Monday Morning, November 4, 2002

Electronic Materials and Devices
Room: C-107 - Session EL+SC+MI-MoM

Semiconductors
Moderator: A. Rockett, University of Illinois

9:00am **EL+SC+MI-MoM3 Low-temperature Epitaxial Growth of the Wide Bandgap Semiconductor SiCAlN**, ***I.S.T. Tsong***, Arizona State University **INVITED**

Two compounds, SiC and AlN, normally insoluble in each other below 2000C, are synthesized as a single-phase solid solution thin film by molecular beam epitaxy (MBE) at 750C using a unimolecular precursor H3SiCN and Al atoms. The growth of epitaxial SiCAlN films with hexagonal structure takes place on 6H-SiC(0001) and Si(111) substrates. The surface morphology, microstructure, and composition of the films are analyzed by atomic force microscopy (AFM), cross-sectional transmission electron microscopy (XTEM), Rutherford backscattering spectrometry (RBS) and high-resolution electron energy loss spectroscopy (EELS). Two structural models for the hexagonal SiCAlN films are constructed based on first-principles total-energy density functional theory calculations, each showing agreement with experimental XTEM observations. The predicted fundamental bandgap is 3.2 eV for the stoichiometric SiCAlN, in good agreement with photoluminescence (PL) measurements. Bandgap engineering is a distinct possibility by varying the composition of the pseudo-binary (SiC)-(AlN) film.

9:40am **EL+SC+MI-MoM5 Evolution of Structure and Optical Properties of GaAsN Films Grown by Reactive Molecular Beam Epitaxy**, ***M.J. Reason***, *W. Ye, X. Weng, V. Rotberg, R.S. Goldman*, University of Michigan

Narrow gap nitride semiconductor alloys have shown significant promise for a wide range of electronic, optoelectronic and photovoltaic applications. At present, the ultimate limit of nitrogen solubility in GaAs, as well as the effects of growth conditions on stress relaxation and optical properties of narrow gap nitride films are not well understood. In this work, we have examined the evolution of nitrogen incorporation, strain relaxation, and optical properties of GaAsN films grown by solid-source molecular beam epitaxy using an N2-rf plasma source. The samples consisted of 500 nm buffer layers of GaAs grown at 580C and 20 nm layers of GaAs grown at 500C, both using a high arsenic flux; followed by 100-500 nm thick layers of GaAsN grown at 400C using a 10% N2/Ar gas mixture at a 0.15 sccm flow rate, with a variety of arsenic beam equivalent pressures (BEP). The structure and properties of the samples were investigated by reflection high energy electron diffraction (RHEED), multi-beam optical stress sensing (MOSS), high resolution x-ray rocking curves (XRC), nuclear reaction analysis (NRA), atomic force microscopy, and photoluminescence. For all of the arsenic fluxes studied, in-situ RHEED during the GaAsN layer growth reveals a pattern similar to that observed during the growth of the GaAs layers. As the arsenic BEP is increased, MOSS shows that the film stress decreases, indicating a lowering of the apparent nitrogen incorporation into GaAsN. Interestingly, variations in the absolute nitrogen concentrations determined from NRA analysis and a Vegard's law interpretation of XRC suggest significant nitrogen incorporation into interstitial sites. We will discuss the effects of arsenic flux on the stress relaxation and optical properties of a variety of GaAsN and InGaAsN films and heterostructures.

This work was supported in part by the DOE (Photovoltaics Beyond the Horizon Program), the Air Force Office of Scientific Research (MURI Program), and the TRW Foundation.

10:00am **EL+SC+MI-MoM6 Effects of LED Processing Steps on the Surface of Doped GaN Epilayers**, ***K.H.A. Bogart***, *D.D. Koleske, A.A. Allerman, A.J. Fischer, K.W. Fullmer, K.C. Cross, C.C. Mitchell*, Sandia National Laboratories

Gallium nitride (GaN)-based materials are critical for the creation of UV optoelectronic devices such as light-emitting diodes (LEDs). Ohmic contacts with low contact resistivities to p-type (<1x10^{-3}Ωcm^{2}) and n-type (<1x10^{-5}Ωcm^{2}) GaN are essential for improving optical device performance. Understanding the characteristics of p- and n-type GaN epitaxial layer surfaces and the interfaces formed with the contact metals is vital for optimization. Fabrication of an LED requires several processing steps including dicing, annealing, surface cleans (to remove native oxides), lithography, metal deposition, and plasma etching. The effects of processing steps on the surface morphology and electrical characteristics of the epitaxial materials and metal contacts have been investigated using scanning probe microscopies and the circular transmission line method (CTLM). One of the first LED processing steps is dicing a 50 mm wafer using photoresist for surface protection, which is later removed with solvents. For p-type GaN (5x10^{17}cm^{3}), AFM analysis showed that the surface roughness nearly doubled after photoresist exposure from an average of 0.24±0.05 nm to 0.50±0.10 nm. The source of the roughness increase was the formation of pits into the surface, ~1 nm in depth. In another LED processing step, n-type GaN is exposed by plasma etching a mesa structure into the p-type GaN overlayer. One half of a wafer with a 1.2µm n-type GaN (1.7x10^{18}cm^{3}) epitaxial film was plasma etched with chlorine-based chemistry. AFM analysis showed that the etched n-type GaN film (RMS=1.11±0.23nm) was not significantly more rough than non-etched n-type GaN film (RMS=1.70±0.59nm). However, after annealing (500°C/N^{2}), the plasma etched film had more Ohmic behavior by (CTLM) than did the non-etched film. More extensive experiments following the GaN epitaxial layers in processing will be presented and effects on contacts discussed.

10:20am **EL+SC+MI-MoM7 Hydrogen Removal Mechanisms from Gallium Nitride**, ***B.D. Thoms***, *Y. Yang, J. Lee*, Georgia State University **INVITED**

The reaction between hydrogen and GaN is important since hydrogen is often present (sometimes in abundance) during growth and processing and since it produces significant effects. For instance, the effect of hydrogen on the efficacy of Mg dopants has been widely reported and both annealing and electron exposures have been used to remove hydrogen. In addition, recombinative desorption of hydrogen is an important part of many dry etching processes. Removal of hydrogen requires both the transport of hydrogen to the surface and desorption from the surface. In this talk, the authors will discuss characterization of surface and subsurface hydrogen on GaN(0001) and its removal by annealing and by electron exposure.

11:00am **EL+SC+MI-MoM9 N-type Diamond Electronics With Nitrogen Doped Ultrananocrystalline Diamond**, ***J.E. Gerbi***, Argonne National Laboratory, *B.W. Alphenaar*, University of Louisville, *O. Auciello*, Argonne National Laboratory, *J. Birrell*, University of Illinois at Urbana-Champaign, *J.A. Carlisle, D.M. Gruen*, Argonne National Laboratory

Thin diamond films have extremely attractive properties for electronic device applications: high thermal conductivity, carrier mobility, and breakdown fields. However, efforts to create diamond based electronic devices have been hampered by the difficulty in incorporating dopants. Attempts to dope diamond films have resulted in low p-type carrier concentrations or unstable p-type surface layers. N-type doping has been even less successful, and it has not yet been possible to synthesize n-type diamond films with sufficiently high room-temperature conductivities. Ultra-nanocrystalline diamond (UNCD) is a fine-grained (3-5nm), phase-pure diamond material with atomically abrupt grain boundaries. Synthesized by microwave CVD using Ar-rich Ar/CH$_4$ plasmas, both the structure and electronic properties of UNCD can be tailored by doping with a controlled amount of N$_2$ in the plasma. As the N$_2$ content in the plasma increases to 20% , the grain size and grain boundary width of the UNCD films increase. This microstructural change correlates with a striking increase in room-temperature conductivity . Most importantly, nitrogen doped UNCD films are n-type with activation energies as low as 0.05 eV. This is striking, as traditional nitrogen substitutional doping of diamond produces a very deep state of 1.7eV, rendering the material useless for room-temperature applications. We use this material to demonstrate the first n-type diamond MESFET that can be operated at room temperature. We have characterized the films using Raman spectroscopy, NEXAFS, SIMS, Hall mobility measurements, and HRTEM, and measure device properties such as I-V curves and transconductance. The ohmic vs. Schottky behavior of various contacts to nitrogen doped UNCD as a function of growth chemistry has also been studied. A discussion of the microstructure-property relationship of nitrogen-doped UNCD films will be presented in the context of the UNCD-based MESFET performance.

11:20am **EL+SC+MI-MoM10 Electronic Structure and Spin-Polarization of Mn-containing Dilute Magnetic III-V Semiconductors**, ***L. Kronik***, *M. Jain, J.R. Chelikowsky*, University of Minnesota **INVITED**

The systematic use of electron spin, in addition to its charge, holds great promise for a new class of semiconductor devices with unprecedented functionality. Recently, Mn-containing, "dilute magnetic", III-V semiconductors have emerged as candidate materials for such a technology. They can potentially produce charge carriers with well-defined spin, yet are compatible with already existing semiconductor technologies. In order to assess the performance limits of such materials theoretically, we present first principles pseudopotential - density functional calculations for the

electronic structure of the dilute magnetic semiconductors $Mn_xGa_{1-x}As$ and and $Mn_xGa_{1-x}N$, with an experimentally relevant realistic x=0.063, in their ordered ferromagnetic phase. We predict that both materials allow, in principle, for a theoretical limit of 100% spin-injection, and that spin-polarized transport can be attained in both materials in the context of a simple band picture. This is because in MnGaAs, hybridization of As 4p and Mn 3d orbitals splits the valence band, resulting in a ~0.5 eV energy range where holes have a well-defined spin and an effective mass comparable to that of GaAs. In MnGaN, the situation is even more favorable: hybridization of Mn 3d and N 2p orbitals results in the formation of a ~1.5 eV wide impurity band, which supports effective mass transport. We will discuss the technological impact of these findings and compare our results to pertinent experimental data.

Electronic Materials and Devices
Room: C-107 - Session EL+SC+MI-MoA

Metal-Semiconductor Interfaces
Moderator: C.J. Palmstrom, University of Minnesota

2:00pm **EL+SC+MI-MoA1 Spin Transport in Ferromagnet-Semiconductor Schottky Diodes**, ***P.A. Crowell***, *A.F. Isakovic, B.D. Schultz, J. Strand, C.J. Palmstrom*, University of Minnesota **INVITED**

We have completed an investigation of spin injection in semiconductor heterostructures using a Schottky contact between Fe and n-Al$_{1-x}$Ga$_x$As as an injector and an Al$_{1-x}$Ga$_x$As/GaAs/Al$_{1-x}$Ga$_x$As quantum well (QW) as the detector. The injector and detector are combined in a single device in which the QW is placed in the depletion region of a p-n junction. The Schottky contact is δ-doped, so that a tunneling current can be obtained under moderate reverse bias.[1] The injected electrons recombine in the QW with holes from the p-contact, and the polarization of the resulting electroluminescence (EL) is used to infer the spin state of the recombining carriers. We demonstrate that the doping profile chosen for the QW has a dramatic effect on the apparent spin-detection efficiency. EL polarizations over 10% are obtained in optimally biased devices in which the QW is intentionally p-doped. The field-dependence of the EL polarization closely matches the magnetization of the Fe electrode. However, the largest polarizations are not observed from ordinary ground-state recombination in the quantum well. The maximum polarization observed from ground-state recombination is approximately 4% and appears to be less sensitive to the doping profile. In contrast, the EL polarization in control samples is less than 2%, does not track the magnetization of the ferromagnetic electrode and depends only weakly on bias voltage. The interpretation of these measurements will rely on a thorough understanding of the QW spin detector and the identification of background contributions. For example, we show using optical pumping measurements that the spin detection efficiency of the QW is a function of the bias voltage, as is the background photoluminescence polarization. This work was supported by DARPA, ONR, and NSF (MRSEC).

[1] H.J. Zhu et al., Phys. Rev. Lett. 87, 016601 (2001); A.T. Hanbicki et al., Appl. Phys. Lett. 80, 1240 (2002).

2:40pm **EL+SC+MI-MoA3 Characterization of an Fe/AlGaAs Tunnel Barrier Interface for Electrical Spin Injection**, *A.T. Hanbicki*, ***R.M. Stroud***, *B.T. Jonker*, Naval Research Laboratory

Electrical injection of spin-polarized carriers from a contact into a semiconductor is essential for the success of spintronic devices. Ferromagnetic metals are attractive contact materials because of their ample supply of spin-polarized electrons, but the use of these materials has been limited by small injection efficiencies in the diffusive transport regime.[1] The use of a tunnel barrier between a metal and semiconductor.however. should facilitate usable spin currents.[2] Recent experiments reported spin injection from Fe into a AlGaAs/GaAs-based LED which produced an electron spin polarization of 15% in the GaAs quantum.[3] This was attributed to tunneling through the Schottky barrier. We have characterized the Fe/AlGaAs contact reported in reference 3 to verify the tunneling nature of the contact and to investigate the physical nature of the interface. Samples were grown by molecular beam epitaxy and were specifically engineered to utilize the Schottky barrier between the Fe and the semiconductor as a tunnel contact. Current vs voltage measurements were made through the structure at different temperatures. The conductance shows an asymmetric parabolic dependence on the voltage. Further, there is a weak insulating-like behavior of the zero-bias resistance as a function of temperature, a reliable indication that this is a tunneling process based on the Rowell criteria for tunneling.[4] High-resolution TEM measurements indicate an atomically abrupt interface between the metal and semiconductor. Current-in-plane measurements and the relation of bias voltage to spin polarization will also be discussed. This work was supported by the DARPA SpinS program and ONR.

