f@sub T@ and f@sub max@ simultaneously exceeding 100GHz. Our best small-area (0.4 × 3.0 @micron@@super 2@) HBTs feature an f@sub T@ of 215GHz, a V@sub be@ of 0.35V, and a @beta@ of 60. Using similar devices, we have successfully fabricated the world's first InAs-based integrated circuit - - - a divide-by-sixteen circuit operating at 27GHz. The divider consists of 62 transistors fabricated on a 3" wafer. The promise that HBTs nearly-lattice-matched to InAs potentially operate at higher frequencies and with lower power-delay products than current technologies motivated this work. Nevertheless, we have had to overcome several materials-related obstacles in order to achieve these results. For example, insulating substrates for the 6.1@Ao@ family of materials do not exist, and the nature of the band alignments in these materials dictate that at least one, if not all, the layers in the structure be strained. We employed two approaches to deal with the substrate issues. InAs transistors were grown by molecular beam epitaxy either on InP substrates using semi-insulating, strain-relaxed AlGaAsSb buffers or coherently on 3" InAs substrates. The latter approach required subsequent wafer bonding to sapphire carriers. Our baseline structures utilized either an InAsP or AlInAs emitter and an InAs base. For some devices, the emitter was graded to reduce strain energy. Current gain decreases for base doping levels above 1×10@super 19@ cm@super -3@; however, even with heavily Be-doped (~2 × 19 cm@super -3@) InAs bases, we obtain high @beta@ (>60). Numerical simulations provide an insight into the deleterious implications of Be diffusion, the degree of which can be manipulated through the MBE growth process. The work described in this talk was sponsored by DARPA/SPAWAR under contract number N66000-01-C-8033.

4:40pm **SC-WeA9 Lattice Constant Differences and Their Affect on the Surface Bonding of In@sub 2@O and Ga@sub 2@O on GaAs and InAs**, ***M.J. Hale****, D.L. Winn, J.Z. Sexton, M. Passlack, A.C. Kummel,* University of California, San Diego

The atomic bonding structures formed upon deposition of In@sub 2@O on GaAs(001)-c(2x8)/(2x4) and InAs(001)-c(2x8)/(2x4) were identified through scanning tunneling microscopy and density functional theory calculations. These results were compared to the surface bonding structure of Ga@sub 2@O deposited on GaAs(001)-c(2x8)/(2x4). It was found that In@sub 2@O forms three distinct bonding configurations on the GaAs(001)-c(2x8)/(2x4) surface: two different configurations which span the trough, and one which inserts into row arsenic dimer pairs. When In@sub 2@--O was deposited on the InAs(001)-c(2x8)/(2x4) surface only the row As dimer pair site was observed. This effect is attributed to the In@sub 2@O molecule being large enough to span the 8.0Å trough of the GaAs(001)-c(2x8)/(2x4) surface, but too small to span the 8.6Å trough of InAs(001)-c(2x8)/(2x4). The In@sub 2@O bonding site on InAs(001)-c(2x8)/(2x4) is analogous to the binding site for Ga@sub 2@O on GaAs(001)-c(2x8)/(2x4), where Ga@sub 2@O is found to bond only in row arsenic dimer pairs. The change in lattice constant between InAs and GaAs is also found to have an affect on Fermi level pinning. Through experiments and DFT calculations, we have shown that In@sub 2@O pins GaAs whereas Ga@sub 2@O does not. DFT calculations also show that we should not expect In@sub 2@O to pin InAs. Our results show that a modest change in lattice constant can dramatically alter the adsorbate bonding and electronic structure via a change in site selectivity.

