Electronic Materials and Processing
Room: Dona Ana - Session EM+MI-MoA

Semiconducting and Highly Correlated Oxides
Moderator: L.J. Brillson, The Ohio State University

2:00pm **EM+MI-MoA1 Oxide Superconducting Semiconductors**, ***H.Y. Hwang***, University of Tokyo, Japan **INVITED**

$SrTiO_3$ is the lowest density known bulk superconductor [1]. In addition, it is a dielectric material which is well-known for its very large low-temperature dielectric constant, arising due to the proximity of a ferroelectric instability [2]. With recent advances in complex oxide heteroepitaxy, these physical properties provide a unique opportunity to apply concepts of band structure engineering to this superconducting semiconductor.

At the conducting $LaAlO_3/SrTiO_3$ interface, the superconducting state can be back-gate modulated to induce a 2D superconductor-insulator transition [3]. Using magnetotransport studies in the normal state, we find that the mobility variation is five times as large as the change in sheet carrier density [4]. These results indicate that the relative disorder strength increases across the superconductor-insulator transition, which can be understood to be driven by localization as in previous examples of ultra-thin quenched amorphous superconductors such as Bi [5].

Using heterostructures of Nb:$SrTiO_3$ embedded in undoped $SrTiO_3$, we have studied the crossover from 3D to 2D superconductivity as the thickness of the doped layer is decreased. A notable feature is that the mobility increases in the 2D limit to over 6 times the highest bulk value at comparable doping, in analogy to delta-doping in semiconductors. This aspect suggests that a new regime of 2D superconducting phase transitions can be accessed approaching the clean limit, in contrast to the dirty limit seen at the back-gated $LaAlO_3/SrTiO_3$ interface [6].

This work was done in collaboration with Y. Kozuka, C. Bell, M. Kim, S. Harashima, Y. Hikita, and B. G. Kim.

[1] J. F. Schooley *et al.*, Phys. Rev. Lett. **12** (1964) 474.

[2] K. A. Mueller and H. Burkard, Phys. Rev. B **19** (1979) 3593.

[3] A. D. Caviglia *et al.*, Nature **456** (2008) 624.

[4] C. Bell *et al.*, Phys. Rev. Lett. **103** (2009) 226802.

[5] A. M. Goldman and N. Markovic, Physics Today **226** (1998) 39.

[6] Y. Kozuka *et al.*, Nature **462** (2009) 487.

3:00pm **EM+MI-MoA4 X-ray Photoemission Spectroscopy of Sr_2FeMoO_6 Film Stoichiometry and Valence State**, ***M.M. Rutkowski***, *A.J. Hauser, F.Y. Yang, R. Ricciardo, T. Meyer, P.M. Woodward, A. Holcombe, P.A. Morris, L.J. Brillson*, The Ohio State University

We have used a combination of monochromatized X-ray photoemission spectroscopy and Rutherford backscattering spectrometry to determine bulk compound stoichiometry and charge state of Sr_2FeMoO_6 epitaxial films. Complex oxides are an attractive class of materials for the creation of novel electronic devices due to their diverse properties. Sr_2FeMoO_6 (SFMO) is one such material due to the discovery of low field colossal magnetoresistance at room temperature and its half metallic character making it suitable in applications from magnetic read heads and nonvolatile magnetic random access memory to spin injectors in spintronic devices. But in order to create functional devices from such materials, it is necessary to have complete control over the crystal stoichiometry and ordering. Complicating this is that many of these materials, SFMO included, are not point compounds and small changes in stoichiometry can lead to the formation of other material phases which would strongly influence the materials properties.

Using standard samples with known stoichiometries of Fe_2O_3 and $SrMoO_3$ we were able to obtain sensitivity factors relative to oxygen for Sr, Fe, and Mo. In conjunction with RBS measurements, these sensitivities allowed us to determine sensitivity factors specific to SFMO for measuring stoichiometry. These studies also identify an optimum ion sputtering process for removing surface contaminants and an SrMoO4 overlayer while avoiding preferential sputtering of film constituents or alteration of their characteristic valence states. For Sr_2FeMoO_6, low energy (500 eV), glancing incidence Ar^+ sputtering for short (tens of seconds) periods is successful in achieving stoichiometric compositions and characteristic charge states of the film constituents. Furthermore, the adventitious surface carbon content dropped from 10% to less than 2% in the first 15s of sputtering. With longer sputtering times we observed the oxygen content to fall below its stoichiometric value (60%) and continue to fall with further sputtering indicating the preferential removal of oxygen from the film. We also observed the emergence of a metallic component to the iron and molybdenum valence states after 120s of sputtering indicating damage to the crystal lattice. Thus XPS reveals both a different surface overlayer stoichiometry as well as a 'window' of sputter time that provides bulk stoichiometry. The evolution of composition and valence state with sputtering provides a guide to measure stoichiometry and charge state of SFMO and complex oxide thin films in general.

