Tuesday Morning, October 26, 1999

Surface Science Division
Room 606 - Session SS1+EM-TuM
Nitrides and Compound Semiconductors

Moderator: A.C. Kummel, University of California, San Diego

8:20am **SS1+EM-TuM1 Reconstructions and Growth Kinetics of GaN Surfaces with and without Adlayers**, ***R.M. Feenstra***, Carnegie Mellon University **INVITED**

Reconstructions of the gallium nitride (0001) Ga-face and N-face surfaces have been studied using scanning tunneling microscopy, with growth performed by molecular beam epitaxy. Distinct families of reconstruction are observed on each face, with most of the structures involving the presence of one of more adlayers of gallium bonded to underlying nitrogen atoms. For the N-face, this Ga-adlayer is in a 1x1 arrangement and further reconstructions are formed by additional Ga adatoms weakly bonded on the Ga-adlayer. For the Ga-face, the Ga-adlayer is incommensurate with the GaN lattice. For both the Ga- and N-face, growth under Ga-rich conditions yields smooth surfaces whereas growth under N-rich conditions produces rough surfaces. The latter case is indicative of limited surface diffusion rates. However, in the presence of surfactant layers such as Mg or As, smooth growth is also obtained in the N-rich regime. For sufficiently high surface coverage of Mg, a remarkable transition is observed in which Ga-polar material converts to N-polarity, with the inversion domain boundary extending along the c-plane. For growth of InGaN alloys, the role of surface metal layers (mainly indium) is also found to play an important role in the growth kinetics and incorporation efficiency. @FootnoteText@ Work supported by Office of Naval Research and National Science Foundation, and performed in collaboration with V. Ramachandran, H. Chen, A. Smith, D. Greve, J. Northrup, J. Neugebauer, W. Sarney, and L. Salamanca-Riba.

9:00am **SS1+EM-TuM3 Increase of Electrical Conductivity in p-GaN by Immersion in H@sub2@O@sub2@ Solution***, ***B. Liu***, *M.H. Ahonen, P.H. Holloway,* University of Florida

Immersion in a peroxide solution was found to increase electrical conductivity in p-GaN films. Auger electron spectroscopy (AES), current-voltage and Hall measurements were used for characterization. All samples in this study were grown on the c-plane of sapphire substrates by metallorganic vapor phase epitaxy (MOVPE) with a carrier concentration of 1.1x10@super 17@ cm@super -3@. The samples were first cleaned in boiling aqua regia (3HCl+3HNO@sub 3@) for 10min, rinsed in DI water, and blown dry with N@sub 2@. Metal contacts (10nmNi/100nmTi/100nmAu) were deposited with an electron beam evaporator (~10@super -6@ Torr). After metal deposition, samples were immersed in a H@sub 2@O@sub 2@ solution (1H@sub 2@O@sub 2@ : 5H@sub 2@O or 1H@sub 2@O@sub 2@ : 1H@sub 2@O, in volume) for different time (30sec to 300sec). This was followed by DI water rinse and N@sub 2@ blowing dry. Surface composition analysis using AES showed differences in N concentration versus treatments with the highest increase of N (5.67at%) found after immersion in 1H@sub 2@O@sub 2@ : 1H@sub 2@O for 300sec. Corresponding to this increase in N, improved electrical conductivity was confirmed by current-voltage data. The highest (a factor of two) increase of conductivity was measured for the sample with the highest increase of N concentration. No increase of carrier concentration was found in these samples with Hall measurement. The increase of N atoms at the sample surface and improvement of electrical conductivity will be discussed based on the chemical reaction of H@sub 2@O@sub 2@ with GaN and the effects of N vacancies in p-GaN. * This work is supported by EPRI and DARPA under agreement W08069-07.