5:00pm **SC-WeA10 An Atomic Understanding of the Sub-Monolayer Interface formed Upon the Deposition of SiO on GaAs(001)-c(2x8)/(2x4)}**, ***D.L. Winn****, M.J. Hale, J.Z. Sexton, M. Passlack, A.C. Kummel,* University of California, San Diego

Scientists have been trying to develop a GaAs-based MOSFET device in an effort to reduce standby power and gate leakage. To achieve this it is important to understand the chemistry at the oxide/semiconductor interface. The interface formed upon deposition of SiO on GaAs(001)-c(2x8)/(2x4) was studied using STM, scanning tunneling spectroscopy (STS) and DFT. STM images show that SiO molecules bond Si end down in three distinct locations: into row and trough As dimers and between row As dimers. It was also observed that when SiO bonds between row As dimers, the two adjacent dimers along the [1bar10] direction each contain an inserted SiO molecule forming a chain of three molecules (triple site). STS measurements show that ~5% of a monolayer of SiO pins the Fermi level at mid gap. This is consistent with SiO absorbates withdrawing charge from surface As atoms, causing charge on the As atoms to grossly deviate from the charge on bulk As atoms. Multiple SiO sites were simulated using DFT, the lowest energy structure however was not observed in STM. An energy versus chemical potential plot was used to explain and identify the most stable bonding structures in the coverage studied with STM. This plot showed that at low SiO coverages the most stable sites were single sites but at higher coverages the most stable sites shifted to sites involving three SiO molecules including the triple site. This work demonstrates the key role of coverage in determining the most stable bonding structure. For oxides on semiconductors there are usually multiple nearly degenerate bonding configurations and the coverage is the key variable in determining the relative chemical potentials

Semiconductors
Room 304B - Session SC+EM-ThM
Wide Bandgap Semiconductors

Moderator: D.D. Koleske, Sandia National Laboratories

8:20am **SC+EM-ThM1 HVP-CVD: A Novel Chemical Vapor Deposition Approach for Zinc Oxide Synthesis***, **T.M. Barnes**, J. Leaf, C. Fry, C.A. Wolden,* Colorado School of Mines

Zinc oxide (ZnO) is a versatile II-VI semiconductor that has generated tremendous interest due to its unique combination of optical, electronic and mechanical properties. High vacuum plasma-assisted chemical vapor deposition (HVP-CVD) is introduced as a novel technique for the deposition of zinc oxide and the study of the associated surface chemistry. An inductively coupled plasma (ICP) source was used for the generation of atomic oxygen and other radicals. Radicals from the ICP source and organometallic precursors diffuse into a high vacuum environment where they combine to form metal oxide thin films on a heated substrate. The process is differentiated from conventional CVD approaches in that the collisionless environment precludes gas-phase reactions with the metal precursor. Advantages of the HVP-CVD approach were demonstrated for zinc oxide growth using dimethyl zinc. Notable achievements include high growth rates of highly oriented material, room temperature formation of (002)oriented ZnO, and nitrogen doping. The underlying process chemistry was investigated using a combination of in-situ diagnostics and ex-situ materials characterization. Optical emission spectroscopy (OES) and quadrupole mass spectrometry (QMS) were used to monitor the ICP source and deposition environment, respectively. In the case of intrinsic ZnO, the growth kinetics were found to be first order in dimethyl zinc and zero order in atomic oxygen. QMS analysis suggests that growth proceeds through an elegant pathway in which the methyl ligands simply desorb without oxidation. Nitrogen doping was achieved by replacing oxygen with N@sub 2@O in the ICP source. The mechanism of nitrogen incorporation is discussed in light of film properties and characterization of the deposition environment.

8:40am **SC+EM-ThM2 Realization of Mg(x=0.15)Zn(1-x=0.85)O based Metal-Semiconductor-Metal UV Detector on Quartz and Sapphire***, S. Hullavarad,* University of Maryland*; **R. Vispute**,* Bluewave Semiconductors, Inc.*; T. Venkatesan, S. Dhar, I. Takeuchi,* University of Maryland

MgZnO is a novel oxide based UV sensitive material. The band gap of MgxZn1-xO can be tuned by varying the composition of Mg to achieve band gaps corresponding to UV-A, UV-B, UV-C regions of UV spectrum. This material is of significant importance for various applications in flame sensors, UV index monitors and missile plume detection. The interesting property that makes this material unique is its existence in multiple phases for different Mg compositions. This allows picking up desired Mg composition corresponding to suitable UV sensitive window and growing on lattice matched substrate. In this paper we present the growth of MgZnO on non-conventional substrates like quartz and on sapphire for comparison of the device reliability. MgZnO films are characterized by X-Ray Diffraction, UV-Visible spectroscopy and Rutherford Back Scattering - channeling techniques. We are reporting for the first time the highly oriented growth of MgZnO on quartz by Pulsed Laser Deposition technique with a RBS channeling yield of 50% showing highly ordering. The morphology of the films is studied by Atomic Force Microscopy. The metal-semiconductor-metal device was fabricated on the MgZnO film to study the device response under proper UV irradiation.