[1] G. Schmidt, et al, Phys.Rev.B 62, R4790 (2000)
[2] E.I. Rashba, Phys.Rev.B 62, R16267 (2000)
[3] A.T. Hanbicki, et al., Appl.Phys.Lett. 80, 1240 (2002)
[4] B.J. Jönsson-Åkerman, et al., Appl.Phys.Lett. 77, (2000).

3:00pm **EL+SC+MI-MoA4 A Schottky Tunnel Barrier Contact for Electrical Spin Injection into a Semiconductor**, ***B.T. Jonker***, *A.T. Hanbicki, G. Kioseoglou*, Naval Research Laboratory, *G. Itskos, R. Mallory, A. Petrou*, SUNY at Buffalo

Electrical injection of spin polarized electrons into a semiconductor heterostructure is a critical issue for semiconductor-based spintronic devices. While very encouraging results have been obtained using magnetic semiconductors as injecting contacts,[1] the desire for room temperature operation at low magnetic fields leads one to consider other materials and avenues. Ferromagnetic (FM) metals offer high Curie temperatures and can be rapidly switched (~ 300 ps) at low applied fields. However, theory has indicated that only very small spin injection (~0.01%) can be expected for typical FM metals as diffusive contacts.[2] We report here electrical spin injection from an Fe Schottky contact into an AlGaAs/GaAs LED structure, with spin injection efficiencies above 34% which extend to room temperature. These robust effects are attributed to spin tunneling[3] through the tailored Schottky barrier contact. The samples are grown by MBE, and the width of the depletion region at the Fe/AlGaAs interface is controlled by the semiconductor doping profile. Under reverse bias, electrons tunnel from the Fe into the semiconductor, and radiatively recombine in the GaAs quantum well. The circular polarization of the surface emitted electroluminescence (Faraday geometry) provides a quantitative, model independent measure of the QW spin polarization, and hence the injection efficiency.[1] The spin tunnel current is dominated by minority spin carriers, in contrast to previous work using Al$_2$O$_3$ tunnel barriers and a superconducting film detector. The temperature dependence of the polarization will also be discussed. These results will be compared with previous work[4] and theoretical modeling of Schottky barrier injection. Work supported by the DARPA SpinS program and ONR.

[1] R. Fiederling, et al Nature (1999); B.T. Jonker et al, PRB (2000)
[2] G. Schmidt et al, PRB (2000)
[3] E.I. Rashba, PRB (2000)
[4] H.J. Zhu et al, PRL (2001).

3:20pm **EL+SC+MI-MoA5 Contact Metallurgy for the Antimonide Based Compound Semiconductors**, ***S.E. Mohney***, *W.E. Liu, H.S. Wang, J.A. Robinson*, Penn State University **INVITED**

Antimonide based compound semiconductors are promising candidates for both high frequency, low power electronic devices and optoelectronic devices, and the performance of electrical contacts to these semiconductors is critical for some of the devices currently under development, particularly the electronic devices. Control of the interfacial reactions between the contact metals and the semiconductors is necessary during device processing and packaging since interfacial reactions between the metals and semiconductors occur at very low temperatures. Therefore, we have examined the condensed phase equilibria in the metal-III-Sb systems to guide our selection of shallow, thermally stable contact metallizations. We have performed thermodynamic calculations to estimate ternary phase diagrams in the transition metal-Ga-Sb, transition metal-In-Sb and selected metal-Al-Sb systems. We find that W, Re, and Os are the only transition metals predicted to be in thermodynamic equilibrium with both GaSb and InSb under the conditions considered in our calculations, while W is the only transition metal predicted to be in equilibrium with AlSb. Finally, we give an example of our use of the information we have gathered for the design of a very shallow, thermally stable low resistance ohmic contact to p-type GaInSb. Since we have observed using transmission electron microscopy that Pd reacts uniformly with GaSb at low temperatures, we chose a very thin layer of Pd as the first metal in our contact. We then deposited W because of our prediction that it would be in thermodynamic equilibrium with both GaSb and InSb and that it could serve as a diffusion barrier between layers. Finally, we capped the films with Au, which was important for lowering the metal sheet resistance. A contact resistance of 3 x 10^{-7} ohm-cm^2 was measured with good stability at 250 °C for 100 h, as verified using contact resistance measurements and Auger depth profiles.

4:00pm **EL+SC+MI-MoA7 Electrical Contact Behavior of Ni/C60/4H-SiC**, ***W. Lu***, Fisk University, *W.C. Mitchel*, Air Force Research Laboratory, *J.R. Landis*, University of Dayton Research Institute, *T.R. Crenshaw*, Fisk University, *S.R. Smith*, University of Dayton Research Institute, *W.E. Collins*, Fisk University

Ohmic contact formation of Ni/C60 film on n-type 4H-SiC was investigated. A C60 interfacial layer between Ni film and SiC improves ohmic contact properties significantly. The C60 film was deposited by Langmuir-Blodgett method prior to the Ni film deposition on SiC using DC sputtering method. High quality ohmic contact of Ni/C60/4H-SiC is formed after annealing at 800°C in Ar for two hours with a specific resistance of 1.6

$x\ 10^{-6}\ \Omega cm^2$ for the SiC with a doping concentration of $1.8 \times 10^{19} cm^{-3}$. Raman spectra reveal that the formation of graphitic carbons by Ni catalytic effects result in the formation of ohmic contact on SiC, and the nano-size graphitic flakes identified by Raman spectroscopy play a key role for ohmic contact formation on SiC. Scanning electron microscopy (SEM) and atomic force microscopy (AFM) show a direct relationship between the graphitized morphological features on the film and ohmic contact behavior.

4:20pm **EL+SC+MI-MoA8 Electrical Characterization of AlN MIS/MIM-structures**, ***F. Engelmark***, *J. Westlinder, I.V. Katardjiev, J. Olsson, S. Berg*, University of Uppsala, Sweden

The electrical properties of insulating ceramic films such as AlN, Ta_2O_5, HfO_2, ZrO_2, Al_2O_3, etc. are of substantial interest for a number of microelectronic and electro-acoustic applications owing to their chemical stability in harsh environments along with some very interesting electrical properties. In this work, emphasis has been put on the electrical properties of Aluminum nitride (AlN) films. Thin AlN films have been deposited onto Si(100) and Mo/Si(100) substrates. The sputter deposited Mo is polycrystalline, showing a predominant (110) orientation. AlN film growth is performed using different process conditions in a reactive PVD (Physical Vapour Deposition). Both fully textured (0002) polycrystalline and XRD amorphous films have been grown and studied. MIS- and MIM-structures have been fabricated and electrical properties such as dielectric constant, leakage current as well as their high frequency behaviour are investigated. The measurements indicate that the dielectric constant does not vary with crystallinity of the films, and remains constant at a value of 10. Further, the high frequency behaviour of the dielectric constant have been studied in the range 100 MHz to 20 GHz. The leakage current mechanism is also similar for different films and is believed to be Poole-Frenkel controlled. C-V (Capacitance-Voltage) measurements for MIS structures revealed the presence of charges in the interface between the substrate and the dielectric layer. Trapped charge density was estimated to be $3.5*10^{10}\ cm^{-2}$.

Electronic Materials and Devices
Room: C-107 - Session EL+SC-TuM

Heterojunctions
Moderator: R.S. Goldman, University of Michigan

8:20am **EL+SC-TuM1 Epitaxial Growth and Characterization of CdS Layers Grown on InP (001) using Molecular Beam Epitaxy from Atomic Sulfur Beam and Thermally Evaporated Cd**, ***J.W. Choi***, *M.-A. Hasan, A. Bhupathiraju*, University of North Carolina at Charlotte

Recent progress in epi-ready InP(E_g=1.35 eV) wafer growth has prompted new applications of heterojunction devices and quantum structures based on closely lattice matched epitaxial films on InP. Cadmium sulfide (CdS), a direct bandgap material (E_g=2.5 eV), has a small lattice mismatch to InP (0.63%) that can facilitate optoelectronic integration on InP. In this work, growth of CdS on InP (001) substrates is investigated using modified molecular beam epitaxy (MBE). Two growth methods are investigated. In the first method, epitaxial growth is conducted by atomic sulfur (S) beam from an RF atomic source with H_2S as the source gas while Cd is supplied from a cracker cell. The RF source is operated at 13.56 MHz and produces an intense monoatomic sulfur beam (λ= 930.5 nm emission peak measured by plasma spectroscopy). In the second method, deposition is performed using CdS sublimation from a solid CdS using a conventional Knudsen cell. Rinsing by methanol is used to clean the epi-ready InP (001) substrates. Final substrate cleaning is achieved by thermal desorption (530-550°C) in vacuum. RHEED shows InP (001) 2x1 surface after thermal cleaning. In both methods, in-situ RHEED measurement indicates epitaxial growth of zincblende CdS; Auger electron spectroscopy (AES) shows stoichiometric CdS within the AES resolution limit. AES depth profiles also indicate an abrupt InP/CdS interface for all temperatures investigated. The growth rate of CdS is primarily governed by Cd flux as indicated by the activation energy measured from the flux-dependence of the growth rate. Atomic force microscopy (AFM) shows measurable dependence of surface roughness on growth method. For growth using an RF atomic source, average surface roughnesses of 1-2 nm is measured for all growth temperatures, layer thicknesses, and flux ratios with no evidence of island formation; higher roughness values (10-20nm) were typically measured for growth from solid CdS.

8:40am **EL+SC-TuM2 Structure of InAs/InP Interfaces Formed During Metalorganic Vapor-Phase Epitaxy**, ***D.C. Law***, *Y. Sun, C.H. Li,* University of California, Los Angeles, *S.B. Visbeck,* Siemens & Shell Solar Gmbh, *G. Chen, R.F. Hicks,* University of California, Los Angeles

We have studied the initial stages of heterojunction formation during the metalorganic vapor-phase epitaxy of indium arsenide on indium phosphide. Exposing an InP (001) film to 10 mTorr of tertiarybutylarsine below 500 °C results in the deposition of a thin InAs layer from 1.5 to 5.0 atomic layers thick (2.3 to 7.5 Å). The surface of this epilayer remains atomically smooth independent of arsenic exposure time. However, in an overpressure of tertiarybutylarsine at or above 500 °C, the arsenic atoms diffuse into the bulk, creating strained InAsP films. These films form three-dimensional island structures to relieve the built-up strain. The arsenic transport into InP can be described by a constant-source diffusion model with the arsenic number density given by: $N_{As} = 0.5\ N_T \mathrm{erfc}\ (x/2\sqrt{(D_{eff}t)})$. The activation energy and pre-exponential factor for arsenic diffusion into indium phosphide are: $D_o = 2.3\pm1.0\ x10^{-7}\ cm^2/s$ and $E_d = 1.7\pm0.2$ eV.

9:40am **EL+SC-TuM5 Device Quality III-V Compound Semiconductor Epitaxy on Si Via SiGe Interlayers**, ***S.A. Ringel***, *C.L. Andre, A. Khan, M. Gonzalez, M.K. Hudait,* Ohio State University, *E.A. Fitzgerald,* Massachusetts Institute of Technology, *J.A. Carlin, M.T. Currie, C.W. Leitz, T.A. Langdo,* AmberWave Systems Corporation **INVITED**

Integration of III-V compounds with Si using direct epitaxial approaches has been an area of intense interest for years. Achieving this would enable a complement of electronic and optoelectronic capabilities that would generate new circuit functions with higher speed, and potentially simpler architecture. There is also substantial interest in III-V/Si integration where the primary purpose for Si is as an alternative substrate for III-V solar cells, which are conventionally grown on Ge or GaAs substrates. Compared to Si, these substrates are expensive, brittle and heavy, which are issues for this application. For both of these directions, the materials issues of how to integrate III-V compounds with Si without degrading electronic properties due to the mismatch in structural, thermal and chemical properties so that high performance devices can be achieved are the same. Here we show that growth of compositionally graded SiGe interlayers to accommodate lattice strain between a Si wafer and III-V epitaxial structures, coupled with monolayer-scale control over the formation of the initial III-V/IV interface to eliminate anti-phase domain disorder and block interface diffusion, together yield high quality AlGaAs/GaAs and InGaP/GaAs layers, heterostructures and minority carrier devices. Time resolved photoluminescence measurements of III-V double heterostructures reveal record high minority carrier lifetimes for GaAs on Si in excess of 10 nanoseconds, which is attributed to the simultaneous elimination of anti-phase domains and reduction of residual threading dislocation densities to below $1x10^6$ cm^{-2}. SIMS and capacitance-voltage measurements show that autodoping is effectively eliminated for GaAs grown on Ge/SiGe/Si, with no additional background impurities detected in the GaAs layers grown on these substrates. Solar cells are used as examples of minority carrier devices to show that high performance comparable to similar devices grown on conventional substrates has been achieved, with record voltage output for III-V cells grown on Si.