9:20am **SS1+EM-TuM4 Structure of GaN(0001)-1*1: Holography Study of Mg Adsorption on GaN(0001) Surface**, ***G.J. Lapeyre***, *S.H. Xu, H. Cruguel, Y. Yang,* Montana State University; *J.F. Schetzina,* North Carolina State University

The adsorption site and surface atomic structure of Mg on GaN(0001)-1*1 surface has been studied by photoelectron holographic imaging technique. The results clearly show that Mg adsorbs on T4 site and there is one monolayer Ga adatoms on the surface. They are on H3 sites.

9:40am **SS1+EM-TuM5 Angle Resolved Photoemission Studies of the Surface Electronic Structure of GaN(0001)**, ***K.E. Smith***, *Y.C. Chao, P. Ryan, J. Downes, C.B. Stagarescu, R. Singh, T.D. Moustakas,* Boston University; *D. Hanser, R.F. Davis,* North Carolina State University

The physical properties of GaN are under intense study due to its use in optoelectronic and high temperature semiconductor devices. However, the surface electronic structure of GaN remains poorly understood. Numerous reconstructions of GaN are observed, but very little is known about the detailed electronic structure of clean, ordered GaN surfaces. We report the results of an extensive synchrotron radiation excited angle-resolved photoemission study of n-type and p-type wurtzite GaN(0001)1x1 surfaces. GaN thin films were grown both by MOCVD on SiC, and by MBE on Al@sub 2@O@sub 2@. Surfaces were cleaned by repeated cycles of N@super 2+@ ion bombardment followed by annealing in UHV. We have observed a number of different surface states on these materials. For n-type MBE samples we find a non-dispersive surface state just below the valence band maximum that is highly sensitive to surface contamination and disorder. This state shows no dispersion perpendicular to the surface and exists across the surface Brillouin zone in a region devoid of bulk states. Polarization measurements reveal that this feature originates from a state with sp@sub z@ character. Destruction of this state only partially removes the observed band bending. For n-type MOCVD samples, cleaned in an identical fashion, we find at least two surface states. One is similar to that seen on the MBE material, while the second is a highly dispersive back bonding state, extending to the bottom of the valence band at points in the surface Brillouin zone. Removal of these states does not alter the observed band bending. For p-type MBE samples, we also find a surface state in the fundamental band gap, above the valence band maximum. Such states are not observed for the n-type material. We will discuss the surface electronic structure of GaN in the context of these measurements. @FootnoteText@ Work supported in part by NSF grant DMR 95-04948. Experiments were performed at the NSLS, which is supported by US DOE.

10:00am **SS1+EM-TuM6 The Reaction of Oxygen with GaN(0001)**, ***B.D. Thoms***, Georgia State University, US; *V.J. Bellitto, Y. Yang,* Georgia State University; *D.D. Koleske, A.E. Wickenden, R.L. Henry,* Naval Research Laboratory

In addition to optoelectronic applications, Group III Nitrides also exhibit properties appropriate for their use in high power and high temperature transistors. Oxidation of the surface influences several aspects of device fabrication including surface passivation and the production of metal contacts. We have characterized the reaction of oxygen with MOCVD-grown GaN(0001) using low energy electron diffraction (LEED), Auger electron spectroscopy (AES), energy loss spectroscopy (ELS), high resolution electron energy loss spectroscopy (HREELS), and temperature programmed desorption (TPD). AES of GaN(0001) following exposure to O2 at room temperature results in an increased O(KLL) Auger intensity which saturates after approximately 200 L. AES following heating shows that oxygen is present to temperatures of 900 C. No surface reconstruction is observed by LEED, but rather a reduction in contrast between diffraction spots and background with increasing oxygen exposure. The reaction with oxygen produces a reduction in the ELS intensity at loss energies of 3.5 and 6 eV. A similar reduction is observed after exposure to atomic hydrogen, consistent with the reaction of both oxygen and hydrogen with surface dangling bonds. Oxygen exposure also produces an increase in ELS intensity at 10 eV. In HREEL spectra acquired following oxygen exposures up to 200 L, no adsorbate vibrational features are resolved from Fuchs-Kliewer phonon losses at integer multiples of 700 cm-1. These data are consistent with the chemisorption of oxygen on Ga sites.