9:00am **SC+EM-ThM3 A Non-Traditional Approach to Low-Temperature Nitride Thin Film Deposition and Nanoscale Device Fabrication***, **M.A. Hoffbauer**, A.H. Mueller, E.A. Akhadov, M.A. Petruska, V.I. Klimov,* Los Alamos National Laboratory **INVITED**

Using energetic neutral atoms to control interfacial chemistry opens new opportunities for low temperature materials processing and device fabrication at the nanoscale. We are developing a unique low-temperature thin film growth and etching technology, exclusive to LANL, called Energetic Neutral Atom Beam Lithography/Epitaxy (ENABLE) that utilizes neutral reactive atomic species (e.g. N and O) with kinetic energies comparable to chemical bonds strengths (a few eV) for growing nitride and oxide thin films at low temperatures and for etching very high-aspect-ratio features into polymers. Co-depositing metals onto substrates simultaneously exposed to energetic N-atoms permits device quality GaN-based semiconducting films to be grown at temperatures ranging from ambient to greater than 500 C on a variety of substrates (including plastics). Characterization details regarding film crystallinity, epitaxy, stoichiometry, and optical properties will be discussed. Low-temperature GaN film deposition permits semiconducting nanocrystals (NCs) synthesized by colloidal chemistry and having size-controlled emission wavelengths to be encapsulated in a GaN-based matrix. Devices based on p-i-n structures show direct charge injection and electroluminescence from the NCs. Using energetic oxygen atoms to selectively etch various nanoscale features in polymeric films yields sub-100 nm features with aspect ratios exceeding 35:1. Examples will be shown where ENABLE is used to directly grow patterned nitride thin film structures by combining the capability to etch polymer templates with subsequent low-temperature thin film growth. Future prospects and challenges for low-temperature ENABLE-based nanoscale fabrication along with progress towards an efficient multicolor (white) light source based on a NC LED device will be presented.

9:40am **SC+EM-ThM5 Confined Epitaxial Growth of GaN for Defect Reduction and Device Development***, **C.R. Eddy, Jr.**, R.T. Holm, R.L. Henry, M.E. Twigg, N.D. Bassim, L.M. Shirey, F.K. Perkins,* Naval Research Laboratory*; M.C. Peckerar,* University of Maryland*; E.J. Cukauskas,* Sachs Freeman Associates

The family of III-V nitride materials has been the subject of many device technology development efforts, including visible and ultraviolet light emitters and detectors and high power rf transistors. Another area of interest is the development of vertically conducting device technologies for power electronics. In such applications it is critical that the threading dislocations inherent in this heteroeptixial materials system (no native substrate) be eliminated, particularly in the active region of the device. These threading dislocations have been identified as sources of leakage currents and premature failure of voltage blocking devices. In this work, an approach to reduce/eliminate vertical threading dislocations is described and initial results presented. The approach involves confined homo- or hetero-epitaxy of GaN materials using sputtered oxide masks to delineate growth regions. Growth is carried out using conventional MOCVD and conditions that inhibit lateral growth over the mask. The resulting confined epitaxial material is terminated with equilibrium crystal facets that form hexagonal mesas. The material contains a reduced dislocation density (approximately one order of magnitude as determined by TEM) compared to the underlying template layer for homoepitaxial growth. This reduction in dislocation density is believed to be the result of reduced strain in the epitaxial volume and the presence of the free surfaces represented by the sidewalls of the mesa. Characterization of pn junction diodes grown in this manner reveals significantly reduced leakage currents in as-grown structures (1 @mu@A/cm@super2@), which can be further reduced with application of passivation coatings. The approach is well suited to the development of distributed diode device technologies appropriate for power device applications. Issues such as doping variations in the confined epitaxial regions and the impact of additional device filtering techniques will also be presented.