4:00pm **EM+MI-MoA7 Electronic Structure of Ferrimagnetic $Co_{1-x}Fe_{2+x}O_4$ Determined by Soft X-ray and Ultraviolet Spectroscopies**, ***J.A. Moyer***, *C.A.F. Vaz*, Yale University, *D.A. Arena*, Brookhaven National Laboratory, *V.E. Henrich*, Yale University

Developing new materials with large spin polarizations, high Curie temperatures and resistivities similar to those of semiconductors would greatly benefit the field of spintronics. Cobalt ferrite ($CoFe_2O_4$), like its parent compound magnetite (Fe_3O_4), is a promising material for spintronic applications due to its high Curie temperature (T_c=793 K) and large predicted spin polarization; however, $CoFe_2O_4$ is an insulator. Cobalt ferrite becomes an *n*-type conductor when doped with excess iron – $Co_{1-x}Fe_{2+x}O_4$; the origin of the conduction is electron hopping between Fe^{2+} cations in octahedral sites. The strong localization of electrons on the Fe^{2+} cations in this highly correlated oxide keeps the conductivity in the semiconducting range. In this work, heteroepitaxial $Co_{1-x}Fe_{2+x}O_4$ thin films have been grown on MgO (100) and $MgAl_2O_4$ (100) and (110) with *x* ranging from 0 to 0.5. The electronic band structure near the Fermi energy is measured with ultraviolet photoelectron spectroscopy (UPS), and the results are correlated with resistivities determined from transport measurements. This range of doping allows for the resistivity to be tailored over two orders of magnitude. The cation valence states and occupation sites are determined with x-ray photoelectron spectroscopy (XPS) and x-ray absorption spectroscopy (XAS). Bulk magnetic moments are obtained with SQUID magnetometry, while bulk and site specific orbital and spin magnetic moments are obtained using x-ray magnetic circular dichroism (XMCD). The XMCD measurements provide a view of the spin polarization of the Fe^{2+} octahedral cations responsible for conduction. The wide variety of measurements enables us to determine the electronic structure of $Co_{1-x}Fe_{2+x}O_4$, an important development for the goal of determining the viability of $Co_{1-x}Fe_{2+x}O_4$ as a spin-polarized source or detector in spintronic devices.

This research is primarily supported by NSF Grant MRSEC DMR-0520495.

4:20pm **EM+MI-MoA8 Effects on the Electronic Band Structure of EuO Films upon Gd Doping**, ***J.A. Colón***, *J. An, K.D. Belashchenko*, University of Nebraska - Lincoln, *Y.B. Losovyj*, Louisiana State University, *P. Liu, X.J. Wang, J. Tang*, University of Wyoming, *P.A. Dowben*, University of Nebraska - Lincoln

High quality films of EuO and Gd doped EuO were successfully grown on Si (100) via pulse laser deposition (PLD). The addition of 4% Gd introduces considerable affects the texture growth direction, although the crystal structure remains intact. This Gd doping also have a strong influence in the electronic structure of these films, in particular the apparent band offsets, making the material appear considerably more n-type in combined photoemission and inverse photoemission studies. There are also concomitant changes to the conductivity properties. To further elucidate the influence of Gd doping on the electronic band structure of the EuO films, heterojunction devices were constructed resulting in diodes with very distinct properties a negative differential current that depends on magnetic field.

