Surface Science

Room: 611 - Session SS2-ThM

Surface Structure of Compound Semiconductors

Moderator: Y.J. Chabal, Rutgers University

8:00am **SS2-ThM1 Structural and Surface-Morphological Analysis of InN Layers Grown by HPCVD**, ***G. Durkaya***, *M. Alevli, R. Atalay,* Georgia State University*, W. Fenwick, I. Ferguson,* Georgia Institute of Technology*, N. Dietz*, Georgia State University

InN, a promising group III-nitride material for development of advanced optoelectronic structures, has still many not understood growth specific physical properties. InN layers investigated in the contribution were grown by high-pressure chemical vapor deposition (HPCVD) method, a technique that has been developed to counter the vast different partial pressures in this material system. In this study, we utilize and correlate Raman, XRD and AFM data to analyze the structural and electrical properties of the InN layers. The line shape analysis of the InN E2(high) Raman line is correlated to the crystalline quality of the layers and compared with the XRD pattern and AFM surface morphology studies for various growth conditions. The Raman line shapes for the A1(LO) phonon mode in these layers are analyzed and fitted to theoretical simulations in order to provide an estimate on the free electron concentration. The estimates are linked to results obtained by IR reflectance spectroscopy.

8:20am **SS2-ThM2 Desorption of Hydrogen from the Indium Nitride Surface Studied by HREELS**, *R.P. Bhatta,* ***B.D. Thoms***, *M. Alevli, N. Dietz*, Georgia State University

Thermal desorption of hydrogen from the N-polar InN surface has been studied by acquiring vibrational spectra using high resolution electron energy loss spectroscopy (HREELS). The reductions in intensity of the N-H stretching and bending vibrations in HREEL spectra upon annealing indicated loss of surface hydrogen and was attributed to recombinative desorption. Annealing to 375 °C for 15 min resulted in a small amount of hydrogen desorption while heating to 425 °C for the same amount of time resulted in complete removal of surface hydrogen. A shorter anneal time of 30 s raised the temperatures for both the onset and completion of desorption by about 50 °C. Since temperatures are typically 500 °C or greater for many of the common growth techniques, this result indicates that desorption of surface hydrogen is occurring during growth and may be an important mechanism for the production of reactive sites during the growth of InN. In addition to the desorption of hydrogen, an increase in the carrier concentration of the film was also observed upon annealing to 475 °C or higher as shown by a shift of the conduction band plasmon excitation to higher energy .

8:40am **SS2-ThM3 Preparation and Characterization of β-Si_3N_4 Surfaces**, ***V.M. Bermudez***, Naval Research Laboratory **INVITED**

β-Si_3N_4 is an important electronic material with numerous device applications. Yet, in contrast to other such materials, relatively little is known about its fundamental surface properties. This talk will discuss recent theoretical and experimental work relating to the preparation and properties of β-Si_3N_4 surfaces. The growth and characterization (via IR spectroscopy and XPS) of thin films will be examined, together with methods for preparing an atomically-clean and stoichiometric surface in UHV. Ab-initio calculations of the physical and electronic structure of the (0001) surface, which provide insight into the interpretation of electron-spectroscopic data, will be described. In particular the nature of the relaxation and the electronic states at the surface will be discussed. Data from Auger, photoemission (UPS and XPS) and electron energy-loss spectroscopies will be examined in relation to the theoretical results, and preliminary chemisorption data will be presented. Strong surface-charging effects are observed in UPS and XPS which take the form of rigid shifts of the spectra by 1 eV or more with adsorption and with x-ray or VUV irradiation. These will be examined in the context of electron and hole trap states in the band gap. Brief mention will also be made of IR internal-reflection studies of wet-chemical processing of β-Si_3N_4 films.