10:20am **EL+SC-TuM7 Interdiffusion, Alloying, and Defect Formation at GaN-Sapphire Interfaces**, ***X.L. Sun***, *S.T. Bradley, G.H. Jessen, L.J. Brillson*, The Ohio State University

The chemical and electronic structure at GaN/sapphire interfaces has a major influence on the electronic quality of epitaxial GaN films. In particular, degenerate doping usually occur near hydride vapor phase epitaxy (HVPE) grown GaN/sapphire interfaces that can affect lateral transport in overgrown devices. Near the interface, impurity diffusion, alloying, and related defect formation can occur at the high (1150°C) growth temperatures that is important to understand and control. We have used Auger electron (AES) and cathodoluminescence (CLS) spectroscopies in a UHV scanning electron microscope (SEM) to probe the chemical and electronic features at the HVPE GaN/sapphire interface in cross section in a nanometer scale. Specimens were cleaved and Ar sputtered in UHV to prepare clean interfaces with well-defined AES, CLS, and secondary electron images. AES images reveal dramatic evidence for diffusion of O from sapphire typically decreasing exponentially ~ 1 µm into GaN from 60% to the detection limit of < 1% surface coverage. The AES O intensity line profile mirrors corresponding SIMS O depth profiles and a donor level CLS emission vs. depth normal to the interface found in similar samples. Conversely, N with plateau concentrations of ~5 % extend ~ 2 µm into the sapphire and correspond spatially to a 3.8 eV defect emission attributed to Al-N-O complexes. While Ga exhibits no strong diffusion, interface Al decreases from 10% to < 1% over ~1 µm into the GaN and support evidence for AlGaN alloy formation, based on ~3.6 eV CLS emission above the GaN band gap at the buried interface. Depending on surface pretreatment and growth conditions, such interfaces can be abrupt to < 200 nm or can exhibit interdiffusion on a micron scale. These results illustrate a new approach to probe chemical and electronic interactions at semiconductor heterojunctions and reveal that both interdiffusion and alloying can occur and lead to extrinsic electronic effects.

10:40am **EL+SC-TuM8 Growth and Characterization of Heterjunction Diode Made of AlN on Si(111)**, ***K. Sundaresan***, *M. Jenkins, M.-A. Hasan,* University of North Carolina, *M. Sardela Jr.*, University of Illinois

Single crystalline hexagonal AlN(001) was grown on Si(111) using surface-reconstruction induced epitaxy. The Si(111)7x7 surface, generated under thermal etching under UHV, was first passivated by deposition of ~0.3 monolayer (ML) of Al at 650-700 °C. Each Al atom bonds to 3 Si atoms on the surface, which give rise to the well-known Si(111)root3xroot3 surface. The well ordered, Al-passivated Si(111)root3xroot3 surface was then used as a template to initiate epitaxial growth of AlN on Si. The growth was conducted by using an atomic N flux from a RF atomic source and thermal Al evaporation. X-ray diffraction showed single crystalline hexagonal AlN(001) with a full width at half maximum (FWHM), measured from the layer peak, equal to that of the Si substrate indicating highly oriented AlN layer. Epitaxial growth was achieved over a wide range of Al/N flux ratio and growth temperatures extending from 350 to 850 °C. AlN/Si heterojunction diode, fabricated using this method showed a breakdown voltage in excess of 350 V and a leakage current below 100 nA indicating high quality interface.

11:00am **EL+SC-TuM9 Observation of a Long-range Strain Field under SiO_2/Si Interface by using Multi-wave X-ray Diffraction**, ***W. Yashiro***, National Institute of Advanced Industrial Science and Technology (AIST), Japan, *K. Sumitani, T. Takahashi*, The University of Tokyo, Japan, *Y. Yoda*, Japan Synchrotoron Radiation Research Institute (JASRI), *K. Takahashi, T. Hattori*, Musashi Institute of Technology, Japan

In order to further improve the speed of VLSI circuits, new materials and device structures are being proposed in recent year. In particular there has been considerable interest in strained Si because it can lead to high-performance metal-semiconductor (MOS) devices. Transmission electron microscopy (TEM) is a technique to investigate local strains, e.g. around a dislocation at a phase boundary. In contrast with TEM, x-ray diffraction is powerful to investigate long-range ordered structures in crystals. In the present paper, we propose a new method that is sensitive to very small and long-range strains near surfaces of crystals by using multi-wave x-ray diffraction technique. To date, the Bragg reflection of x-ray diffraction is used to investigate such long-range strain fields. Recently Emoto et al. have indicated using the Bragg reflection that there exist very small strain fields on the side of the Si substrates if even ultra-thin layers are formed on them.[1] Our method is also a method using the Bragg reflection, but with the important distinction that we use a phenomenon, intensity modulation of the CTR scattering under a Bragg condition. This makes it possible to determine total displacements due to small lattice distortions, rather than local lattice spacing. The method was applied to a Si(001) wafer whose surface is covered with an oxide layer about 5 nm thick formed by microwave-excited high density Kr/O_2 plasma oxidation. We found that the total displacement of -0.18 Å in the direction normal to the surface exists under the interface between the oxide layer and the substrate.

[1] Emoto et al. Surf. Sci. 493 (2001) 221-226.

11:20am **EL+SC-TuM10 Measurement of Fermi Level Pinning Kinetics at Si-SiO_2 Interfaces: Implications for CMOS Transistor Manufacture**, ***K. Dev***, *M.Y.L. Jung, R. Gunawan, R.D. Braatz, E.G. Seebauer*, University of Illinois

Excessive transient enhanced diffusion (TED) of boron in silicon has been a major inhibitor to forming ultrashallow junctions for CMOS device applications. Current technology for junction formation relies on ion implantation into Si through SiO_2 to introduce dopants into the substrate, followed by rapid thermal annealing. We have investigated a previously unknown effect in this process sequence: charge build-up at the Si-SiO_2 interface and the resulting Fermi level pinning that can occur just after implant. Fundamentally, the charge build-up occurs in response to the ion-induced formation of dangling bonds that introduce energy states into the Si surface bandgap. The present work uses the optical technique of photoreflectance to demonstrate experimentally that these effects indeed exist and to measure their evolution kinetics. Photoreflectance is one of a class of modulation spectroscopies in which a semiconductor is periodically perturbed, and the resulting change in dielectric constant is detected by reflectance. The presence of a photoreflectance spectrum demonstrates unequivocally the existence of Fermi level pinning. The spectral amplitude scales linearly with the magnitude of built-in surface potential. Thus, we can deduce the pinning kinetics from the variation in amplitude. Our data demonstrate the existence of substantial pinning just after implant with 500 eV ions. Healing begins to occur in the vicinity of 400°C - within the temperature stabilization step in which interstitial clusters form. TED simulations using electrostatic boundary conditions derived from the photoreflectance experiments show that pinning deepens the pn junction significantly by transforming the Si-SiO_2 interface into a reflector of charged bulk interstitials.

11:40am **EL+SC-TuM11 Effects of Interface Properties on Degradation and Reliability of CMOS Devices with RPECVD Stacked Oxide/Nitride and Oxynitride Dielectrics**, *G. Lucovsky*, ***Y. Lee***, North Carolina State University, *Y. Wu*, Advanced Micro Devices, *C. Bae, J.G. Hong*, North Carolina State University

The effects of interface properties on device degradation and reliability of sub-2nm stacked oxide/nitride and oxynitride gate dielectrics prepared by the remote plasma enhanced CVD (RPECVD) technique under constant voltage stress (CVS) are investigated. Time evolutions of the transient SILC effect and threshold voltage (Vt) changes have been demonstrated to illustrate the breakdown behaviors and charge trapping during stress. More negative Vt shifts were observed for both P- and N-MOS devices, indicating the increases of hole trapping at the Si/SiO_2 interface. The p-channel transistors with stacked gate dielectrics received interface N_2/He nitridation and effectively suppress positive off-state leakage current, resulting in less device degradation as compared to the transistors without interface nitridation. This improvement is attributed to approximately one monolayer of N at the Si/SiO_2 interface which suppresses hole trapping. In addition, the influence of remote-plasma-assisted oxidation (RPAO) thickness on oxynitride device degradation and reliability is also studied. It is found that the devices with 0.6 nm RPAO exhibit improved C-V characteristics, lower post-breakdown current and higher TDDB reliability compared to the devices with 0.8 nm RPAO. The generation of interface states and the correlation between carrier conduction mechanism and TDDB are also discussed.

Magnetic Interfaces and Nanostructures
Room: C-205 - Session MI+EL+SC-TuM

Ferromagnetic Semiconductors
Moderator: B.T. Jonker, Naval Research Laboratory

8:20am **MI+EL+SC-TuM1 ab initio Magnetic Exchange Interactions in DMS and TiO_2**, ***M. van Schilfgaarde***, Arizona State University **INVITED**

The electronic structure of TM-doped TiO2 is studied within the ab initio local spin-density approximation and compared to more traditional TM-doped III-V DMS semiconductors. The conduction band of TiO2 consists mainly of Ti d character. Substituting a 3d TM for Ti, localized levels split off the conduction band; they are spin-split by an on-site exchange interaction and are responsible for the magnetism. The deepest level is of t2 symmetry and sweeps deeper in the gap in the series TM=V,Cr,Mn,Fe,Co. In the dilute alloy, the impurity level broadens into a narrow band. Thus the conductivity is expected to occur through a hopping mechanism, increasing with decreasing temperature as is observed in Co:TiO2. The character of this level is compared to TM d levels in the III-V DMS alloys (Cr,Mn,Fe):(Al,Ga,In)(N,P,As). Using a linear-response technique, the LSDA is mapped analytically onto a magnetic hamiltonian, which was used to investigate exchange interactions in random TM:TiO2 and (Cr,Mn):(Al,Ga,In)(N,P,As) alloys. Several novel phenomena will be described in the DMS case; for example Tc is predicted to increase monotonically with concentration for Cr:III-V, while for Mn:III-V Tc reaches a maximum at about 10% Mn concentration. The exchange interactions are found to have elements in common with both the carrier-mediated model and the double exchange/superexchange model, but also show important differences. For (V,Cr,Mn,Fe,Co):TiO2, the filling, magnetic moment and exchange interactions change systematically and are well described by a double exchange/superexchange model. However, for Tc to reach the observed RT in Co:TiO2, a source of holes is needed.

9:00am **MI+EL+SC-TuM3 $Co_xTi_{1-x}O_2$ Anatase Heteroepitaxy on Si(001)**, ***T. Droubay***, Pacific Northwest National Laboratory, *A.C. Tuan*, University of Washington, *S.A. Chambers*, Pacific Northwest National Laboratory

With a Curie temperature above 700K, high remanence, and respectable coercivity, Co-doped TiO_2 anatase ($Co_xTi_{1-x}O_2$) is one of the more magnetically robust dilute magnetic semiconductor (DMS) materials currently under investigation. The future of this material for near-term device use as a spin injector requires deposition on and compatibility with traditional semiconductors such as silicon. Successful growth of crystalline oxides on silicon without oxidizing the underlying substrate is a formidable challenge. Our goal in this work is to grow epitaxial $Co_xTi_{1-x}O_2$ on Si(001) by using a suitable template layer, and then determine the resulting magnetic and electronic properties. We have previously shown that polycrystalline $Co_xTi_{1-x}O_2$ grown on Si(001) with its native oxide is ferromagnetic at room temperature. We are now working on $Co_xTi_{1-x}O_2$ heteroepitaxy on Si(001) using an ultrathin epitaxial $SrTiO_3$ buffer layer to prevent formation of titanium silicide and SiO_2 at the interface that result from a thermodynamic instability. An added benefit of the $SrTiO_3$ buffer layer is to generate a nearly zero conduction band offset to Si, which is essential for efficient n-type spin injection. A detailed analysis of the growth and properties of this heteroepitaxial system will be presented.

9:20am **MI+EL+SC-TuM4 Epitaxial Growth and Properties of Co-doped TiO_2 Anatase on $LaAlO_3$(001)**, ***S.A. Chambers***, *T. Droubay, C.M. Wang, S.M. Heald, S. Thevuthasan, A.S. Lea, C.F. Windisch, Jr.*, Pacific Northwest National Laboratory, *R.F.C. Farrow, L. Folks, J.-U. Thiele, M.G. Samant, R.F. Marks*, IBM Almaden Research Center

We are investigating Co-doped TiO_2 anatase heteroepitaxy on $LaAlO_3$(001) by oxygen plasma assisted molecular beam epitaxy. This material is of considerable interest because it is ferromagnetic well above room temperature. Thus, it may be a useful DMS for spintronics. The use of a higher growth rate (0.04 nm/sec) results in the nucleation of nanocrystals of rutile, the more stable form of TiO_2, within the continuous anatase film. The density of rutile nanocrytals increases as the quality of the substrate surface decreases. A lower growth rate (0.01 nm/sec) results in a much better film morphology, although a low density of smaller nanocrystals remains. Unlike the fast-grown films, these films show no evidence for any phase other than anatase. A number of techniques reveal that Co substitutes for Ti in the lattice and exhibits a +2 oxidation state; there is no evidence for elemental Co in any form. Each Co(II) substitution for Ti(IV) requires an O^{-2} anion vacancy in order to maintain charge neutrality, and evidence for such a vacancy is forthcoming from preliminary Co K-shell EXAFS. Such vacancies do not generate free carriers because they are uncharged. Hall effect and XPS measurements show that the films are n-type, the most likely cause being the presence of O atom vacancies that form during growth. These vacancies are independent of the presence of Co, and are negatively charged, thereby providing a source of free electrons from shallow donor states. The magnetization depends critically on free carrier concentration, as expected for a DMS. The exact Curie temperature is currently being determined, but appears to be in excess of 700K.

