Tuesday Afternoon, October 19, 2010

Electronic Materials and Processing
Room: Dona Ana - Session EM-TuA

Defects in Semiconductors and Oxides
Moderator: J. Drucker, Arizona State University

2:00pm **EM-TuA1 Influence of N-induced Point Defects on the Electronic Properties of Dilute Nitride GaAsN Alloys**, ***Y. Jin***, *R.M. Jock, H. Cheng, C. Kurdak, R.S. Goldman*, University of Michigan **INVITED**

(In)GaAsN alloys with a few percent nitrogen have potential applications in long wavelength optoelectronic devices, such as infrared laser diodes, heterojunction bipolar transistors, and high efficiency solar cells. However, due to the large size and electronegativity differences between As and N, the formation of several point defect complexes has been predicted, likely leads to the limited optical emission efficiency and minority carrier transport properties in (In)GaAsN alloys. In this work, we investigate the influence of two types of N-related point defect complexes, Si-N complexes and N interstitials, on the electronic and optical properties of InGaAsN alloys.

The presence of Si-N defect complexes is first suggested by a decrease in carrier concentration, n, with increasing N-composition observed in GaAsN:Si films but not in modulation-doped heterostructures. In addition, for GaAsN:Te (GaAsN:Si), n increases substantially (minimally) with annealing-T, suggesting a competition between annealing-induced Si-N complex formation and a reduced concentration of N-related traps. Since Si-N complex formation is enhanced for GaAsN:Si growth with the (2 x 4) reconstruction, which has limited group V sites for As-N exchange, the $(Si\text{-}N)_{As}$ interstitial pair is identified as the dominant Si-N complex.

For the investigation of N interstitial defects, we compared the structural and electronic properties of GaAsN films before and after annealing. Nuclear reaction analysis (NRA) reveals an annealing-induced decrease in the interstitial N concentration, f_{int}, while the total N composition remains constant. Corresponding signatures for the reduced f_{int} are apparent in Raman spectra. For as-grown GaAsN films, low T transport measurements reveal two distinct *T*-dependent regimes of *n*: a T-independent regime > 150K, and a thermally-activated regime <150K. Meanwhile, persistent photoconductivity effect (PPC) was observed up to 160K, with the photo-capture barrier determined to be 350 - 400 meV. These two phenomena are reminiscent of the behavior of n-type AlGaAs due to the presence of DX-center levels, suggesting the presence of similar N-induced defect levels in GaAsN. After annealing, the thermal activation of n and the PPC effect are both suppressed, accompanied by the decrease in f_{int} revealed by NRA, suggesting the association of these two phenomena with N interstitials.

This work is supported by NSF-FRG, grant # DMR-0606406, monitored by L. Hess

2:40pm **EM-TuA3 Identification of the Dominant Recombination Centers in Dilute Nitrides**, ***I.A. Buyanova***, *M. Chen*, Linköping University, Sweden **INVITED**

Dilute nitride alloys have in past years sparked a considerable interest because of their unusual physical properties and their potential device applications in visible light emitting diodes (LEDs), long wavelength telecommunications lasers on a GaAs substrate and highly efficient hybrid solar cells. Up to now, however, a major obstacle for full exploration of these devices is degradation of the radiative efficiency and carrier mobility of dilute nitrides when N content increases, mainly due to severe non-radiative (NR) recombination and carrier scattering. Many theoretical and experimental efforts were devoted to identifying the NRR centers, however, their origin is still being debated.

In this talk we will review our recent experimental results that have positively identified Ga interstitial defects as the dominant NR defects in Ga(In)NP and Ga(In)NAs epilayers and quantum wells by optical and spin resonance spectroscopy. Their formation is shown to strongly depend on growth methods (MBE or MOCVD) and conditions (growth temperature, bombardment by N ions, N flow, etc) as well as post-growth rapid thermal annealing and hydrogenation. In Ga(In)NAs, the carrier recombination process via these defects is shown to be strongly spin-dependent, which opens a door for spin manipulation of the process [1]. We demonstrate that strong spin-blockade of NR carrier recombination via these Ga interstitial defects can be achieved once the defect electrons are spin polarized. This results in a significant enhancement of light emission efficiency by up to 8 times, accompanied by a sizable increase in the non-equilibrium carrier lifetime. The defects formation is concluded to become thermodynamically favorable under the presence of N, possibly because of local strain compensation and seems to be unavoidable at least with the current technology. Therefore, demonstrated spin blockade of the associated carrier recombination appears to offer an attractive approach to strongly suppress NR shunt path.