10:00am **SC+EM-ThM6 Conductive Atomic Force Microscopy Studies of Forward and Reverse Current Conduction in GaN Films***, **A.A. Baski**, J. Spradlin, S. Dogan, H. Morkoc,* Virginia Commonwealth University

We have investigated the current conduction of homo- and heteroepitaxial GaN-based films using conductive atomic force microscopy (C-AFM). For the case of a homoepitaxial film grown by MBE on HVPE template, C-AFM shows premature current breakdown at the centers of hillocks associated with screw dislocations, consistent with the results of other groups. Local C-AFM current-voltage curves of such dislocations indicate a Frenkel-Poole mechanism for forward conduction on defective regions, as opposed to field emission on non-defective regions. In the case of heteroepitaxial GaN films grown on sapphire, C-AFM data do not show a straightforward correlation between topography and current conduction. We observe, however, that films with more rectifying Schottky behavior via standard I-V measurements produce forward and reverse bias C-AFM images with strong asymmetry. In addition, standard I-V data indicate a field emission (forward bias) or hopping (reverse bias) mechanism for a high quality rectifying film, and a Frenkel-Poole mechanism for a lower quality film. This behavior is consistent with the C-AFM I-V data of defective regions on the homoepitaxial film, which also show Frenkel-Poole conduction in forward bias.

10:20am **SC+EM-ThM7 Thin-Film Diamond Electronics: Progress and Expectations***, **J.E. Gerbi**,* Argonne National Laboratory **INVITED**

Diamond has long been thought to have the potential to revolutionize electronics due to its exceptional single-crystal properties, including extremely high thermal conductivities and carrier mobilities. Unfortunately, major roadblocks exist for both the growth of affordable single-crystal diamond, and especially for the doping of such material. Non-single crystal diamond, while suffering the degradation of some important single crystal diamond properties, does nevertheless show promise as an extremely useful electronic material. A review of such materials will be given, with emphasis on how the structure of various types of polycrystalline diamond affects key electronic properties. The ability to dope polycrystalline diamond in non-traditional ways will be discussed, as will the integration of diamond thin films in a device environment. Finally, prototype room-temperature device fabrication and performance will be discussed. The emphasis will be made that the field of d iamond electronics continues to make significant progress, especially for niche applications such as MEMS and chemical sensors. This work was supported by the DOE-Office of Science-Materials Science under Contract No. W-31-109-ENG-38.

11:00am **SC+EM-ThM9 X-ray Absorption and Emission Studies of Diamond Nanoparticles***, T. van Buuren,* Lawrence Livermore National Laboratory*; C. Bostedt,* HASYLAB at DESY, Hamburg, Germany*; **T.M. Willey**, R.W. Meulenberg,* Lawrence Livermore National Laboratory*; J.Y. Raty,* University of Liege, Belgium*; G. Galli, L.J. Terminello,* Lawrence Livermore National Laboratory

Carbon nanoparticles, produced in detonations, are found to have a core of diamond with a coating fullerene-like carbon. X-ray diffraction and TEM show that the nanodiamonds are crystalline and approximately 4 nm in diameter. These nano-sized diamonds do not display the charateristic property of other group IV nanoparticles: a strong widening of the energy gap between the conduction and valence bands owing to quantum-confinement effects. For nano-sized diamond with a size distribution of 4 nm, there is no shift of the band energies relative to bulk diamond@footnote 1@. The C 1s core exciton feature clearly observed in the K-edge absorption of bulk diamond is attenuated and broadened in the nanodiamond case due to increased overlap of the excited electron with the core hole in the small particle. Also the depth of the second gap in the nanodiamond spectra is shallower than that of bulk diamond. A feature at lower energy in the X-ray absorption spectra that is not present in the bulk samples is consistent with a fullerene like surface reconstruction. By exposing the diamond nanoparticles to an Argon / Oxygen plasma then annealing in a UHV environment, we have obtained a hydrogen free surface. The nanodiamonds processed in this manner show an increase fullerene type contribution in the carbon x-ray absorption pre-edge. High spatial resolution EELS measurements of the empty states of a single nanodiamond particle acquired with a filed emission TEM also show the core of the particle is bulk diamond like whereas the surface has a fullerene like structure. Density-functional theory calculations on clusters show an increase in bandgap only for clusters smaller than 1 nm, and confirm the fullerene-like surface reconstruction. @FootnoteText@ This work is supported by the U.S. DOE, BES Materials Sciences under contract W-7405-ENG-48, LLNL.@footnote 1@ J. Y. Raty, G. Galli, C. Bostedt, T. van Buuren, L. J. Terminello, Phys. Rev. Lett. 90, p.401 (2003) .