9:40am **MI+EL+SC-TuM5 Ferromagnetism in Mn-implanted Single Crystal Oxides**, ***D.P. Norton***, *S.J. Pearton, B.S. Jeong, Y.W. Heo, A.F. Hebard, N.A. Theodoropoulou,* University of Florida, *L.A. Boatner,* Oak Ridge National Laboratory, *Y.D. Park,* Seoul National University, Korea, *R.G. Wilson*, Consultant

Several semiconducting oxides, including ZnO, offer significant potential in providing spin-based functionality. Theoretical predictions suggest that room-temperature carrier-mediated ferromagnetism should be possible in Mn-doped p-type ZnO. In this paper, we report on the synthesis and properties of magnetically-doped semiconducting oxides, including ZnO. While previous efforts report no ferromagnetism in Mn-doped ZnO that is n-type due to group III impurities (consistent with theory), we find ferromagnetism in n-type ZnO that is co-doped with Mn and Sn. Hysteresis was observed in magnetization versus field curves for Mn-implanted n-type ZnO:Sn. Differences in zero field-cooled and field-cooled magnetizations persists up to ~ 150 K for Sn-doped ZnO crystals implanted with 3 at % Mn. These results indicate that ZnO doped with Mn and Sn may prove promising as a ferromagnetic semiconductor for spintronics.

10:00am **MI+EL+SC-TuM6 Self-compensation in Manganese-doped Ferromagnetic Semiconductors**, ***S.C. Erwin***, *A.G. Petukhov*, Naval Research Laboratory

We present theoretical evidence that the observed hole compensation in manganese-doped ferromagnetic semiconductors is due to interstitial manganese. We show that under the non-equilibrium conditions used during growth, interstitial Mn is readily formed near the surface by a simple low-energy adsorption pathway. In GaAs, isolated interstitial Mn impurities are electron donors, each compensating two substitutional Mn acceptors under p-type conditions. We show that partial compensation is a prerequisite for ferromagnetic order below the metal-insulator transition, and that the Curie temperature is highest when 1/6 of the Mn is interstitial.

10:20am **MI+EL+SC-TuM7 Ferromagnetic Semiconductor Heterostructures[1]**, ***N. Samarth***, Penn State University **INVITED**

The molecular beam epitaxy (MBE) of ferromagnetic semiconductor heterostructures provides model systems for exploring fundamental issues in semiconductor spintronics. We provide an overview of heterostructures that combine the ferromagnetic semiconductor (Ga,Mn)As with conventional III-V and II-VI semiconductors, as well as with the metallic ferromagnet MnAs. After an introduction to the properties of MBE-grown (Ga,Mn)As, we discuss two classes of heterostructures: (a) hybrid ferromagnetic metal/semiconductor tunnel junctions that allow us to unambiguously probe spin injection into semiconductors using all-electrical techniques and (b) hybrid ferromagnetic/semiconductor photodiodes that serve as toy spintronic "devices" whose photo-response is magnetically controlled.

[1] This work is carried out in collaboration with S. H. Chun, K. C. Ku, S. J. Potashnik, and P. Schiffer, and is supported by grants from NSF, ONR and DARPA

11:00am **MI+EL+SC-TuM9 Epitaxial Growth of the Diluted Magnetic Semiconductor Cr_xGe_{1-x}**, ***G. Kioseoglou***, *A.T. Hanbicki,* Naval Research Laboratory, *Y.D. Park,* Seoul National University, Korea, *S.C. Erwin, B.T. Jonker*, Naval Research Laboratory

Ferromagnetic semiconductors (FMS) provide an opportunity to control spin-dependent behavior in semiconductor device heterostructures. Although much effort has focused on III-Mn-V materials such as GaMnAs , the mechanism of ferromagnetic order remains unclear; in particular the precise roles played by the dopant and the semiconductor host. We have explored this issue recently by developing a new Group-IV FMS, MnGe.[1] Here we report our work to develop an elemental FMS using a different dopant, Cr-doped Ge. This choice was motivated partly by our density-functional theory (DFT) calculations, which indicate that CrGe and MnGe should have comparable Curie temperatures. We report the epitaxial growth of Cr_xGe_{1-x} and describe the structural, magnetic and transport properties. The samples were grown on GaAs(001) substrates by molecular beam epitaxy at substrate temperatures of 40-500°C and the crystallinity was confirmed by the RHEED pattern. The Cr concentration used was 2-3% as determined from X-ray fluorescence. The RHEED pattern indicates single crystal growth for substrate temperatures above 200°C, with sharp 1x1 streaks. Growth at 40-70°C is initially single crystal, but the pattern becomes increasingly diffuse with film thickness. The samples are strongly p-type, and the hole density varies with the Cr concentration. SQUID measurements were performed on all samples to investigate the magnetic character of the Cr:Ge system. Samples grown at the higher growth temperatures exhibit only paramagnetic order. Co-doping with both Mn and Cr is also investigated. This work was supported by the DARPA SpinS program and ONR.

[1] Y.D. Park, et al., Science 295, 651 (2002).

11:20am **MI+EL+SC-TuM10 Cr-Doped III-V Ferromagnetic Semiconductors**, ***M.E. Overberg***, *G.T. Thaler, R.M. Frazier, C.R. Abernathy, S.J. Pearton, N.A. Theodoropoulou, A.F. Hebard,* University of Florida, *R.G. Wilson,* Private Consultant, *J.M. Zavada*, U.S. Army Research Office

Ferromagnetic semiconductors, consisting of a semiconductor host material doped with transition metal ions, are becoming increasingly prevalent in the literature as a candidate for incorporating the spin degree of freedom into device structures. To date, the vast majority of work in this area has centered on the incorporation of Mn into both II-VI and III-V materials by a variety of techniques. However, recent theoretical work has indicated that Cr may be a more suitable dopant for achieving room-temperature ferromagnetism within these materials.[1] In this paper, we will report on the preparation of GaCrN, GaCrP, and AlGaCrP by the direct implantation of Cr. The magnetic and magneto-transport (anomolous Hall Effect) properties of these films will be quantified both versus implantation dose (x=0.04, 0.06, 0.10) and versus post-implantation annealing, to identify an optimum combination of dose and annealing conditions. Analysis by SQUID magnetometry of the GaCrN with 6% Cr indicates the presence of a strong ferromagnetic phase with a Curie temperature above the 350 K limit of the magnetometer. High resolution x-ray diffraction (HRXRD) and transmission electron microscopy (TEM) results from the implanted films will also be presented to address the issue of the formation of second phases within these materials. HRXRD rocking curves of the implanted materials will also be used to trace the evolution of the implantation-induced lattice damage with annealing as well as strain-related effects due to the incorporation of Cr into substitutional lattice sites.

[1] K. Sato, and H. Katayama-Yoshida, Jap. J. Appl. Phys., Pt. 2, 40 (5B), p. L485 (2001).

11:40am **MI+EL+SC-TuM11 Suppression of Phase Segregation during MBE Growth of GaMnN Using Nitrogen-Hydrogen Plasma**, *Y. Cui,* ***L. Li***, University of Wisconsin-Milwaukee

Epitaxial growth of GaMnN by electron-cyclotron-resonance plasma-assisted molecular beam epitaxy using nitrogen-hydrogen plasma was studied by reflection high-energy electron diffraction, scanning electron microscopy, energy dispersive spectroscopy, and x-ray diffraction. The electron diffraction pattern changed from streaky to spotty when hydrogen was added to the nitrogen plasma, indicating that the effective N/Ga ratio was increased. Films grown with nitrogen plasma are phase segregated into GaN and manganese nitrides. In contrast, when nitrogen-hydrogen plasma was used, the films are single phase Ga1-xMnxN, with x can be as high as 0.06. These results indicate that phase segregation can be suppressed by adding hydrogen to the nitrogen plasma during growth.

Electronic Materials and Devices
Room: C-107 - Session EL+SC-TuA

Semiconductor Characterization
Moderator: P.H. Holloway, University of Florida

2:00pm **EL+SC-TuA1 Active-Device Scanning Voltage Microscopy Studies on a Forward and Reverse Biased InP pn Junction Sample**, ***ST.J. Dixon-Warren***, *R. Dworschak, G. Este, AJ. SpringThorpe, J.K. White,* Nortel Networks, Canada, *D. Ban, E.H. Sargent*, University of Toronto, Canada

Active-Device Scanning Voltage Microscopy (SVM) is a new Scanning Probe Microscopy (SPM) technique in which a two-dimensional voltage map is obtained on the cross-section of a biased semiconductor sample. The voltage is measured using a very high impedance voltmeter that is connected to a conductive doped-diamond coated SPM tip. Recently obtained results on a molecular beam epitaxy (MBE) grown InP pn junction sample will be reported, under both forward and reverse bias conditions. The results are compared to those obtained with Scanning Spreading Resistance Microscopy (SSRM) measurements under zero bias on the same sample. The SVM and SSRM results will be discussed in terms of the semi-classical model of the pn junction. The physics of the SVM measurement process will also be discussed. Finally, the results obtained on the simple pn junction sample will be compared with those obtained on more complex samples, such as InP based ridge waveguide and buried heterostructure laser samples under forward bias.

2:20pm **EL+SC-TuA2 Scanning Tunneling Microscopy Imaging of Charged Defects on Clean Si(100)-(2x1)**, ***G.W. Brown***, *H. Grube, M.E. Hawley,* Los Alamos National Laboratory, *S.R. Schofield, N.J. Curson, M.Y. Simmons, R.G. Clark*, University of New South Wales, Australia

We have used scanning tunneling microscopy (STM) to image charged defects on the clean Si(100)-(2x1) surface. In the absence of "C"-type defects, band bending can occur during STM imaging, allowing near surface charge to influence the state density contributing to the tunnel current. As in the case of cleavage faces of III-V semiconductor crystals, the charge-induced band bending produces long range enhancements superimposed on the periodic surface lattice. We observe this in empty-state STM images taken on n-type Si(100). No band bending signature is seen in the filled-state images. This can be understood by considering the band structure at the surface, which has surface states within the gap. The charged defects observed in this work are of the types commonly observed in clean Si(100)-(2x1) STM studies, however, not all defects of a given type appear charged. This would indicate subtle differences in defect structure or the influence of impurities. This work demonstrates the ability to observe charged features on the clean Si(100) surface, which will be important for current and future research focussed on producing atomic scale electronic structures. Predictions for signatures on p-type material will also be made.

2:40pm **EL+SC-TuA3 The Surface Photovoltage and Photoelectron Spectroscopy**, ***J.P. Long***, Naval Research Laboratory **INVITED**

Frequently, the surface of a semiconductor in equilibrium exhibits "band bending," an electrostatic shift of the surface relative to the bulk that arises from the built-in electric field associated with a surface depletion layer. When such a surface is illuminated, photogenerated electrons and holes move to screen the built-in field, thereby reducing the band bending and shifting the surface energy levels, an effect known as the surface photovoltage (SPV). Because the energy levels measured by photoelectron spectroscopy shift with the electrostatic potential of the surface, the technique is sensitive both to equilibrium band bending, a fact often exploited to characterize Schottky barrier heights, and to the SPV, which makes photoemission a useful SPV detector. However, under certain conditions, the ultraviolet or x-ray photoemission source itself can induce a sizable SPV that seriously hampers the measurement of equilibrium energy levels. This talk will introduce the SPV at a tutorial level, and will discuss the interplay between photoelectron spectroscopy and the SPV. Illustrations of photoemission as a SPV detector include the use of synchrotron radiation to characterize SPV decays in laser-excited Si and to detect, via SPV-induced band-flattening, inhomogeneous band bending on GaAs caused by Ga islands. In addition, the problem of SPV's induced by photoemission sources themselves will be addressed. Usually encountered below room temperature where the SPV is enhanced, source-induced SPV's become an important issue at and above room temperature in wide band-gap materials, which are acutely prone to a SPV when large equilibrium band bending is present. A striking example of current relevance is p-type GaN, which exhibits source-induced SPV's at room temperature exceeding a volt when examined by ordinary UPS and XPS laboratory sources.