4:40pm **EM+MI-MoA9 Catalytic Performance for Soot Combustion of Lanthanum-Based Cobalt-Iron Perovskite Materials**, ***L.M. Petkovic***, *S.N. Rashkeev*, Idaho National Laboratory, *V. Utgikar*, University of Idaho

Perovskite-type oxide materials with a general formula La0.8A0.2Fe(1-y)Co(y)O(3-delta), where A is Sr or Ba and y=0.4 or 0.5, were prepared and tested in the combustion of carbon black, which can be regarded as a conservative soot model. Maximum combustion rates under temperature programmed combustion conditions were found at temperatures about 150°C lower than blank combustion experiments. A combination of density-functional-theory (DFT) calculations and characterization analyses such as surface area, infrared spectroscopy, X-ray diffraction, and temperature programmed oxidation and reduction were applied to elucidate the main processes that contribute to the activity of these catalysts for soot combustion. The results suggest the importance of the kinetics of oxygen adsorption and reaction at the surface and oxygen migration in the bulk.

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

Contacts and Transport
Moderator: L. Porter, Carnegie Mellon University

8:00am **EM-TuM1 Resistivity Increase due to Electron Surface Scattering in Nanoscale Metal Films**, ***J.S. Chawla***, *D. Gall*, Rensselaer Polytechnic Institute

The resistivity increase due to electron surface scattering can be reduced by facilitating specular scattering, as demonstrated by *in-situ* transport measurements on single crystal Cu, Ag, and TiN layers. However, metal barrier layers and surface exposure to oxygen/air perturb the periodic surface potential, causing diffuse electron scattering which increases the resistivity. These findings are important for the development of future generation narrow low-resistivity Cu interconnects and TiN metal gates. Epitaxial Cu(001), Ag(001), and TiN(001) layers exhibit a minimum continuous thickness of 20, 50, and 1.8 nm, respectively, when grown on MgO(001) substrates by ultra-high vacuum magnetron sputter deposition at 80, 140, and 750 ° C, respectively, while Cu grown on a 2-nm-thick TiN(001) buffer layer at room temperature shows a minimum continuous thickness of 4 nm. X-ray diffraction θ-2θ scans, ω-rocking curves, and pole figures show the layers are single crystals with a cube-on-cube epitaxy. The surface and interface roughness, and layer thickness were determined by Rutherford backscattering spectrometry, x-ray reflectometry, and *in-situ* scanning tunneling microscopy. *In-situ* electron transport measurements at room temperature show a resistivity increase with decreasing thickness d, from (*i*) 1.7 to 6.4 μΩ-cm for Cu layers with d = 1400 to 4 nm, (ii) 13 to 150 μΩ-cm for TiN layers with d = 760 to 1.8 nm, and (iii) 1.6 to 2.1 μΩ-cm for Ag layers with d = 1250 to 50 nm. The data for Cu and Ag layers is consistent with the Fuchs-Sondheimer model and indicates specular scattering at metal-vacuum boundary with an average specularity parameter p = 0.6 and 0.4, respectively. In contrast, layers measured *ex-situ* show completely diffuse surface scattering (p = 0) due to sub-monolayer oxidation.

In-situ deposition of 0.3 to 7 nm thick Ta barrier layers on Cu(001) films leads to a resistance increase that indicates transition to p = 0, independent of the Ta thickness. *In-situ* exposure of Cu(001) layers to O_2 between 10^{-3} and 10^5 Pa-s results in a sequential increase, decrease and increase of electrical resistance which is attributed to partial specular surface scattering for smooth clean Cu(001) and for surfaces with a complete adsorbed monolayer, but diffuse scattering at partial coverage and after chemical oxidation. A model relates the surface coverage to p and provides values for the oxygen adatom and advacancy scattering cross-sections of 0.8 and 0.06 nm^2, which are qualitatively validated by non-equilibrium *ab initio* transport simulations. The rates for resistance change are proportional to the O_2 pressure, indicating a high-sensitivity gas sensing mechanism.

8:20am **EM-TuM2 Extracting Inelastic and Elastic Hot Electron Attenuation Lengths from nm-Thick Metal Films using BEEM**, ***J.J. Garramone***, *J.R. Abel, I.L. Sitnitsky, V.P. LaBella*, University at Albany

Measuring the scattering of electrons in nm-thick structures of metals such as Cu and Ag is both technologically and fundamentally significant. For example, sidewall and grain boundary scattering in nanoscale Cu-metal interconnects dramatically increases the resistance, which is detrimental to device performance. A highly accurate method for studying hot electron transport on the nanometer length scale is ballistic electron emission microscopy (BEEM). BEEM is a three terminal scanning tunneling microscopy (STM) based technique, where electrons tunnel from a STM tip into the grounded metal base of a Schottky diode [1]. The BEEM current is a measurement of the electrons that traverse the metal film and are collected in the semiconductor. Results from BEEM measurements of the hot electron attenuation length of the metal films will be presented. A Fermi liquid based model is utilized to extract the inelastic and elastic contributions to the scattering. The metal films are deposited on H-terminated Si(001) under ultra-high vacuum (UHV). The BEEM measurements are taken at 77K under UHV. Recently we fabricated a contact to the metal layer on the silicon utilizing standard lithography prior to deposition of the metal in UHV [2]. This allowed these BEEM measurements to be performed *in situ*. The process utilized to fabricate this contact will be presented along with the *in situ* BEEM results.