9:20am **SS2-ThM5 Linear Smoothing Coefficient in Epitaxial Growth of GaAs on Rough Substrates**, ***M.B. Whitwick***, *T. Tiedje, T. Li*, University of British Columbia, Canada

By a combination of theoretical and experimental work, using GaAs as a model system, we show that time evolution of surface morphology during epitaxial growth can be used to obtain rather detailed information on step densities and adatom dynamics. From in-situ light scattering we find that homoepitaxial growth on randomly rough GaAs (100) substrates causes the surface to smooth towards a characteristic surface roughness determined by kinetic roughening. A recent theoretical model for the surface morphology as a function of growth time,[1] based on a Burton-Cabrera-Frank picture of crystal growth[2] in which adatoms incorporate at step edges, suggests that the smoothing of GaAs can be described by a conservative Kardar-Parisi-Zhang type equation in which the dominant linear term in the growth equation is due to a negative Ehrlich-Schwoebel potential barrier for adatom migration at step edges. The surface smoothing rate is found experimentally to depend on the deposition rate and temperature during growth. In the model the coefficient of the linear term in the growth equation is inversely proportional to the step density (~F/S), where F is the flux of deposited adatoms and S is the step length density. Although the full growth equation is nonlinear, for low amplitude roughness the linear term dominates. We have used this fact to determine the linear smoothing coefficient as a function of substrate temperature (400-610 C) and growth rate (0.01-10 ML/s) by in-situ UV (244 nm) diffuse light scattering along the [011] and [01-1] directions. The coefficient of the linear smoothing term was found to have a power law dependence on flux with exponent of 0.7 and an exponential temperature dependence on temperature with activation energy 0.50 eV. The surface step density was measured ex-situ by AFM. The step density was found to be ~0.10±0.05 1/nm with a tendency towards higher density at high growth rates. This step density is in good agreement with the step density inferred from theoretical expression for the linear smoothing coefficient. The coefficient of the nonlinear smoothing term is also found to be in good agreement with theory.

[1] A. Ballestad and T. Tiedje, Phys. Rev. B 74, 153405 (2006).
[2] W.K. Burton, N. Carrera, F. Frank. Phil. Trans. Roy. Soc. 243(866):299-358. (1951).

9:40am **SS2-ThM6 Spectroscopic Study of Acid and Base-Activated Thioacetamide Passivation of GaSb and InAs Surfaces**, ***R. Stine,*** U.S. Naval Research Laboratory*, D.Y. Petrovykh,* U.S. Naval Research Laboratory and University of Maryland*, E.H. Aifer, L.J. Whitman*, U.S. Naval Research Laboratory

A wide range of III-V semiconductor heterostructure devices are under development for applications in electronics, optoelectronics, and sensing. However, the performance of III-V devices following processing is often detrimentally affected by the formation of mid-bandgap electronic states and the subsequent pinning of the surface Fermi level. Chemical passivation of the device surfaces can stabilize their properties by inhibiting the regrowth of native oxides that can otherwise contribute to Fermi level pinning. Traditionally, this passivation has been accomplished by the formation of surface sulfide groups through wet chemical treatment with an inorganic sulfur-containing compound, such as ammonium sulfide or sodium sulfide. More recently, though, the use of thioacetamide (TAM), an organic sulfur containing compound, has been shown to have a number of advantages over traditional inorganic methods,[1-3] including milder reaction conditions and a higher degree of control over the reaction. Although studies have shown the effect of TAM passivation on the electronic properties of devices, little information has been available on the actual chemical reactions that take place at the surfaces. Here, we present detailed X-ray photoelectron spectroscopy (XPS) studies of these surface reactions on gallium antimonide and indium arsenide-important materials for infrared optoelectronics. A comparison of TAM passivation performed under acidic versus basic conditions shows that acidic-TAM treatment produces a thicker sulfide layer that is better suited to the prevention of re-oxidation than that formed under basic-TAM treatment, regardless of exposure time or TAM concentration. We have determined the relative amounts of III-sulfides versus V-sulfides and tracked the rate of re-oxidation for each component independently over time.