3:20pm **EL+SC-TuA5 Direct Measurement of the Electrical Potentials in GaInP$_2$ Solar Cells**, ***C.-S. Jiang***, *H.R. Moutinho, J.F. Geisz, D.J. Friedman, M.M. Al-Jassim*, National Renewable Energy Laboratory

We report the application of electrostatic force microscopy (EFM) to photovoltaic devices. The built-in electric field plays a major role in photovoltaic devices, because it collects photo-excited carriers and is a key factor in determining the open-circuit voltages of solar cells. However, the measurement of the built-in potential has been limited to indirect ways such as the characteristics of current-voltage and capacitance-voltage. In these measurements, it is hard to distinguish the contributions from the multi-junctions or interfaces of a modern solar cell device. In this presentation, we report a direct measurement of the electric potential on cross-sectional planes of a GaInP$_2$ device both quantitatively and spatial-resolvedly, by using the Kelvin probe force model of the EFM technique. Two features on the potential profile are assigned respectively to the p-n junction of GaInP$_2$ and the band offset between the GaInP$_2$ base and the GaAs substrate materials. With varying the light intensities irradiated at the sample, we found that, in addition to the flattening of the p-n junction, two changes in the potential profile happened in the locations of the front window or the back surface field (BSF) layers under the condition of a lower or a higher light intensities, respectively. The two potential changes, together with the flattening of the p-n junction, contribute positively to the open-circuit voltage of the device, indicating the importance of the window and the BSF layers in solar cell designs. Furthermore, the potential change at the window layers is understood in terms of the band offset between the AlInP$_2$ window and the GaInP$_2$ emitter layers, and the potential change at the BSF layer is understood in terms of the total effect of the photo-induced flattening of the band bending and the band offset at the interface between the base and the BSF, respectively.

3:40pm **EL+SC-TuA6 Deep Level Defect Characterization of InGaAsN Layers Grown by Molecular-Beam Epitaxy**, ***S.W. Johnston***, *R.K. Ahrenkiel, A.J. Ptak*, National Renewable Energy Laboratory

The quaternary alloy In$_x$Ga$_{1-x}$As$_{1-y}$N$_y$ can be grown lattice-matched to GaAs and can potentially be used as the 1-eV bandgap material in a four-junction, high-efficiency solar cell. We have characterized a series of In$_x$Ga$_{1-x}$As$_{1-y}$N$_y$ samples with varying N content by measuring deep level transient spectroscopy (DLTS). The samples were grown by rf plasma-assisted molecular-beam epitaxy and contain N concentrations $0 \leq y \leq 0.02$. Our data show that each as-grown sample contains a hole trap whose peak occurs near 350 K for the 0.2-ms rate window. Analysis of these peaks indicates activation energies of 0.62, 0.62, and 0.75 eV for samples with y = 0.003, 0.013, and 0.02, respectively. Electron traps were also detected, even though the DLTS measurements were performed with Schottky contacts deposited on p-type material. This is attributed to a large Schottky barrier. For the sample with y = 0.003, an electron trap with an activation energy of 0.50 eV was detected. As N-content increased, the detected electron-trap activation energies decreased to 0.22 and 0.27 eV for the y = 0.013 sample, and to 0.13 eV for the y = 0.02 sample. We also show DLTS data correlating to varying growth conditions and the effects of annealing processes.

4:20pm **EL+SC-TuA8 Thermal Quenching and High Temperature Cathodoluminescent Degradation of Sulfide-Based Powder Phosphors**, ***B.L. Abrams***, *L.C. Williams, J.-S. Bang, P.H. Holloway*, University of Florida

Temperature effects on cathodoluminescent (CL)intensity, spectrum and degradation of ZnS:Ag,Cl powder phosphor have been investigated. Thermal quenching was studied by increasing the phosphor temperature without exposure to a continuous electron beam and measuring the decreased CL intensity. A characteristic thermal quenching temperature of 150^{o}C with an activation energy (E_a) of 0.87eV was observed for ZnS:Ag,Cl. Along with reduced CL intensity, the spectra shifted to longer wavelengths and changed shape at elevated temperature. The shift was dominated by band gap narrowing at high temperatures. Shape change was attributed to Cu contamination from the heater stage. The CL spectral distribution and intensity were 100% recoverable upon cooling back to room temperature when electron beam exposure was minimal (<1C/cm^2). With continuous electron beam exposure, CL intensity upon cooling to RT (after 24C/cm^2, 2keV primary beam energy) was <40% of the original intensity before heating. The loss of CL intensity at high temperatures was less than at RT for the same primary beam energy and coulombic dose. This is consistent with the Electron Stimulated Surface Chemical Reaction

(ESSCR) Model of degradation which predicts that elevated temperatures will reduce the mean stay time of physisorbed gases, decreasing the rate of the surface reactions leading to CL degradation. Electron beam heating was calculated using a simple heat transfer model and was significant for powder samples. This is consistent with morphological erosion observed on the surface of the ZnS particles degraded at elevated temperatures or high power densities. It is speculated that at temperatures of about 300°C, surface chemical reactions in combination with heating leads to removal of S and evaporation of Zn. Work supported by DARPA Grant MDA 972-93-1-0030 through PTCOE.

4:40pm **EL+SC-TuA9 Analysis of Ion Implantation Damage in Silicon Wafers by a Contactless Microwave Diagnostic**, ***R.K. Ahrenkiel***, National Renewable Energy Laboratory, *B. Lojek*, Atmel Corporation

Rapid thermal annealing (RTA) of ion implantation damage is required to maintain the integrity of submicron integrated circuit devices. A quick, efficient, and contactless diagnostic of the implantation damage is highly desirable. The residual radiation damage drastically reduces the recombination lifetime in the implanted region. Here, we will demonstrate the use of resonance-coupled photoconductive decay (RCPCD) technique allows us to to probe this region in boron and arsenic-implanted silicon wafers. Using a tuneable optical excitation source, we excite electron-hole pairs in the implanted region only. We compare these recombination times with those of the non-implanted bulk of the crystal. The lifetime is independent of excitation wavelength for the as-grown, oxidized wafers with typical values larger than 50 ms in semiconductor-grade silicon. After ion implantation with either arsenic or boron, the near-surface (711 nm) lifetime drops more than two orders of magnitude because of recombination at implantation-produced defects. After an RTA process, the lifetimes increase and again approach the bulk lifetime. One first group of wafers was processed in a standard rapid thermal processing (RTP) system SHS 2000 with a Hotliner. A second set of wafers were exposed to constant wavelength irradiation with maximum photon energy of approximately 1.4 eV for about 5 seconds, which has been called a "spike anneal". Our studies showed that the latter process produces wafers of lower recombination center density that the standard process. We propose some possible models to explain the improved properties of the "spike-annealed" wafers.

5:00pm **EL+SC-TuA10 Gas-phase Nanoparticle Formation during AlGaN MOCVD**, ***J.R. Creighton***, *W.G. Breiland, M.E. Coltrin,* Sandia National Laboratories

The AlGaN MOCVD process is often plagued by parasitic chemical reactions that diminish the group-III deposition efficiency and make it difficult to control alloy composition. We have explored many possible mechanisms for the parasitic reactions using a variety of experimental techniques and complex reactive flow simulations. Results indicate that the reactions require high temperatures and occur in the boundary layer near the growing surface. These reactions ultimately lead to the formation of nanoparticles, which we have recently observed using in situ laser light scattering. Thermophoresis keeps the nanoparticles from reaching the surface, so the material tied-up in nanoparticles cannot participate in the thin film deposition process. In the case of AlN, the particle size was determined to be 48 nm, and the particle density was in the range of 10^{8-9} cm^{-3}. At these densities a significant fraction (20% or more) of the input Al is converted into nanoparticles. Analysis of the polarization dependence of the scattering from GaN nanoparticles indicates that they are non-spherical. This makes determination of their size and density more difficult, but they are in the range observed for AlN nanoparticles. For GaN and AlN nanoparticles the balance of thermophoretic and viscous forces results in a sharp height distribution centered at ~6 mm above the surface, which is in good agreement with the theoretical prediction.[1]

[1] Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

Organic Films and Devices
Room: C-102 - Session OF+EL+SS+SC-WeM

Metal-Organic Interfaces
Moderator: L.J. Guo, University of Michigan

8:20am **OF+EL+SS+SC-WeM1 Interfaces between Metals and Conjugated Organic Materials: From Physisorption to Covalent Bonding**, ***N. Koch***, Princeton University, *J. Ghijsen,* Facultes Universitaires Notre-Dame de la Paix, Belgium, *A. Rajagopal,* Rutgers University, *C. Chan,* Princeton University, *J.J. Pireaux,* Facultes Universitaires Notre-Dame de la Paix, Belgium, *J. Schwartz, A. Kahn*, Princeton University **INVITED**

The electronic properties of interfaces formed between conjugated organic materials (polymers and small molecules) and other organic and inorganic materials are of paramount importance in terms of the performance of organic-based devices (e.g., light emitting diodes, thin film transistors). The alignment of energy levels at such interfaces is a direct consequence of the physical and chemical interactions between the materials. Using mainly photoemission spectroscopy (PES), we show that the nature of interaction between low work function metals and phenylene-based electroluminescent oligomers and polymers covers the whole range from physisorption (aluminum and samarium) to chemical reduction (calcium), and to charge transfer reactions (alkali metals). Although PES is a very powerful experimental tool to determine electronic properties of interfaces, great care must be taken in the interpretation of the data when wide band-gap materials, such as conjugated organic materials, are being investigated. We demonstrate that the observation by PES of a finite density of occupied states at the Fermi-level on an organic film in which alkali metal atoms have been intercalated does not necessarily imply metallicity nor the presence of negative polarons (radical anions), as previously proposed. From a combination of ultraviolet PES and Kelvin probe measurements, evidence is obtained that the substrate and the surface of the organic film are not necessarily in thermodynamic equilibrium, leading to potential misinterpretations of the Fermi level position at the surface of organic films.

9:00am **OF+EL+SS+SC-WeM3 Structural and Electronic Properties of the Interfaces between Au(111) and the Organic Semiconductors Pentacene and p-sexiphenyl**, ***C.B. France****, P.G. Schroeder, B.A. Parkinson*, Colorado State University

Thorough understanding of the interface between organic semiconductors and metal contacts is important because of charge transfer events that take place in new devices based on organic semiconductors. Transistors[1] and photovoltaic devices[2] have been fabricated using pentacene as the organic semiconductor. In the interest of understanding the structural and electronic environments of these interfaces we have investigated thin films of pentacene and p-sexiphenyl on the Au(111) surface in ultrahigh vacuum using multiple characterization techniques. The entergetics of these heterojunctions have been measured using photoemission spectroscopy. Large interfacial dipole barriers exist at the interface of both systems. Temperature programmed desorption has been used to investigate the binding environment of the organic semiconductors on the metal substrate. Two different binding environments have been uncovered for both molecular semiconductors on the Au(111) substrate. Scanning tunneling microscopy has been used to investigate the coverage dependant structures that are formed by thin films of semiconductor molecules on the Au(111) surface. Pentacene was found to generate many overlayer structures at differing film thickness. Structures found on low coverage, monolayer and multilayer films will be discussed.

[1] Schön, J. H.;Berg, S.;Kloc, C.;Batlogg, B. Science 2000, 287, 1022.

[2] Schön, J. H.;Kloc, C.;Bucher, E.;Batlogg, B. Nature 2000, 403, 408. .

9:20am **OF+EL+SS+SC-WeM4 Growth of Organic Molecules on Ferromagnetic Substrates for Hybrid Organo-metallic Spintronic Devices**, ***M.V. Tiba****, O. Kurnosikov, B. Koopmans, J.T. Kohlhepp, C.F.J. Flipse, W.I.M. de Jonge, U.S. Schubert*, Eindhoven U. of Technology, CNM, The Netherlands

Motivated by the success of polymer based- and molecular electronics, a challenging new field is emerging. Recent work has demonstrated the feasibility of hybrid organo-metallic spintronics, in which the spin degree of freedom is explicitly being used. Application in future magnetic sensor and memory technology has been proposed. Improved characteristics of such devices require very clean interfaces, therefore deposition of organic molecules in UHV environment is desirable. A severe complication of growing ordered structures of organic molecules on transition metal ferromagnetic substrates is their high reactivity. In this work we investigate the influence of substrate passivation on the bonding to the substrate (and hence the molecular ordering) for different organic molecules. Selection of the molecules is based on their electronic properties as well as their tendency to form well ordered layers. In the particular case of PTCDA molecules deposited on a Ni(111) substrate we show that quarter monolayer of oxygen reduces enough the reactivity of Ni to enable the molecules to form an ordered structure.[1] Current activities aiming at the fabrication of organo-metallic hybrid magnetic tunnel junctions having polycrystalline Co electrodes and organic barriers will be addressed as well.

[1] M.V.Tiba et al. Surf. Sci. 498 (2002) 161.

9:40am **OF+EL+SS+SC-WeM5 Controlling Metallic Contacts to Molecular Electronic Devices**, ***A.V. Walker****, T.B. Tighe, O. Cabarcos, B.C. Haynie, D.L. Allara, N. Winograd*, Pennsylvania State University

In the development and design of molecular electronic devices, it is vital to understand the nature of the metal-organic monolayer interaction. To fully characterize these interactions, we employ a multi-technique approach using time-of-flight secondary ion mass spectrometry (ToF SIMS), infrared spectroscopy (IRS), x-ray photoelectron spectroscopy (XPS) and density functional theory (DFT) calculations. Using an unfunctionalized molecular wire (4-[4?-(phenylethynyl)-phenylethynyl]-benzenethiol) monolayer on Au, we demonstrate that the metal-monolayer contact can be varied from complete destruction of the monolayer to contact formation at the monolayer terminus to complete penetration through the layer. For example, we show that upon deposition of Cu or Ag, the Cu and Ag atoms simultaneously interact with the terminal phenyl ring and penetrate to the Au/S interface. In contrast, Au penetrates through the monolayer at all coverages studied. By using metals specifically tailored for the chemistry of the device molecule as well as for electronic states, the characteristics of the metal-molecule contact can also be controlled. These types of data provide a foundation for rational design of contacts in molecular electronic devices.