11:20am **SC+EM-ThM10 Direct Electronic Sensing of Biological Binding Events on Diamond Thin Films***, **W. Yang**,* University of Wisconsin-Madison*; J.E. Butler, J.N. Russell, Jr.,* Naval Research Laboratory*; R.J. Hamers,* University of Wisconsin-Madison

The chemical and physical inertness of diamond combined with its semiconducting electrical properties make it an attractive substrate for biological sensing. We have investigated the direct covalent modification of diamond with a variety of biomolecules including DNA and antibodies, and have investigated the relationships between the interfacial structure and the resulting electrical response observed upon DNA hybridization and antibody-antigen binding. The biological sensitivity and selectivity on diamond surfaces have been optimized using traditional fluorescence methods. By using electrical impedance spectroscopy (EIS), we have been able to detect DNA hybridization and antigen-antibody interactions in real time with high sensitivity. EIS measurements allow us to map out the impedance response as functions of both frequency and potential, helping to separate the electrical properties of the diamond space-charge region, the molecular layers, and the remaining solution. At low frequencies binding can be detected by the ion diffusion through the modified interfacial layers. At higher frequencies binding can be detected through a field effect induced in the diamond. The field effect mechanism allows us to directly detect biological molecules based on the different molecular charges. Complementary measurements on n-type and p-type silicon confirm the overall picture of the transduction process. Our results suggest the possibility of fabricating biological FET devices on diamond thin films.

11:40am **SC+EM-ThM11 Enormous Photocurrent for Hydrogenated Single-crystalline B-doped Diamond Epilayers Grown by Microwave-excited Plasma Chemical Vapor Deposition.***, **Y.K. Koide**,* National Institute for Materials Science (NIMS), Japan

Diamond with energy band-gap of 5.5 eV is an attractive semiconductor for applying to a visible-blind photodetector operated at ultraviolet wavelength smaller than 240 nm. Although there have been several reports for challenges to develop such the photodetector (PD), tremendous efforts were made by applying polycrystalline diamond films to the PDs. Enormous photocurrent (PC), persistent photoconductivity (PPC), and relatively-large thermally-stimulated current (TSC) were reported by several groups to be observed for the polycrystalline diamond DUV-PDs, and the mechanisms of the PPC and TSC were proposed to be due to bulk deep levels, surface states, and/or interface states at grain boundaries in the polycrystalline diamond films. In order to understand the defect-related mechanism of the PPC and TSC, it is required to investigate the photoresponse properties of PD fabricated by single-crystalline diamond epilayer, which will lead to development of high-efficiency diamond DUV-PD with high reliability. Also, it is essential to investigate influences of diamond surfaces terminated by hydrogen and oxygen (named by hydrogenated and oxidized surfaces, respectively) on photoresponse properties, which will provide an important information on effect of surface states on the mechanism of PPC. The purpose of this paper is, as a first step to develop reliable, high-efficiency diamond PD, to explore the PC and PPC for homoepitaxial B-doped diamond epilayer with hydrogenated and oxidized surfaces. The PC's with gain larger than 105 and the long-term PPC were observed in illuminating UV-light to metal/p-diamond/ metal photodiodes fabricated on hydrogenated surfaces of the single-crystalline B-doped p-diamond epilayer. Saturation of PC with increasing applied voltages and phototransistor action against incident optical power densities were observed. The PC with large gain and the PPC were believed to be due to surface states on hydrogenated surface.