Besides the Ga interstitial defects, we will show that severe nitrogen ion bombardment under non-equilibrium growth conditions during solid-source MBE could also trigger formation of an interfacial defect at a GaNP/GaP interface. The defect is identified to involve a P_{Ga} antisite or a P_i interstitial with a neighboring partner aligned along a <111> direction . The defect could be important in restricting carrier mobility in the related transistor structures and in reducing radiative efficiency of the GaNP-based LEDs.

[1] X.J. Wang, I.A. Buyanova, F. Zhao, D. Lagarde, A. Balocchi, X. Marie, C.W. Tu, J.C. Harmand and W.M. Chen, Nature Materials, 8, 198 (2009).

4:00pm **EM-TuA7 Band Bending and Surface Defects in Ga_2O_3**, ***T.C. Lovejoy***, *R. Chen, S.X. Zheng*, University of Washington, *E.G. Villora, K. Shimamura, H. Yoshikawa, Y. Yamashita*, NIMS, Japan, *S. Ueda, K. Kobayashi*, SPring-8, Japan, *S. Dunham, F.S. Ohuchi, M.A. Olmstead*, University of Washington

Wide-band-gap oxides like Ga_2O_3, In_2O_3, SnO_2, and ZnO, are of key importance as transparent conductors and gas sensing materials. The conductivity in these materials is almost-always observed to be n-type, although the mechanism is under debate. An inverse correlation between oxygen partial pressure, p(O2), during growth and measured conductivity has been reported, leading to a commonly held model that oxygen vacancy defects in the crystals are responsible for the conductivity. This model is supported by some density functional theory (DFT) calculations, in SnO2 for example, but excluded by others. beta-Ga2O3 has the largest band gap of the oxides listed above, ~(4.8 eV), making it unique among them for near-UV applications. We report on a combined experimental and theoretical study of beta-Ga2O3 single crystals. Using density functional theory we compute the formation energies of various intrinsic defects as function of the Fermi level position relative to the valence band maximum (E_F-E_VBM). We show by a combination of hard x-ray photoemission (HXPS) and Hall measurements that the near-surface value of E_F-E_VBM is very different from that in the bulk due to band bending. By comparing the experimental results with the calculations we conclude that oxygen vacancies have too high an activation energy in the bulk to contribute substantially to the conductivity, but band bending enables them to play a role near the surface.

4:40pm **EM-TuA9 Control of Oxygen Diffusion in Titanium Dioxide for Nanoelectronic Applications**, *A. Hollister, P. Gorai*, ***E.G. Seebauer***, University of Illinois at Urbana-Champaign

The technologically useful properties of semiconductor oxides such as titania often depend on the concentration and motion of defects. Native point defects such as interstitial atoms and vacancies strongly affect the operation of nanoelectronic gas sensors, light emitting diodes and memory resistors. Past work in our laboratory with silicon has shown that semiconductor surfaces serve as efficient pathways for generation and annihilation of point defects in the underlying bulk. Such pathways should play an especially important role in nanoelectronics fabrication, where devices have high surface-to-volume ratios. The present work extends the findings for silicon to the oxide semiconductor TiO_2, wherein we have identified a new pathway for interstitial-mediated diffusion of oxygen in titanium oxide. Oxygen diffusion rates were measured by exposing natural-abundance single-crystal rutile TiO_2 to isotopically labeled oxygen gas. The resulting profiles were measured by secondary ion mass spectrometry and subsequently modeled with continuum equations for the reaction and diffusion of the key point defects that control oxygen diffusion. The exponential diffusion profile shapes, together with the increase of the diffusion coefficients with oxygen pressure, strongly suggest the diffusion is mediated by oxygen interstitials. The measured diffusion coefficients were nearly two orders of magnitude higher than those expected from the literature, but could be decreased substantially by the adsorption of submonolayer quantities of sulfur to saturate surface dangling bonds. These latter observations suggest that the pristine TiO_2 surface is especially efficient at creating oxygen interstitials that then sink into the bulk and mediate diffusion there.