10:20am **SS1+EM-TuM7 Deep Level Electronic States of Clean GaN (0001)(1x1) Surfaces Prepared by In Decapping**, ***A.P. Young***, *L. Brillson,* Ohio State University; *C. Tu,* University of California, San Diego

The tremendous interest in the properties of GaN surfaces and interfaces has created a need for new techniques for preparing clean, ordered surfaces under ultrahigh vacuum (UHV) conditions. Furthermore, the electronic properties associated with different interface preparations are not well understood at present. In contrast to surfaces prepared by N+ bombardment or Ga overcoat annealing cycles at 900C, clean and ordered GaN (0001) (1x1) surfaces can be produced directly from MBE-grown surfaces after removal of an In cap layer at 650C. These surfaces are comparable to those clean, ordered surfaces reported elsewhere. We have used electron-excited nanometer luminescence spectroscopy (EENLS) to measure these states in the band gap of MBE-GaN deposited on a GaN/sapphire composite substrate. The GaN was cleaned in UHV via thermal desorption of a thin (~50 ML) metallic In layer deposited prior to removal of the specimen from the growth chamber. This relatively low temperature desorption presents a benign method of transporting and processing GaN for device applications. Auger Electron Spectroscopy (AES) results show that if the In can uniformly cover the surface, it can prevent contamination during atmospheric exposure without reacting or diffusing into the GaN layer. The as-prepared surface morphology, measured via ex situ atomic force microscopy (AFM), indicated significant islanding of the In on the surface with approximate lateral size of 250 nm and height of 30 nm. Furthermore, a Ga signal, probably in the form of an oxide, was observed via AES indicating that some of the surface was not covered by In. The In was selectively desorbed from the GaN without reacting to produce InGaN. 8 ML of Ga were then deposited and the surface flashed once to 690C to reduce residual O and C contamination yielding a sharp (1x1) low energy electron diffraction (LEED) pattern. EENLS at a probe energy of 350 V (probe depth » 3 nm) indicated substantial "yellow" (YL) emission within the bandgap centered at 2.22 eV (FWHM = 0.4 eV) with only minimal near band edge (NBE) emission. YL emission remains constant while NBE increases with depth of excitation, indicating only states intrinsic to the GaN bulk. Subsequent AFM reveals Ga droplets residual to the flash annealing. Thus, In decapping introduces no new states at the clean, ordered GaN surface.

10:40am **SS1+EM-TuM8 Characterization of MOCVD ZnO Buffer Layers for CIS Solar Cells*, L.C. Olsen,*** Washington State University*; G.J. Exarhos,* Pacific Northwest National Laboratory*; F.W. Addis, L. Huang,* Washington State University

This paper concerns studies carried out to characterize MOCVD ZnO films grown for buffer layers in CIGS solar cells which have exhibited efficiencies between 12 and 14%. Further understanding of properties of these devices are required in order to increase efficiencies above 18% as demonstrated by CIGS cells with CdS buffer layers. Work is focusing on buffer layers grown with a two step process involving nucleation of ZnO at 250 C and subsequent growth at 100 C to achieve a total film thickness on the order of 800 A. The purpose of this work is to characterize the physical and electro-optical properties of MOCVD ZnO layers, and relate the results to device processing. All ZnO films examined were grown onto copper-indium-diselenide (CIS) substrates. XPS examination of films for which the growth was terminated at various stages of the two-step process show that good coverage of CIS is achieved after 100 A of growth, although some outdiffusion of indium does occur. XPS analyses of 800 A films indicate the MOCVD ZnO films have no major impurities and that films are slightly oxygen deficient. Ellipsometry studies indicate that results for the index of refraction and extinction coefficient vs photon wavelength are well understood if one assumes that there are no secondary phases between the ZnO buffer layer and CIS, and that the ZnO band structure is characterized by three transitions, one at 3.2 to 3.4 eV, one at 3.8 to 4.0 eV, and one at 4.8 to 5.2 eV. The transitions are fairly consistent with theoretical results for the ZnO band structure. Raman spectroscopic studies of the ZnO buffer layers are also being carried out. Finally, results for ZnO buffer layers grown with the two-step process will be compared to characteristics of films grown with different procedures and which yield poor performing cells.