References:

[1] L. D. Bell and W. J. Kaiser, Phys. Rev. Lett. 61 2368 (1988)

[2] J. J. Garramone, et al., J. Vac. Sci. Technol. A (in press) (2010)

8:40am **EM-TuM3 Influence of Spontaneous Polarization and Intrinsic Gap States in Schottky Contacts to ZnO**, ***M.W. Allen***, University of Canterbury, New Zealand, *S.M. Durbin*, University at Buffalo **INVITED**

Zinc oxide is an interesting test case for evaluating theoretical Schottky contact formation models as it is significantly more ionic than most semiconductors. This results in weaker Fermi level pinning, which in turn allows the barrier height of Schottky contacts to vary with metal properties. Equally important is the fact that contacts can be prepared on laterally homogeneous, bulk-grown, single crystals with minimal surface processing as there is no requirement, as with most semiconductors, to remove native surface oxide layers with potentially damaging etching treatments. As a result, we have been able to fabricate very low ideality factor, laterally homogeneous Schottky contacts to 'intrinsic' ZnO surfaces for a wide variety of metals using a novel eclipse pulsed laser deposition technique. Using these contacts, we have evaluated the two leading contemporary Schottky contact formation models – Tung's 'chemical bond polarization model' and Mönch's 'metal induced gap states and electronegativity model'. The lack of broad agreement with either of these models suggests the involvement of additional mechanisms, perhaps involving the large spontaneous polarization of ZnO and ionic surface charge screening effects, with important consequences for other oxide semiconductors.

9:20am **EM-TuM5 Dynamics of the Charge Transfer through the Individual Molecules in Alkanethiolate Self-Assembled Monolayers**, *P. Kao,* Pennsylvania State University, *S. Neppl, P. Feulner,* Technische Universität München, Germany, *D.L. Allara,* Pennsylvania State University, ***M. Zharnikov***, Universität Heidelberg, Germany

Emergence of molecular and organic electronics as frontier fields of modern science and technology require reliable experimental data regarding the charge transport (CT) in individual molecules and their functional units. Whereas static conductance of molecules arranged in self-assembled monolayer (SAM) fashion on a suitable substrate has been extensively studied, little is known about the CT dynamics in these systems. By the example of alkanethiolate films on Au(111), we show that the latter phenomena can be successfully addressed by resonant Auger spectroscopy, using the core hole clock method. The charge transfer pathway was unambiguously defined by resonant excitation of the nitrile tailgroup attached to the alkyl backbone. The length of this backbone was varied to monitor the respective dependence of the CT time. It was found that, similar to the static conductance, this dependence can be coarsely described by an exponential function with an attenuation factor of 0.93 per a methylene unit. As a result, the CT time is quite long even for a relatively short alkyl chain; in particular, it is ca. 100 fs for the chain consisting of only four methylene units. In contrast, the CT time associated with the thiolate headgroup anchor was found to be quite short, viz. 2.3 fs (upper limit), which suggests an efficient interfacial electronic coupling between the aliphatic backbone of the molecules and substrate over the thiolate-gold linkage.

9:40am **EM-TuM6 Electronic Properties and Assembly of Zinc Metalloporphyrin Islands on Au(111) Surfaces**, ***A.E. Schuckman***, *K.M. Webb, L.M. Perez,* Texas A&M University, *M. Jurow,* Hunter College of the City University of New York, *L.H. Yu,* National Institute of Standards and Technology, *C.M. Drain,* Hunter College of the City University of New York, *J.G. Kushmerick,* National Institute of Standards and Technology, *J.D. Batteas*, Texas A&M University

Porphyrins are stable, highly conjugated compounds and the choice of metal ion and substituents bound to the macrocycle as well as other effects such as chemical surrounding and cluster size modulate the electronic and photonic properties of the molecule. Porphyrins and their derivatives are relatively non-toxic, and due to their very rich photo- and electro-chemistry as well as their small HOMO-LUMO gaps, this makes them outstanding candidates for use in molecularly-enhanced electronic applications.