5:00pm **EM-TuA10 Effect of Vacuum Ultraviolet and Ultraviolet Irradiation on Capacitance-Voltage Characteristics of Low-k-porous Organosilicate Dielectrics**, *H. Sinha, J. Lauer,* ***M. Nichols****, A. Sehgal,* University of Wisconsin-Madison, *N.M. Russell, M. Tomoyasu,* Tokyo Electron Limited, *G.A. Antonelli,* Novellus Systems, Inc., *Y. Nishi,* Stanford University, *J.L. Shohet,* University of Wisconsin-Madison

High frequency capacitance-voltage (C-V) measurements are used to determine the effects of vacuum ultraviolet (VUV) and ultraviolet (UV) irradiation on defect states in porous low-*k* organosilicate (SiCOH) dielectrics. The dielectric was deposited by plasma enhanced chemical vapor deposition (PECVD) on silicon with 15-nm layer of thermally grown oxide. We determined from VUV spectroscopy that defect states are present in the band gap of the dielectrics.[i] [#_edn1] A non-zero flat-band voltage obtained from C-V characteristics also confirmed the presence of defect states in the dielectric. In addition, the defect states are a source of electrons that can move in the dielectric under influence of electric fields. This causes hysteresis loops observed in the C-V characteristics. VUV photon irradiation depopulates trapped electrons from defect states within the dielectric. Depopulation results in photoemission of the electrons creating trapped positive charge.[ii] [#_edn2] This is evidenced by a negative shift in the flat-band voltage of the C-V characteristic. Some of the depopulated electrons are not able to overcome electron affinity and reside in conduction band. Thus, more charge is available in the dielectric to move under the influence of electric field. Hence, after VUV irradiation the hysteresis loop of C-V characteristic widens. UV irradiation reverses both the shift in the flat-band voltage and the widening of the hysteresis loop, by repopulating the defect states with electrons photoinjected from the silicon substrate.[1,2] Thus, UV reduces the number of trapped positive charges in the dielectric and can effectively repair processing-induced damage.

This work was supported by the Semiconductor Research Corporation under Contract Number 2008-KJ-1781. We thank Tokyo Electron Limited and Novellus Systems for providing samples. The UW Synchrotron is supported by NSF Grant DMR-0084402.

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[1] J.L. Lauer, H. Sinha, M.T. Nichols, G. A. Antonelli, Y.Nishi and J.L. Shohet, "Charge Trapping within UV and VUV Irradiated low-k porous organosilicate dielectrics," *Journal of the Electrochemical Society* (submitted for publication)

[2] H. Sinha, J.L. Lauer, M.T. Nichols, G.A. Antonelli, Y. Nishi and J.L. Shohet, *Applied Physics Letters* **96** 052901 (2010)

5:20pm **EM-TuA11 Effect of Strain Relaxation on Electron Mobility in InAs/GaAs Nanowire Heterowires**, ***K.L. Kavanagh***, Simon Fraser University, Canada, *J. Salfi, I. Saveliev,* University of Toronto, Canada, *D. Susac,* Simon Fraser University, Canada, *M. Blumin, H. Ruda,* University of Toronto, Canada

The structure and electrical properties of InAs-GaAs core-shell nanowires grown by molecular beam epitaxy on GaAs (001) substrates has been investigated by scanning transmission electron microscopy (STEM) and field-effect measurements of nanowire conductance. Zincblende and wurtzite phase wires are found growing preferentially along

(001) directions. The InAs core radii varied from 10 to 60 nm, with GaAs shell thicknesses from 3 to 20 nm, depending on the growth time.

The ZB wires show a rectangular cross-section with <110> side facets while the WZ are hexagonal in cross-section. Strain relaxation via dislocations in individual wire is observed from the analysis of electron diffraction and Moire fringe patterns. Close to complete relaxation (95%) occurs preferentially in the longer radial <110> direction while a large residual strain of 30% to 50% is found along the wire length. Less strain relaxation in the perpendicular radial <110> direction is occurring consistent with a large radius of curvature in the wire morphologies.

The room temperature field effect mobility of unencapsulated InAs nanowires increases from approximately 1000 to several thousand as diameter increases from 30 to 80 nm, consistent with scattering from charged surface states or surface roughness. In comparison, InAs-GaAs core-shell nanowires have lower field effect mobility which does not increase with increasing diameter. A different, diameter-independent scattering mechanism related to strain relaxation limits the electronic mean-free-path in InAs-GaAs core-shell nanowires.

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