10:00am **OF+EL+SS+SC-WeM6 DLC Thin Film as Electron Injection Layer in Organic LEDs**, ***M. Cremona***, Pontificia Universidade Catolica do Rio de Janeiro, Brazil, *R. Reyes,* Universidad Nacional de Ingeniería, Perú, *C.A. Achete, P.I. Guimarães, S.S. Camargo, Jr.*, Universidade Federal do Rio de Janeiro, Brazil

Recently, there has been an increased interest in organic light emitting diodes (OLEDs) due of their potential applications to color flat panel displays and in new optoelectronic components. These devices are assembled using three organic molecular materials: an electron injection layer, the emitting one and finally the hole injection layer. However, in most cases the electron injection is more difficult to achieve than hole injection. In this work two different diamond like carbon (DLC) thin films cathode were used to decrease the electron injection barrier. The first kind were nitrogen-doped amorphous hydrogenated hard carbon films deposited by rf glow discharge from methane-nitrogen mixtures onto the TPD/Alq_3 layer structure thermally deposited. DLC films were obtained for different N_2 partial pressures (bias voltage V_b=â€“370 V and total pressure P=8 Pa). Next, amorphous carbon nitride thin films (a-CN_x) have been deposited using a rf diode sputtering system onto the same organic structure. In this case the DLC films were deposited in reactive nitrogen-argon atmospheres. The partial pressure of nitrogen ranged from 0% to 100% at two different deposition pressures (P = 2 Pa and P = 8 Pa). In both cases a thick (150 nm) aluminum electrode were deposited onto the whole structure. The deposition process for the organic compounds is performed in high vacuum environment (6x10^{-6} Torr) on glass substrates coated with an hole injecting ITO transparent layer. A preliminary investigation was conducted on the properties of the OLED device with the two DLC intermediate layers. The relationship between the properties of the DLC deposited films on the electroluminescent characteristics of the different devices are investigated. The refractive index of the DLC film deposited, their conductivity and optical absorption, the OLED I-V curves, a preliminary photoluminescent and electroluminescent OLED results are presented and discussed.

10:20am **OF+EL+SS+SC-WeM7 Self-assembly of Molecular 1D wires on Cu(110)**, ***Y. Naitoh****, F. Rosei, P. Thostrup, M. Schunack, F. Besenbacher*, University of Aarhus, Denmark

The adsorption of a large organic $C_{90}H_{98}$ molecule, known as the Lander molecule, is studied by Scanning Tunneling Microscopy (STM) on a Cu(110) surface.[1] By exposing the surface to low doses of oxygen at elevated temperatures, we form a nanopattern of alternating bare Cu(110) regions and (2x1)-O reconstructed regions aligned parallel to the [001] direction. The oxygen-induced reconstruction reveals a long-range ordering of Cu-O rows 20-50 Å wide. When deposited on this template, Lander molecules adsorb preferentially on bare Cu regions. By tuning the oxygen dosing, thereby adjusting the lateral periodicity of the template, and by varying molecular coverage in a controlled manner we can form long 1D rows of molecular wires. This type of assembly opens new possibilities for ordering organic molecules on surfaces.

[1] F. Rosei et al., Science 296, 328 (2002).

10:40am **OF+EL+SS+SC-WeM8 Dip Pen Nanolithography on Insulating Substrates**, ***S.E. Kooi***, *P.E. Sheehan*, *L.J. Whitman*, Naval Research Laboratory

Methods of assembling nanoscale components at chosen locations on a surface are needed to produce nanoscale electronic and sensor devices. Dip pen nanolithography (DPN) has been successful in producing such features as small as ~10 nm wide and one monolayer thick in several different molecule - surface combinations. The most studied systems have been alkyl and aryl thiol depostion on gold surfaces; however, DPN has also been demonstrated for inorganic salts on silicon, biomolecules on gold, and silazanes on semiconductor surfaces. We explore the application of DPN to write functional molecules on a technologically important insulating surface, namely silicon oxide. We have written several different trichlorosilane molecules directly onto thermally-grown silicon oxide substrates. By choosing an appropriate trichlorosilane and post-deposition chemical modification of the written molecules, we can direct the deposition of other nanostructures (such as carbon nanotubes, semiconducting nanowires, or nanoparticles). For example, by writing 10-undecenyltrichlorosilane onto silicon oxide, we can create a terminal carboxylic acid group with a post-deposition chemical oxidation. Subsequent deprotonation of the patterned carboxylic acid groups produces a negative charge that directs the deposition of positively-charged nanostructures. The ability to place nanoscale components at chosen locations on a surface, in combination with traditional (e-beam) lithographic techniques, opens up the possibility of interfacing nanoscale components with traditional devices.

Electronic Materials and Devices
Room: Exhibit Hall B2 - Session EL+SC-WeP

Poster Session

EL+SC-WeP1 Mechanistic Aspects of SiC Oxidation, *C. Radtke,* ***F.C. Stedile****, I.J.R. Baumvol,* UFRGS, Brazil, *I.C. Vickridge, I. Trimaille, J.-J. Ganem, S. Rigo*, Universite de Paris 6 et 7, France

SiC is the material of choice in the field of high band-gap semiconductors used in high-power, high-frequency, high-voltage, and/or high temperature applications. The possibility of obtaining an oxide film with good electrical characteristics (SiO_2) by thermal oxidation is one of its major advantages. In order to develop an oxidation model, the knowledge of the oxidation mechanism is of great importance. We investigated the incorporation of oxygen in surface and interface regions during different stages of the oxidation process of the C-face of 6H-SiC(0001) wafers as well as its dependence with the gas pressure. Oxidations in natural ultra dry O_2 followed by oxidations using isotopically enriched oxygen ($^{18}O_2$) were performed. Different times of oxidation in the natural gas and chemical etching of grown oxides were used to obtain samples representing different starting conditions. Amounts of incorporated ^{18}O and depth profiles were determined using nuclear reactions in plateau and resonance regions of their cross-section curves, respectively. The results evidence that in the whole range of oxidation times studied, the oxidation process was limited by the reaction rate of diffusing oxygen with SiC. These results present a new dynamical mechanism with remarkable differences from the oxidation of Si.

EL+SC-WeP2 Comparison of the Decomposition of Metacarborane and Orthocarborane, ***A.N. Caruso****, P.A. Dowben*, University of Nebraska, Lincoln

It is now recognized that there are several different polytypes of B_5C (boron carbide) for which the electronic structure has remained obscure. We present a novel B_5C polytype that is radically different from previous polytypes in that it forms an n-type semiconductor. Decomposition of closo-1,7 dicarbadodecaborane (metacarborane) and closo-1,2 dicarbadodecaborane (orthocarborane) due to adsorption of photons (32eV soft x-rays) has been observed. We compare adsorption and decomposition for these molecules and attempt to address why molecules with the same basic structure create materials that are wildly different in their electronic (semiconducting) properties.

EL+SC-WeP3 Non Destructive Evaluation of Alternative Substrate Quality Using Glancing Incidence X-Ray Diffraction and Raman Spectroscopy, ***H.J. Haugan****, A.M. Cain, T.W. Haas, K.G. Eyink,* Air Force Research Laboratory, *C.J. Eiting,* Uniroyal Optoelectronics, *D.H. Tomich, L. Grazulis, J.D. Busbee*, Air Force Research Laboratory

Alternate substrate technology holds promise for the growth of high quality lattice mismatched epitaxial films. Unfortunately, the technology has been plagued by difficulties in reproducibility of results. Some of this problem resides in a lack of characterization of the thin, twist bonded layer used as the template for subsequent epitaxial growth. In this work, grazing incidence diffraction (GID) and micro-Raman spectroscopy were used to characterize the alternative substrate prior to growth. The 14 nm and 50 nm thin GaAs layers were bonded to (100) GaAs substrates and subsequently exposed by standard thinning and etching techniques. The crystalline quality of the thin bonded substrates was studied by GID. The full widths at half maximum (FWHM) of the 004 peaks were used to monitor optimum bonding condition. The measured FWHM varied from 29 to 601 arcseconds with smooth surfaces exhibiting the lowest values. The effect of bond pressures on template layers were studied for a series of 50 nm alternative substrates prepared using pressures ranging from 75 psi to 25 psi with a constant bonding temperature of 450 °C. All transferred template layers prepared within this pressure range showed poor quality (FWHM ranged from 324 to 601 arcseconds) when compared to the bulk-GaAs of 12 arcseconds. Micro-Raman measurements were also carried out on these samples. A transverse optical (TO) phonon line is seen and the intensity ratio of the TO to longitudinal optical phonon were much higher than that of GaAs substrate, confirming that the bonding process is causing damage to the thin template layer.

EL+SC-WeP4 Design and Simulation of AlGaN/GaN Heterojunction Bipolar Transistors, ***K.P. Lee****, S.J. Pearton, F. Ren,* University of Florida, *J.-I. Chyi*, National Central University, Taiwan, *A. Dabiran, P.P. Chow*, SVT Associates

The progress in developing AlGaN/GaN HBTs has been very limited compared to HEMT devices in the same materials system.HBTs would have advantages of better linearity,higher output power,better radiation resistance and more uniform threshold voltage compared to field effect transistors.To date,dc current gains in HBTs have been limited to <30 at room temperature and the rf performance is poor.The high base resistance is one of the limiting factors in npn structures.We have used a drift-diffusion model to simulate the dc characteristics of a variety of structures designed to improve the HBT performance.These include a superlattice base to enhance the hole concentration due to incomplete ionization of the Mg acceptors,base grading and a regrown base contact structure.The anisotropy in transport properties of the superlattice base have been taken into account.Base transport enhancement is predicted by the introduction of a quasi-electric field in the base layer.The minority carrier lifetime in the base is also a critical parameter determining the HBT performance.A comparison will be given of the relative strengths of the different device structures and their prospects for realizing a high gain,high speed,robust AlGaN/GaN HBT technology.

EL+SC-WeP6 Growth of Gallium Nitride on Silicon Substrate by MOCVD Using Multiple Buffer Layers, *M.A. Al-Tamimi,* ***D.A. Gulino***, Ohio University

An attempt has been made to improve the crystalline quality of MOCVD-grown gallium nitride on silicon (111) substrate by the insertion of a second aluminum nitride buffer layer. The conventional method for growing GaN on heterosubstrates has been to first grow a thin, low-temperature layer of typically aluminum or gallium nitride to act as a compliant, or "buffer," layer to reduce the degree of crystalline defects and threading dislocations in the subsequently-grown GaN epilayer. In the work reported here, a second, low-temperature AlN buffer layer was grown on top of the first GaN epilayer, and this was followed by a second GaN epilayer. We have found improvement in the crystalline quality of the second GaN epilayer as measured by x-ray diffraction rocking curves. We also experimented with ramping the temperature during growth of both the first and second AlN buffer layers, and we discovered that the best quality GaN film obtained in this work occurred when the first buffer layer was grown as the temperature was ramped from 800 to 1060°C and the second buffer layer grown at a fixed temperature of 800°C.

EL+SC-WeP7 Edge Termination Design and Simulation for Bulk GaN Rectifiers, ***K.H. Baik***, University of Florida, *Y. Irokawa*, Toyota Central Research Laboratories

GaN bulk rectifiers show excellent on-state resistances (in the milli-ohm.cm-2 range) forward turn-on voltages of ~1.8V and reverse-recovery times of <50ns. A key requirement is to develop effective edge termination techniques in order to prevent premature surface-induced breakdown. We have performed a simulation study of the effects of varying the dielectric passivation material(SiO2,SiNX,AlN,Sc2O3 or MgO),the thickness of the this material, the extent of metal overlap onto the dielectric and the ramp oxide angle on the resulting reverse breakdown voltage(VB) of bulk rectifiers. We find that SiO2 produces the highest VB of the materials investigated, that there is an optimum metal overlap distance for a given oxide thickness and small oxide ramp angles produce the highest VB. Initial experimental results on small-area devices show good agreement with the trends identified by the simulations. The dc characteristics are still dominated by the defect density in the substrate for large-area rectifiers.

EL+SC-WeP8 Photoelectrochemical Oxidation of GaN and Fabrication of Metal-oxide-semiconductor Structures using Ga-oxide Dielectrics, ***D.J. Fu****, T.W. Kang*, Dongguk University, Korea

GaN metal-oxide-semiconductor (MOS) capacitors were fabricated by using Ga oxide formed by photoelectrochemical oxidation of GaN. The electrical properties of the MOS structures as characterized by capacitance-voltage measurement were found to be dependent on the oxidation time and post-treatment. Positive flatband voltage was observed in devices with thin oxide layers indicating the existence of negative oxide charge. Very thin oxide exhibits high capacitance and reverse leakage, which can be reduced by rapid thermal annealing. Passivation of the interface by the annealing is partially responsible for the improvement. Thicker oxide layers exhibit improved electrical properties. Low density of interface states was obtained in the Ga-oxide/GaN structure grown under optimized conditions.