11:00am **SS1+EM-TuM9 Photoelectron Diffraction of GaSe Bilayer Grown on Si(111)*, S. Meng,*** *B.R. Schroeder, A. Bostwick,* University of Washington*; E. Rotenberg,* Lawrence Berkeley National Laboratory*; F.S. Ohuchi, M.A. Olmstead,* University of Washington

Initial nucleation of GaSe on Si(111)7x7 results in formation of a pseudomorphic bilayer, which passivates the substrate dangling bonds and serves as the interface for further film growth. Component-resolved photoelectron diffraction (PED) and low-energy electron diffraction show this bilayer is oriented in a single domain, with the Ga-Se bond aligned with the substrate Si-Si bond. Combining scanned-angle and scanned-energy PED with theoretical calculations reveals the Ga and Se atomic positions. Ga sits directly atop surface Si, and the resultant interface bonding leaves Se lone-pair states on the surface. This makes the Si(111):GaSe surface highly resistant to contamination, and even additional GaSe does not stick for T@sub substrate@@>=@550°C. The measured PED patterns of Ga and Se 3d states show strong forward focusing along Ga-Se bond as well as diffraction rings from in-plane Se-Se scattering. The Ga-Se bond angle is between that for layered GaSe and cubic Ga@sub 2@Se@sub 3@. PED also shows strong (>20%) angular variation of the Ga3d spin-orbit branching ratio, while the Se 3d branching ratio is constant within 5%. This is likely associated with differences in photoionization matrix element and propogation of 3/2 and 5/2 states for the different local environments. * Supported by NSF DMR9801302.

11:20am **SS1+EM-TuM10 An Example of a Compound Semiconductor Surface that Mimics Silicon: The InP (001) (2x1) Reconstruction*, L. Li,*** *Q. Fu, B. Han, M. Begarney, D. Law, C. Li, R.F. Hicks,* University of California, Los Angeles

An InP (001) (2x1) reconstruction was prepared by metalorganic vapor-phase epitaxy. Scanning tunneling micrographs and infrared spectra of adsorbed hydrogen revealed that the (2x1) is terminated with a complete layer of buckled phosphorous dimers, giving rise to p(2x2) and c(4x2) domains. A surface band gap of 1.2 ± 0.2 eV was measured by scanning tunneling spectroscopy. The buckling can be explained by electron correlation among the dangling bonds of pairs of phosphorous dimers. This allows the surface to achieve a lower energy, semiconducting state. This reconstruction mimics the Si (100) (2x1), which is terminated with buckled silicon dimers.

11:40am **SS1+EM-TuM11 STM Studies of Sulfur Passivated InP(100)*, G.P. Lopinski,*** *R.A. Wolkow,* National Research Council, Canada*; C.D. MacPherson,* Nortel Networks, Canada

While sulfur passivation of InP(100) has been extensively studied by a number of techniques the details of the surface structure are still not definitively established. In this work we report STM studies of sulfur passivated InP(001) surfaces, prepared by wet chemical treatment in ammonium sulfide followed by annealing in UHV. Although the as prepared surface is disordered due to the presence of excess sulfur, highly pitted terraces evolve for annealing temperatures above 300C. Further annealing to 450C results in emergence of atomically flat terraces. LEED observations indicate the existence of a (3x1) phase in addition to the previously reported (2x1) structure. Atomically resolved STM images reveal the coexistence of local (3x1) and (2x1) periodicity. These surfaces are found to be stable with respect to brief air exposures.

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