[1] Petrovykh, et al., Appl. Phys. Lett. 86, 242105 (2005)
[2] Petrovykh, et al., Surf. Interface Anal. 37, 989 (2005)
[3] Aifer, et al., Proc. SPIE 6542, in press.

10:00am **SS2-ThM7 STM Imaging and DFT Modeling of the Group III-rich Reconstruction of InAs(100)-c(8×2)/(4×2)**, ***D.L. Winn***, *J. Shen, J.B. Clemens, A.C. Kummel*, University of California, San Diego

The atomic group V reconstruction of the III-V (001) surfaces have been extensively studied since these surfaces are favorable for MBE growth. The

group III rich surfaces are of III-V semiconductor can be readily prepared by heating the group V rich reconstructions. The group III rich surfaces may be favorable for ALD oxides growth since they exhibit a low reactivity to O_2 because the usually lack group V dimers. InAs(001) is well documented to have a (4×2) reconstruction, however, the details of the reconstruction are still under debate. Atomically resolved filled and empty state scanning tunneling microscopy (STM) images of the InAs(001)-c(8×2)/(4×2) surface reveal that the reconstruction is made up of single atom rows that run in the [110] direction which are separated by ~17 Å. In addition, atomically resolved STM images show that the row structure is most likely comprised of undimerized atoms. Cl2 was deposited onto the surface (which has been shown to preferentially react with III atoms on III-V semiconductors) to confirm that the rows were in fact comprised of In atoms. The experimental results suggest that the most probable structure for InAs(001)-c(8×2)/(4×2) is the undimerized or dimerized β3(4×2) reconstruction. The reconstruction consistent of a top layer of bicoordinated or tricoordinated In atoms at the center of the rows and tricoordinated As atoms in the second layer at the edges of the rows. Density functional theory (DFT) STM simulations were used to confirm the experimental findings. DFT reveals that the dimerized and undimerized structures are nearly degenerate consistent with STM images show the In dimerization may be temperature dependent. Both the undimerized and dimerized β3(4×2) structures lack As dimers and have a low reactivity to O2 consistent with a surface which is suitable for ALD gate oxide deposition.

10:20am **SS2-ThM8 Scanning Tunneling Microscopy Study of Interfacial Bonding Structure and Annealing Effect of In_2O/InAs(001)-c(8x2)/(4x2)**, ***J. Shen**, D.L. Winn, A.C. Kummel*, University of California, San Diego

The key to fabricating a III-V MOSFET is forming an electrically passive oxide-semiconductor interface. In an effort to identify an unpinned oxide/semiconductor interface on InAs, a detailed study of In_2O adsorbed to InAs(001)-c(8x2)/(4x2) was performed. Scanning tunneling microscopy (STM) and density functional theory (DFT) were used to ascertaining how In_2O adsorbates bond to the clean InAs(001)-c(8x2)/(4x2) surface. The InAs(001)-c(8x2)/(4x2) surface consists of a top row of In atoms which are bonded to tricoordinated As atoms containing partially filled dangling bonds. STM results showed that the initial In_2O molecules only occupy specific sites at the edge of the rows. These In_2O atoms most likely form new In-As bonds to the surface. This is a favorable bonding structure for oxide/semiconductor interfaces since it avoids As-O bond formation which is likely to create states in the band gap. In addition, the formation of In-As bonds restores the tricoordinated As atoms to a more bulk-like bonding environment. A height analysis was performed to determine growth mechanism. At low coverage (20% monolayer), the In_2O adsorbates formed islands that are elongated in the [110] direction. Prior to all the first layer sites being occupied with In_2O molecules, second layer growth was observed on the islands. Each layer of oxide has a distinct height, however, the second and subsequent layers appear to be amorphous. In addition, the effect of annealing In_2O/InAs(001)-c(8x2)/(4x2) was studied. The annealed samples were more ordered and uniform. The oxide molecules on the annealed samples filled in the troughs and formed ordered islands with rows in [i10] direction. Comparisons of oxide height distributions before and after annealing, show the oxide height is reduced from 1.5 Å to 1 Å. This is consistent with the In-In bond formation between two nearest neighbor In_2O atoms in the [i10] direction. Most importantly, for both room temperature deposition and annealing, the clean surfaces lattice is left unperturbed, the In_2O adsorbates never cause the abstraction of any surface atoms on the InAs(001)-c(8x2)/(4x2) surface and the In_2O molecules only occupied specific sites. The formation of an ordered oxide-interface without disruption of the InAs(100)-c(8x2)/(4x2) lattice is favorable for creating an unpinned oxide-semiconductor interface.