Surface Science
Room 210C - Session SS+EM+SC-ThA

Compound Semiconductor Growth and Surface Structure

Moderator: A.R. Smith, Ohio University

2:00pm **SS+EM+SC-ThA1 III/V Semiconductor Surfaces during Metalorganic Vapor-phase Epitaxy***, **R.F. Hicks**,* University of California, Los Angeles **INVITED**

{Thin films made from compound semiconductors, such as indium phosphide, gallium arsenide and their alloys, have key applications in electronic and photonic devices. These single-crystal materials are fabricated by metalorganic vapor-phase epitaxy (MOVPE). In our laboratory, an ultra-high vacuum system has been connected to a state-of-the-art MOVPE reactor so that the semiconductor surfaces may be characterized in the growth environment. The atomic composition and structure of these materials has been determined by scanning tunneling microscopy, infrared spectroscopy, reflectance difference spectroscopy, x-ray photoelectron spectroscopy, and ab initio molecular cluster calculations. It has been found that indium phosphide and gallium arsenide exhibit very different surface structures under MOVPE process conditions. A disordered double-layer of As atoms with a few alkyl radicals are adsorbed on GaAs (001), while on InP (001), the surface is terminated with H atoms adsorbed on P dimers. This latter structure exhibits a single-domain (2x1) reconstruction. Another interesting example of III/V semiconductor surface chemistry is the formation of InGaAs/InP interfaces. Localized strain produces atomic arrangements that are distinct combinations of InP and InAs reconstructions. The application of this knowledge to the growth of epitaxial device structures will be discussed. @FootnoteText@ invited by David Castner.}

2:40pm **SS+EM+SC-ThA3 Quantitative Analysis of Indium Concentration in InGaAs Quantum Dots and Wetting Layers Using Cross-sectional Scanning Tunneling Microscopy***, N. Liu, S. Govindaraju, A.L. Holmes Jr., **C.-K. Shih**,* University of Texas at Austin

Scanning tunneling microscopy has been employed to explore self-assembled InGaAs quantum dots (QDs) grown by migration enhanced epitaxy (MEE). With atomic resolution, compositional analysis has been done for both the QDs and wetting layers quantitatively. We found that both vertical and lateral segregation play important roles during the formation of the islands and thereafter capping procedure. Depletion of the wetting layer, due to the formation of the QDs, is demonstrated. More importantly, it is found that after capping the amount of existing indium in the QDs and WL is less than that of deposited indium, indicating a portion of deposited indium atoms was evaporated to the vacuum during overgrowth of GaAs. This observation is different from previous results, which proposed indium re-distribution within GaAs matrix after capping growth. Based on the observed data, a growth model is also proposed.

3:00pm **SS+EM+SC-ThA4 Surface Science of Gallium Nitride and Related Alloys***, **R.M. Feenstra**,* Carnegie Mellon University **INVITED**

The formation and structure of various faces of GaN, including adsorbed layers of Al, In, or H, are discussed. The primary preparation method is plasma-assisted molecular beam epitaxy although a comparison of results from metal-organic vapor phase epitaxy will also be presented. Experimental results from scanning tunneling microscopy allow us to broadly determine the characteristics of the surface structures, and first principles theory is then used to determine the precise atomic arrangements. For the case of surfaces grown by vapor phase epitaxy spectroscopic ellipsometry is used to identify the relevant surface phases. In contrast to other semiconductor surfaces, a central feature of many GaN reconstructions is their tendency to form metallic overlayers of metal (Ga, In, or Al) atoms. The terminating layers of metal atoms also leads to novel aspects of the surface kinetics - N atoms are predicted to diffuse easily between the metal layers, thus yielding enhanced surface diffusivity for those surfaces which are terminated by more than one layer of metal atoms. @FootnoteText@ Work performed with Y. Dong, C. D. Lee, H. Chen, A. R. Smith (CMU); J. E. Northrup (PARC); J. Neugebauer (FHI, Berlin); C. Cobet, T. Schmidtling, M. Drago, N. Wollschlaeger, N. Esser, W. Richter (TU, Berlin); and supported by NSF and ONR.