EL+SC-WeP9 Relating Interfacial Structure and Composition of Pt/CdZnTe to Radiation Detector Device Performance, ***D.J. Gaspar***, *M.H. Engelhard*, *V. Shutthanandan*, *S. Thevuthasan*, Pacific Northwest National Laboratory, *A.A. Rouse*, *C. Szeles*, *J.-O. Ndap*, *S.A. Soldner*, eV PRODUCTS

The interfacial structure and composition of platinum/CdZnTe interfaces was examined to establish correlations between surface and interfacial stoichiometry and radiation detector device performance. X-ray photoelectron spectroscopy (XPS), including depth profiling, and Rutherford backscattering spectroscopy (RBS) were used to determine surface and Pt/CdZnTe interfacial composition. The ^{57}Co spectral response of five CdZnTe detector devices formed by deposition of Pt contacts on a CdZnTe crystal was correlated to the interfacial stoichiometry and the ideality factor. Non-ideal contact behavior was correlated to interfacial oxidation and to the bulk series resistance of the diode. XPS depth profiling revealed differences in the formation of the rectifying contacts, which correlated to device electrical performance.

Electronic Materials and Devices
Room: C-107 - Session EL+SS+SC-WeA

Semiconductor Film Growth and Oxidation
Moderator: R.K. Ahrenkiel, National Renewable Energy Laboratory

2:00pm **EL+SS+SC-WeA1 Scanning Tunneling Microscopy and Spectroscopy of Gallium Oxide and Indium Oxide Deposition on GaAs(001)-(2x4)**, ***M.J. Hale***, *J.Z. Sexton,* University of California, San Diego, *S.I. Yi,* Applied Materials, *D.L. Winn, A.C. Kummel*, University of California, San Diego

The surface structures formed upon deposition of Ga$_2$O and In$_2$O onto the technologically important As-rich GaAs(001)-(2x4) surface have been studied using scanning tunneling microscopy (STM) and spectroscopy (STS), low energy electron diffraction (LEED), and density functional theory (DFT) calculations. At submonolayer coverage, the initial bonding sites are different for Ga$_2$O and In$_2$O adsorptions due to the different activation barriers for the two oxides to chemisorb at various sites onto the surface. In$_2$O initially bonds in the trough between the arsenic dimer rows, whereas Ga$_2$O first inserts into the top layer arsenic dimer rows. Conversely, at elevated surface temperatures, both Ga$_2$O and In$_2$O form a crystalline monolayer. Both oxides form crystalline (2x1) surface reconstructions that are electronically unpinned: there are no states within the band gap. Although both oxides form a (2x1) surface reconstruction, the surface structures differ. At monolayer coverage the Ga$_2$O/GaAs surface has a much larger step density while the In$_2$O/GaAs surface shows a broad distribution of row oxide spacing. The DFT calculations confirm the observed surface structures and show that both oxides form unpinned surfaces because the bonding to these oxides restore the charge on the first and second layer As and Ga atoms to near bulk values.

2:20pm **EL+SS+SC-WeA2 Structure-Sensitive Oxidation of the Indium Phosphide (001) Surface**, ***G. Chen***, University of California, Los Angeles, *S.B. Visbeck,* Siemens & Shell Solar Gmbh, Germany, *D.C. Law*, University of California, Los Angeles, *R.F. Hicks*, University of California, Los Angeles; AVS fellow

Abstract The properties of oxide/semiconductor interfaces significantly affect the performance of indium phosphide-based electronic and photonic devices. In this study, indium phosphide films were grown on InP (001) substrates by metalorganic chemical vapor deposition (MOCVD). Then the samples were transferred to an ultrahigh vacuum system, and annealed at 623 and 723 K to produce the (2x1) and delta(2x4) reconstructions with phosphorus coverages of 1.0 and 0.125 ML, respectively. These structures were exposed to unexcited molecular oxygen, and the reaction characterized by X-ray photoelectron spectroscopy (XPS), reflectance difference spectroscopy (RDS) and low energy electron diffraction (LEED). At 298 K and above, the In-rich InP (001) surface rapidly oxidizes upon exposure to O2. The oxygen dissociatively chemisorbs onto the delta (2x4), inserting into the In-P back bonds and the In-In dimer bonds. By contrast, the P-rich (2x1) reconstruction does not absorb O2 up to 500,000 L at 298 K. Above 453 K, the (2x1) becomes reactive with oxygen inserting into both the In-P back bonds and the phosphorus dimer bonds. Based on these results, we conclude that the oxidation of indium phosphide (001) is highly structure sensitive. This means that the oxide/semiconductor interface formed on InP devices can vary widely depending on the process history.

2:40pm **EL+SS+SC-WeA3 The Addition of Sb and Bi 'Surfactants' during GaN Growth by Metal Organic Vapor Phase Epitaxy**, ***T.F. Kuech***, *L. Zhang, H.F. Tang, J. Schieke, M. Mavrikakis*, University of Wisconsin - Madison **INVITED**

The addition of certain impurities has been shown to modify the growth behavior of several lattice-mismatched epitaxial semiconductor systems, most notably SiGe-Si. Of the many impurities studied, antimony and bismuth have been shown to act as 'surfactants' during SiGe epitaxy altering the critical thickness and surface morphology. Such impurities have not been studied in detail in other systems, such as GaN and related materials. We present data on the role and effect of isoelectronic centers, Sb and Bi, on the structure and properties of GaN epilayers during metal organic vapor phase epitaxy. The Sb addition slightly improved the optical and structural properties of GaN epilayer at a low level of Sb incorporation. The addition of Sb resulted in changes in the GaN surface morphology, which was further explored by the lateral overgrowth epitaxy technique through the changes in the growth rates and the facet formation. The presence of Sb in the gas phase greatly enhanced the lateral overgrowth rate and altered the formation of the dominant facets. While Sb altered the growth facet present during LEO, only a small amount of Sb was incorporated into the GaN, suggesting that Sb may be acting as a 'surfactant' during the GaN MOVPE growth. Sb addition produces surface conditions characteristic of a Ga-rich surface stoichiometry indicating both a possible change in the reactivity of NH$_3$ and/or enhanced surface diffusion of Ga adatom species. Other changes in the surface chemistry and transport were studied by the use of state-of-the-art periodic self-consistent DFT calculations. Bismuth has also been studied as a surfactant to alter the surface chemistry and defect structure during the GaN growth. Bi addition resulted in a decrease in surface roughness as measured by atomic force microscopy while no significant Bi was incorporated over a broad range of gas phase concentrations.

3:20pm **EL+SS+SC-WeA5 Surface Reaction Study of Tungsten Nitride Precursors Decomposition on Si(100)-(2 x 1)**, ***Y.-W. Yang***, Synchrotron Radiation Research Center, Taiwan, *J.-B. Wu, Y.-F. Lin, H.-T. Chiu*, National Chiao-Tung University, Taiwan

Reaching an atomic-scale understanding of the surface reaction pathways followed by precursors during MOCVD thin-film growth is a daunting task. We have been studying the transition metal nitride growth on both Cu and Si surfaces. Here, we report a thermal decomposition study of WN precursor on Si(100)-(2 x 1) using TDS and synchrotron-based XPS techniques. The studied precursors are (t-BuN)$_2$W(NHBu-t)$_2$ and (t-BuN)$_2$W(NEt$_2$)$_2$ and their structural characteristics consist of the presence of both W-N and W=N bonds and either the presence or the absence of β-H that influences the thermolysis of the precursors. XPS data show that the metallic tungsten already forms for a submonolayer dose of the precursors at room temperature, suggesting the complete abstraction of the amine ligands by the dangling bonds on Si(100) surface. The evolution of hydrocarbon and amine species during the pyrolysis are followed by the TDS and the results suggests the similarity to the amine adsorption on Si(100). High temperature annealing produces silicon carbides and silicon nitrides. In stark contrast, no metallic tungsten is ever formed during the pyrolysis of the same precursors on Cu(111) and the formation of tungsten nitride is secured through the gradual loss of excessive amine ligands. Based on these results, possible surface reaction mechanism and the structural effect of the precursor are to be discussed.

3:40pm **EL+SS+SC-WeA6 Thermal Decomposition and Desorption Study of Tetrakis(diethylamido)zirconium(TDEAZr) on Si(100) for MOCVD and ALD of ZrO$_2$**, ***K. Yong***, *J. Jeong, S. Lim*, Pohang University of Science and Technology, Korea

Tetrakis(diethylamido)zirconium (TDEAZr) is used as a zirconium-precursor to deposit zirconium oxide by metal-organic chemical vapor deposition (MOCVD) and atomic layer deposition (ALD). Surface reaction study of precursors can aid in describing the kinetics of MOCVD and ALD. Surface reaction and desorption of TDEAZr (Zr(N(C$_2$H$_5$)$_2$)$_4$) on Si(100) were studied using temperature programmed desorption (TPD), X-ray photoelectron spectroscopy (XPS) and Auger electron spectroscopy (AES). During TPD, ethylethyleneimine, diethylamine, acetonitrile, ethylene and hydrogen desorbed as main decomposition products of diethylamido, which was chemisorbed on Si(100) through the scission of zirconium-diethylamido bond in TDEAZr. The formation of silicon-carbide and silicon-nitride was observed on the surface after TPD runs. These results indicated that a complete decomposition of diethylamido also proceeded. A reaction pathway model of TDEAZr/Si(100) was proposed. Also, the coadsorption of TDEAZr with water on Si(100) was studied.

4:00pm **EL+SS+SC-WeA7 Reactions of Organosulfur Compounds with Si(100) for Chemically Controlled Epitaxy of II-VI Semiconductors on Si(100)**, *Z. Zhu, A. Srivastava,* ***R.M. Osgood Jr.***, Columbia University

The growth of silicon-based quantum devices requires precise control of ultrathin Si/wide-bandgap-semiconductor/Si heterostructures. We have investigated the initial stages of chemistry-based low-temperature epitaxy using organosulfur precursors. The approach uses the chemical insight gained from organic functionalization of Si.[1] Thus we have studied the reaction of (CH$_3$S)$_2$, CH$_3$SH, (CH$_3$)$_2$S with Si(100) at room temperature, under UHV conditions for atomic layer growth of functional-group-terminated sulfur on Si(100). This reaction is the first step in the layer by layer self-limiting epitaxy of ZnS, for example, on Si(100). AES studies indicate that each of these organosulfur compounds have different reaction kinetics with the Si(100) surface and reach different levels of sulfur saturation coverage. The differences observed for (CH$_3$S)$_2$ and (CH$_3$)$_2$S reactions have been shown to be explained by the relative bond strengths and the number of sulfur atoms present in the adsorbate molecule. Our TPD studies from 25-825°C show no sulfur-related desorption. Instead AES studies confirm that sulfur atoms remain on surface until ~ 525°C and then diffuse into the Si(100) substrate upon further annealing. TPD studies also indicate evolution of H_2 at temperatures similar to those obtained for H_2 desorption from saturated atomic H on Si(100). In our studies methyl desorption also occur at T > 650° C, temperatures higher than that of H_2 desorption. The amount of m/e = 15,16 fragments is dependent on the organosulfur compound examined. Chemical strategies are now being explored to grow layers of Zn on methyl-terminated sulfur layer as shown in the epitaxy using sequential H_2S/dimethyl cadmium dosing on ZnSe.[2]

[1] Bent SF, J Phys Chem B, 106(11): 2830-2842, 2002.

[2] Luo Y, Han M, Slater DA, Osgood RM, J Vac Sci Tecnol A 18(2): 438-449, 2000.

4:20pm **EL+SS+SC-WeA8 Kinetics and Mechanism of Adsorption and Ultrathin Oxide Growth by Ozone on Si(100)2x1 and Si(111)7x7**, ***K. Nakamura***, *A. Kurokawa, H. Nonaka, S. Ichimura*, National Institute of Advanced Industrial Science and Technology (AIST), Japan

Ozone is one of the promising oxidants to synthesize an ultrathin oxide film on silicon surfaces for the near-future MOSFET because of rapid oxidation rate at low substrate temperature, negligible thickness of structural transition layers in the oxide film, etc.[1] However, to control the thickness of an oxide film precisely and accurately,[2] kinetics and mechanism of initial oxide growth must be clarified. Thus, in this paper, we discuss chemistry of adsorption and ultrathin oxide growth by ozone on silicon surfaces. Si(100)2x1 and Si(111)7x7 were exposed to highly concentrated (>80%) ozone gas and monitored by x-ray photoelectron spectroscopy (XPS) and second harmonic generation (SHG). Kinetic analysis has suggested that initial dissociative adsorption of ozone on Si(100)2x1 and Si(111)7x7 proceed with the mechanism of leaving only one oxygen atom on the surface and of desorbing the other two, possibly, as a molecular oxygen. This adsorption, in contrast to that of oxygen, was featured with structure-insensitive kinetics, no activation barrier for the dissociation, and high sticking probability close to unity. After the adsorption was completed, first three oxide layers were synthesized by random adsorption of oxidant species on each layer in the consecutive manner. The formation of three layers led to the further growth of an oxide film with ozone with linear growth kinetics, but not with molecular oxygen. Each of these initial ozone-oxide layers has distinctively different activation energy for its growth: they were estimated 0 eV, 0.34 eV, 0.68 eV, and 0 eV for first, second, third, and above fourth layers on Si(100), respectively, enabling accurate control of the thickness of an oxide film.