10:40am **SS2-ThM9 Bonding Hybridization in the Group III-rich Reconstructions of InGaAs(100)-(4×2)**, ***T. Song**, D.L. Winn, J. Shen, A.C. Kummel*, University of California, San Diego

The group-V (As or Sb) rich reconstructions of III-V semiconductors have been extensively investigated since these surfaces are favorable for MBE growth. However, the group-III (Ga or In) rich reconstructions can readily be prepared by heating the group-V rich reconstructions, and the group-III rich reconstructions may be favorable for ALD gate oxide deposition due to their low reactivity to oxygen. Although the group-III rich surfaces have several potential applications, many III-V semiconductors, including InGaAs, have unidentified group-III rich reconstructions. Four different group-III rich 4x2 reconstructions of In0.5Ga0.5As(001)-(4×2) were modeled using DFT: ζ (4×2), β2(4×2), β3(4×2), and the undimerized β3(4×2) structures. Multiple polymorphs (Ga and In positions) were investigated. The undimerized β3(4×2) reconstruction most closely matches the experimental room temperature STM images of In0.53Ga0.47As/InP(001)-c(8×2)/(4×2). This reconstruction consists of a top row of undimerized In/Ga atoms which are bonded to tri-coordinated As atoms. In the undimerized β3(4×2) structure, the row In/Ga atoms are sp hybridized. Conversely, in the dimerized β3(4×2) reconstruction, the top row In/Ga atoms are sp2 hybridized. DFT calculations showed that the undimerized β3(4×2) reconstructions are more stable in energy. The density of states (DOS) of the β3(4×2) reconstructions showed that the undimerized β3(4×2) structure had a band gap while the dimerized β3(4×2) structure was metallic. The correlation between hybridization and electronic structure is due to the influence of hybridation and bonding structure on the filling of the dangling bonds.

Authors Index

Bold page numbers indicate the presenter

— A —

Aifer, E.H.: SS2-ThM6, 1
Alevli, M.: SS2-ThM1, 1; SS2-ThM2, 1
Atalay, R.: SS2-ThM1, 1

— B —

Bermudez, V.M.: SS2-ThM3, **1**
Bhatta, R.P.: SS2-ThM2, 1

— C —

Clemens, J.B.: SS2-ThM7, 1

— D —

Dietz, N.: SS2-ThM1, 1; SS2-ThM2, 1
Durkaya, G.: SS2-ThM1, **1**

— F —

Fenwick, W.: SS2-ThM1, 1
Ferguson, I.: SS2-ThM1, 1

— K —

Kummel, A.C.: SS2-ThM7, 1; SS2-ThM8, 2; SS2-ThM9, 2

— L —

Li, T.: SS2-ThM5, 1

— P —

Petrovykh, D.Y.: SS2-ThM6, 1

— S —

Shen, J.: SS2-ThM7, 1; SS2-ThM8, **2**; SS2-ThM9, 2
Song, T.: SS2-ThM9, **2**
Stine, R.: SS2-ThM6, **1**

— T —

Thoms, B.D.: SS2-ThM2, **1**
Tiedje, T.: SS2-ThM5, 1

— W —

Whitman, L.J.: SS2-ThM6, 1
Whitwick, M.B.: SS2-ThM5, **1**
Winn, D.L.: SS2-ThM7, **1**; SS2-ThM8, 2; SS2-ThM9, 2