3:40pm **SS+EM+SC-ThA6 First Scanning Tunneling Microscopy and Spectroscopy Study of c-GaN(001)-4x1 Tetramer Structure and SIESTA Surface Simulation***, **H.A. Al-Brithen**, M.B. Haider, N. Sandler, A.R. Smith,* Ohio University*; P. Ordejon,* Institudo de Cienias de Materiales, Spain

Although early papers of the surface structure of c-GaN(001) reported 2x2 and c(2x2) reconstructions,[a] it was later shown both experimentally[b] and theoretically[c] that the intrinsic reconstruction is 4x1. However, until now, this 4x1 reconstruction has never been reportedly observed in real space. We have grown c-GaN on MgO(001) using radio frequency nitrogen plasma molecular beam epitaxy under Ga-rich conditions. RHEED patterns show that GaN(001) clearly exhibits 1x1 reconstruction during and after the growth; in fact, after cooling to ~ 200 °C a reversible disorder-order transition from 1x1 to 2x occurs, which may have been neglected or confused in earlier experiments with 2x2. This 2x is imaged using STM, finding that it is actually c(4x16) for Ga-rich growth and c(4x20) for more Ga-rich growth; STS spectra suggest that GaN(001)-c(4x16) is metallic. Annealing the film at T@sub s@ ~ 700-800 °C leads to the 4x1 reconstruction, as indicated by RHEED. STM performed on c-GaN(001)-4x1 shows that the surface consists of rows aligned along [110] with row spacing of 12.8 Å. Dual-bias STM images show a 180@super o@ phase shift of the filled and empty states profiles, as the sample bias changes from -1.2 V to +1.2 V, consistent with our recent simulated STM images, calculated using SIESTA code based on the tetramer model, showing that the filled state peak centered on the tetramer corresponds to the empty state minimum. STS acquired on the tetramer surface agrees with the semiconducting nature of 4x1, having a surface gap of 1.3 eV. In fact, the 4x1 tetramer structure was also predicted for c-AlN(001)[d], which widens the importance of understanding this reconstruction. Work is supported by NSF. @FootnoteText@ [a] Brandt et al., Phys. Rev. B R2253 (1995). [b] Feuillet et al., Appl. Phys. Lett. 70(8) (1997). [c] Neugebauer et al., Phys. Rev. Lett. 80(14) (1998). [d] Felice et al., Appl. Phys. Lett. 74(15) (1999).

4:00pm **SS+EM+SC-ThA7 Ion Induced Step Debunching of GaN***, **B. Cui**, P.I. Cohen,* University of Minnesota*; A.M. Dabira,* SVT Associates, Inc.

The development of surface morphology during ion bombardment has been described in terms of the curvature dependence of the sputtering yield [1] and asymmetric kinetics for the attachment of surface adatoms and vacancies at step edges [2]. We have used a Kaufman ion source to study the low energy ion effects during the MBE growth of GaN on sapphire substrates and GaN templates, comparing the results to these models. From a macroscopic point of view our measurements on GaN show quantitative agreement with the curvature driven theories. In particular we use the cross-over between Ga-limited growth and N-limited growth to estimate the N adatom concentration, a key ingredient of the theory. From a microscopic view, however, our RHEED and AFM studies have observed step debunching of multilayer steps and the elimination of hillock spirals. In these measurements, the starting GaN(0001) templates had 20 layer high mesas. After growth, round, nanoscale dimple structures, ranging from 90 nm to 850 nm, with bilayer steps were produced. This was seen with both Ar and nitrogen ions at energies ranging from 100-1200 eV. The size of the dimples and the terrace length of the debunched steps decrease with increasing sample temperature. After ion assisted growth, islands are found at the edges of the debunched steps. By tuning the ion energy and growth rate, uniform distributions of GaN nanoparticles, with means ranging from 50 nm to 200 nm, can be prepared. By combining ion induced step debunching and growth, step flow growth at the debunched steps is obtainable. Partially supported by the NSF and the AFOSR. @FootnoteText@ 1. R. M. Bradley and J. M. E. Harper, J. Vac. Sci. Technol. A 6, 2390 (1988). 2. J. Kim, D. G. Cahill, and R. S. Averback, Phys. Rev. B 67, 045404 (2003).