[1] K. Nakamura, S. Ichimura, A. Kurokawa, K. Koike, G. Inoue, and T. Fukuda, J. Vac. Sci. Technol. A 17 (1999) 1275.

[2] K. Nakamura, A. Kurokawa, and S. Ichimura, Jpn. J. Appl. Phys. 39 (2000) L357.

4:40pm **EL+SS+SC-WeA9 Stress-induced Dissociative Chemisorption of Oxygen on Si(001)**, ***M. Yata***, *Y. Uesugi-Saitow*, National Institute for Materials Science, Japan

We have investigated the role of surface stress in dissociative adsorption process of O_2 on Si(001)-2x1by supersonic molecular beam technique. The tensile stress was externally applied on the surface along[110] direction. The Si(001)-2x1surface reconstructs by dimerization of atoms in adjacent rows. In areas of the surface separated by an odd number of monoatomic steps the orientation of the dimer bonds is rotated by 90° giving 2x1 and 1x2 orientational domains. Their domain populations are changed to relax the stress at the surface and the kinetics of the change depend on the surface temperature.[1] Below room temperature, the domain populations were almost equal during the molecular beam experiments. Two co-existing dissociation channels are seen, a trapping-dissociation channel at low translational energy of incident O_2 and a direct activated channel at high translational energy.[2] In case of the trapping-dissociation, O_2 molecule is trapped to a precursor state and undergoes a kinetic competition between desorption and dissociation. We have estimated a difference in activation barrier heights between desorption and dissociation at 30 meV. The initial dissociative sticking probability for low translational energy of incidence increases as the tensile stress increases. This indicates that trapping-mediated dissociation is enhanced by the stress. We have found that the difference in the activation barrier heights between desorption and dissociation decreases as the stress increases. We will discuss the change of dissociation dynamics with the tensile stress in detail.

[1] F. K. Men, W.E. Packard and M. B. Webb, Phys. Rev. Lett. 61(1988) 2469.

[2] B. A. Ferguson, C. T. Reeves and C. B. Mullins, J. Chem. Phys.110(1999)11574.

5:00pm **EL+SS+SC-WeA10 Direct Detection of D_2O and D_2 on D/Si(111) Surfaces under O Atom Exposures**, ***F. Rahman***, *F. Khanom, A. Aoki, S. Inanaga, A. Namiki*, Kyushu Institute of Technology, Japan

Initial oxidation stage of D/Si(111) surfaces by atomic oxygen (O) have been studied from the absorption point of view. O/D/Si(111) co-adsorbed surfaces were prepared by various O exposure on 1.25ML D/Si(111). TPD measurement shows nearly 50% reduction of D adatoms from the surface for 2 min O exposure indicating the D adatoms abstraction by incident O atoms. Measurement of desorbing species have been done with a QMS during O exposures on the 1ML D/Si(111) surface for various surface temperatures (T_S). D_2O as well as D_2 molecules were observed. Rate curves of both species show an initial rate jump and then a gradual increase having a peak, which is followed by a nearly exponential decay with exposure time. Both D_2O and D_2 rates vs. T_S curves show similar line shape to the similar plot of D_2 rates vs. T_S curve obtained for the reaction system of H + D/Si(111) --> D_2. In a previous work, the later reaction was understood as due to the so-called β_2 TPD desorption arising from a dideuteride phase. Therefore, we consider that the O induced D_2 formation proceeds along the same mechanism as for the β_2-channel TPD. Regarding D_2O formation, it is significant and interesting since the reaction takes place as a result of picking up two D adatoms by single O atom upon collision. We will propose a possible mechanism to explain the O-induced D_2O formation on the D/Si(111) surfaces.

Organic Films and Devices
Room: C-102 - Session OF+EL+SC-WeA

Molecular and Organic Films and Devices
Moderator: N. Koch, Princeton University

2:00pm **OF+EL+SC-WeA1 Recent Developments in Organic Optoelectronics**, ***S.R. Forrest***, Princeton University **INVITED**

The interest in organic materials for optoelectronic device applications has undergone explosive growth in the last several years. This growth has been propelled by advances in organic thin films for displays, and for low cost electronic circuits. With a few successful product introductions employing active electronic organic devices, it is possible that the "age of organic optoelectronics" has finally arrived. This talk discusses some of the recent progress in organic device technology, with an eye to the future which may include making active electronic devices with a single molecule. In particular, we discuss extremely high external emission efficiency organic light emitting devices used for displays and lighting applications. Also, similar progress in high bandwidth, high efficiency of organic photodiodes, and efficient thin film photovoltaic cells are discussed. For example, multilayer organic nanostructure photodetectors are found to have very high frequency response with detection sensitivity in the visible spectral range. Finally, we present some new ideas on organic device fabrication enabling patterning of structures on the nanometer scale in both the vertical and horizontal directions.

3:00pm **OF+EL+SC-WeA4 Electron Transport in Platinum Complex Molecules: An Approach to Molecular Electronics**, *T.L. Schull, J.G. Kushmerick*, ***R. Shashidhar***, Naval Research Laboratory

Molecules that are highly conducting and which can be attached to metal on both sides via a functional chemical group form the basic elements of a molecular electronic device. Electron transport across different types of organic molecules are being actively investigated using different types of measuring test beds. In this paper, we present results of our electron conduction studies across a family of organo metallic molecules using a new cross-wire test bed developed recently.[1] We show that trans-platinum-bis-acetylides show good electron transport across their molecular length that are even better than the properties of the corresponding π-conjugated oligo(phenyleneethynylene) studied by several groups. The dependence of the metal ligands on the electron transport properties of materials is discussed. We have also used a simple extended Huckel Theory coupled with a Green Function approach to calculate the current voltage characteristics of these molecules. These theoretical calculations are compared with experiments.

1. J.G. Kushmerick, D.B. Holt, J.C. Yang, J. Naciri, M.H. Moore and R. Shashidhar, to be published.

3:20pm **OF+EL+SC-WeA5 Organic Light-Emitting Diodes and Solar Cells with Electrically Doped Transport Layers**, ***K. Leo***, TU Dresden, Germany **INVITED**

In classical semiconductor technology, controlled n- and p-type doping has always been a standard technique. In contrast, organic materials for devices such as organic light-emitting diodes (OLED) are usually prepared in a nominally undoped form. We discuss results of a comprehensive study of controlled electrical doping of various thin-film molecular organic materials. The layers are prepared by co-evaporation of matrix materials with acceptor molecules and characterized by several electrical techniques. UPS and XPS measurements directly show the Fermi level shift and the reduction of space charge layer width due to increasing doping.[1] We further show that these electrical doping concepts can be successfully applied in devices. The concept of molecular doping is applicable for amorphous wide-gap hole transporting materials and allows for realizing devices with the lowest operating voltages reported so far for small-molecule devices.[2] The concept of controlled doping has also enabled us to prepare a semitransparent inverted OLED with outstanding performance. It features an inverted layer sequence with ITO efficiently injecting electrons into a highly n-doped layer, despite a very large energy barrier of around 1.8eV. The devices reaches display brightness of 100Cd/m2 at 3.4V, which is far below any other literature result. We will also present first results on doped phosphorescent OLEDs which show that the concept of electrical doping can be extended to high-efficiency emitters. Finally, we will discuss the application of doped transport layers in solar cells. (Work done in collaboration with M. Pfeiffer, J. Blochwitz-Nimoth, X. Zhou, J. Huang, D. Qin, B. Maennig, D. Gebeyehu, A. Werner, J. Drechsel.)

[1] J. Blochwitz et al., Organic Electronics, 2 , 97 (2001)

[2] J. Huang et al., Appl.Phys. Lett. 80, 139 (2002).

4:00pm **OF+EL+SC-WeA7 Understanding Charge Transport Across Metal-Molecule-Metal Junctions**, ***J.G. Kushmerick***, *R. Shashidhar*, Naval Research Laboratory

Charge transport across a metal-molecule-metal junction is regulated by three factors 1) the structure of the molecule 2) the nature of the metal-molecule contacts and 3) the choice of metal electrode. We use an experimentally simple crossed-wire tunnel junction to interrogate how each of these three factors influences the current-voltage characteristics of a molecular junction. Results on symmetric and asymmetric junctions demonstrate that a specific molecular core can act either as a molecular wire or a molecular rectifier depending on its coupling to the metal electrodes. We will also show that the experimentally measured conductance of a molecular wire can be directly related to how well it's π-conjugated backbone mimics an ideal one-dimensional metal.

4:20pm **OF+EL+SC-WeA8 Zero-bias Anomaly in Molecular Monolayer Tunneling**, ***D.R. Stewart***, *D.A.A. Ohlberg, P.A. Beck, R.S. Williams*, Hewlett-Packard Laboratories

Electron tunneling is the dominant transport mechanism in nearly all proposed molecular electronic devices. Standard tunneling theory is normally used to predict device behavior, yet few experimental investigations of molecular tunneling exist due to the difficulty in constructing high quality molecular monolayer films. We describe detailed electronic transport characterization of several planar electrode / Langmuir-Blodgett (LB) molecular monolayer / electrode systems that show a large zero-bias anomaly and an anomalous exponential temperature dependence. Single-species LB monolayers of C_{22}, C_{20}, C_{18}, C_{16} and C_{14} carboxylic acid alkanes were sandwiched between upper and lower platinum electrodes, with active device areas of 7-200µm^2. Current and differential conductance were measured as a function of voltage ±1V and temperature 2-300K. Below 40K, device characteristics were constant. Surprisingly, from 40-300K device currents were exponential in temperature. A very wide ±150mV dip in conductance was also present and temperature activated. Both results contradict standard tunnel theory, indicating that the electronic transport is not yet understood even in this simplest symmetric alkane monolayer system.

4:40pm **OF+EL+SC-WeA9 Lateral Confinement of Interfacial Electrons by a Surface Dipole Lattice**, ***X.-Y. Zhu***, *G. Dutton*, University of Minnesota

Interface formation between molecules and a solid substrate often involves charge redistribution, the extent of which can influence a wide range of physical and chemical phenomena. In high mobility field effect transistors (FETs) based on organic single crystals, charge transport is believed to occur in one to two layers of molecules at the organic-dielectric interface. Such an interface may involve charge redistribution and dipole formation. The presence of surface dipoles may significantly alter lateral charge transport in the thin organic layer. When the interface is disordered, these surface dipoles are scattering centers for band transport. On the other hand, if the interface is ordered, there is essentially a two-dimensional lattice of dipoles. Such a surface dipole lattice should give rise to an electrostatic potential which provides periodic confinement of valence and conduction band electrons. We demonstrate this effect for image electrons on C60 thin film covered Cu(111) using angle resolved two-photon photoemission spectroscopy. Metal-to-molecule electron transfer within the first layer creates a (4x4) superlattice of surface dipoles. Such a surface dipole lattice provides lateral confinement of image electron wavefunction, effectively eliminating parallel dispersion for the n=1 image state on one monolayer C60 covered Cu(111). This is in contrast to the significant dispersion observed at higher coverages. The electrostatic potential from the surface dipole lattice is screened by additional layers of C60 molecules, thus, restoring the expected free electron behavior (parallel to the surface) for image states. Quantum mechanical simulation reproduces experimental findings and reveals the extent of wavefunction localization by the surface dipole lattice.

5:00pm **OF+EL+SC-WeA10 Measurement of the Site Specific PDOS of Organic Electronic Materials via Soft X-ray Emission Spectroscopy[1]**, ***J.E. Downes***, *C. McGuinness, P. Sheridan, K.E. Smith,* Boston University, *J.A. Schlueter, U. Geiser,* Argonne National Laboratory, *G. Gard*, Portland State University

Recent advances in the technique of soft x-ray emission spectroscopy (XES) have produced a method to directly measure the bulk elementally and, in certain cases chemically, specific partial density of states of materials. While the detailed measurement of the valence band electronic structure of solids has traditionally been the realm of photoemission spectroscopies several problems have been encountered with the application of these techniques to organic materials. The principal issue is photon induced damage to the compound that modifies the electronic structure as it is being measured. Another is the fact that photoemission measurements probe the surface electronic structure of a material, which may or may not be representative of the bulk. We will show that the use of XES can avoid both of these problems and allows the detailed valence band electronic structure of recently developed organic electronic compounds to be measured. An overview of the technique of XES and its advantages for studying these organic compounds will be followed by specific results from several organic electronic compounds of current interest in the fields of molecular organic semiconductors, (TDATA, Alq$_3$, TPD, Cu-Pc etc.), and ET based conducting organic charge transfer salts, (β-(ET)$_2$SF$_5$CH$_2$CF$_2$SO$_3$).

[1] Work supported in part by the DOE under DEFG0298ER45680; the SXE spectrometer was funded by the U.S. ARO under DAAH04950014. The experiments were performed at the NSLS which is supported by the U.S. DOE, Divisions of Materials and Chemical Sciences.

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