4:20pm **SS+EM+SC-ThA8 Thermal Desorption of Deuterium from GaN(0001): A Sensitive Probe of Surface Preparation***, **C.M. Byrd**, J.N. Russell, Jr.,* Naval Research Laboratory

Gallium nitride (GaN) is a wide band gap semiconductor with applications in high temperature, power and frequency optoelectronic devices. The surface chemistry of hydrogen on GaN affects growth rates and electronic passivation, while annealing temperatures impact both ohmic contacts and thermal stability. In this work, the preparation of a GaN(0001) thin film surface was investigated as a function of anneal temperature (300-1100K) using Auger electron spectroscopy (AES), electron energy loss spectroscopy (EELS), low energy electron diffraction (LEED), and temperature programmed desorption (TPD). After the GaN(0001) surface was sputter cleaned with nitrogen (N@sub 2@@super +@) ions, N@sub 2@ desorption was observed at 950 K from embedded nitrogen and then above 1200 K from GaN decomposition. EELS and AES showed subtle changes as the anneal temperature increased, and the LEED pattern sharpened. TPD spectra were collected for a series of anneal temperatures. After annealing the surface and cooling to room temperature, the surface was dosed with D atoms. When heated at 1 K/s, D@sub 2@ thermal desorption was observed, but not ammonia or gallane. There were four D@sub 2@ thermal desorption peaks at 430, 600, 730 and 810 K, the appearance and relative intensities of which were related to whether the anneal occurred at, above, or below the embedded nitrogen desorption temperature. Correlation of the anneal temperature dependence of the D@sub 2@ thermal desorption with the EELS, AES, and LEED data aided in identifying the origins of the D@sub 2@ desorption states. This work demonstrates D@sub 2@ thermal desorption is very sensitive to the quality of the GaN(0001), and explains differences in hydrogen on GaN(0001) TPD results in the literature.

4:40pm **SS+EM+SC-ThA9 Metal/Semiconductor Phase Transition in CrN Grown by Molecular Beam Epitaxy and Scanning Tunneling Microscopy***, **C. Constantin**, M.B. Haider, A.R. Smith,* Ohio University

Considerable interest has been of late in transition metal nitrides thin films/surfaces, which have both magnetic and electronic properties with potential applications in spintronics. CrN is a particularly interesting case, having a known correlation of structural and magnetic transition from a B@sub 1@ NaCl-paramagnetic to an orthorhombic-antiferromagnetic at T@sub Neel@=273-286K@footnote 1@. However,the reported electronic properties of CrN are controversial, and there has been no consensus whether the material is a metal or a semiconductor@footnote 2,3@. In this study, CrN is grown on MgO(001) at a substrate temperature of 450°C by a novel molecular beam epitaxy method for obtaining smooth surfaces. Bulk measurements reveal that the films are single crystal, and stoichiometric. The 1x1 face-centered cubic (fcc) surface structure is clearly distinguishable as obtained (for the first time) in room temperature atomic resolution scanning tunneling microscopy. In addition to the atomic resolution, long-range topographic distortions [LTD] are also seen on the surface, as also observed for the semiconductor ScN (001)@footnote 3@ and other nonpolar III-V surfaces. LTDs are characteristic of semiconductor surfaces, and are related to localized charge accumulation from impurities. Resistivity was measured from 77 to 450K; metallic behavior is found up to 260K (in contrast with some earlier reports) and semiconductor behavior above 285K. The bandgap obtained from resistivity data,71±0.315meV, agrees with the tunneling spectroscopy of the surface which show a very small gap. Consistent results have now emerged in which CrN has a semiconductor-metal phase transition corresponding to its magnetic transition. @FootnoteText@ @footnote 1@ A. Filippetti et.al, Phys. Rev. B 59, 7043 (1999)@footnote 2@J. D. Browne et.al, Phys. Status Solidi 1, 715 (1970)@footnote 3@P. S. Herle et.al, J. Solid State Chem. 134, 120 (1997)@footnote 4@H. A. Al-Brithen et.al, submitted to Phys. Rev. B.

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