For this study, the transport properties of self-assembled zinc coordinated tri-pyridyl porphyrin thiol islands inserted into a dodecanethiol matrix on Au(111) were investigated using scanning tunneling microscopy (STM) and cross-wire inelastic tunneling spectroscopy (IETS). The zinc porphyrin thiol islands observed by STM exhibited reversible bias-induced switching at high surface coverage due to the formation of Coulomb islands of ca. 10 nm diameter driven by porphyrin aggregation. Low temperature measurements (~ 4 K) from crossed-wire junctions verified the appearance of a Coulomb staircase and blockade which was not observed for single molecules of this compound or for the analogous free base. Scanning probe lithography via nanografting has been implemented to fabricate nanoscale patterns of the zinc porphyrin thiols on Au surfaces and ultimately ~ 10 nm islands which is the optimal size for the observed switching effect.

10:40am **EM-TuM9 Deposition of Nickel Nanostructures by Electroless Deposition on Micron-Scale Patterned SAMs***, Z. Shi,* ***A.V. Walker***, University of Texas at Dallas

We have investigated the reaction pathways involved in the electroless deposition of nickel on -COOH, -OH, and -CH_3 terminated functionalized alkanethiolate self-assembled monolayers (SAMs) adsorbed on gold, using time-of-flight secondary ion mass spectrometry (TOF SIMS), scanning electron microscopy (SEM) and x-ray photoelectron spectroscopy (XPS) . This work has important applications in molecular/organic electronics as well as other technologies.

We observe that the nickel electroless deposition rate increases as the plating bath pH increases. For -COOH, terminated SAMs, this is effect is very pronounced, with the largest deposition rates observed at above pH = 9. This is most likely due to the –COOH terminated groups deprotonating to form forming carboxylate ions, COO^-. These carboxylate ions can easily complex with Ni^{2+} ions in solution, forming Ni-carboxylate complexes which serve as the nucleation sites for Ni deposition. Furthermore on -COOH terminated SAMs the nickel overlayer forms almost immediately, while on -CH_3 and -OH terminated SAMs the nickel overlayer forms after 15-20 minutes deposition. The nucleation of the Ni overlayer is slightly faster on the hydrophobic -CH_3 terminated SAM than on the hydrophilic -OH terminated SAM.

By exploiting the different nickel deposition rates on -COOH, -OH, and -CH_3 terminated SAMs we demonstrate that a variety of nanostructures can be produced, including nanowires and rings, using micron-scale patterned SAM surfaces.

11:00am **EM-TuM10 Rapid DNA Sequencing via Transverse Electronic Transport***,* ***M. Zwolak****,* Los Alamos National Laboratory*, M. Di Ventra*, University of California at San Diego

A rapid and low-cost DNA sequencing method would revolutionize medicine: a person could have their full genome sequenced so that treatments could be tailored to their specific conditions; doctors could know in advance a patient's likelihood to develop a given ailment; cures to major diseases could be developed faster. These goals of "personalized medicine" is hampered today by the high cost and slow speed of DNA sequencing methods. I discuss a sequencing protocol we suggest that uses the measurement of transverse electronic currents during the translocation of single-stranded DNA through nanopores. I present support for our conclusions using molecular dynamics simulations coupled to quantum mechanical calculations of electrical current in experimentally realizable systems. Several recent experiments also support our theoretical predictions. In addition to their possible impact in medicine and biology, the above methods offer ideal test beds to study open scientific issues in the relatively unexplored area at the interface between solids, liquids, and biomolecules at the nanometer length scale [1].

[1] M. Zwolak, M. Di Ventra, "Physical Approaches to DNA Sequencing and Detection", Rev. Mod. Phys. 80, 141 (2008).

11:20am **EM-TuM11 Using Scanned-Probe Microscopy to Study Surface-Induced Fluctuations as a Tool for Microscopically Probing Organic Materials***,* ***N. Hoepker***, Cornell University

The development of organic electronics calls for new tools to study organic thin films. By measuring the frequency noise experienced by a cantilever near a surface, we are able to microscopically probe organic materials. In previous work, we have used custom-fabricated ultrasensitive cantilevers to measure frequency noise ("jitter") due to dielectric fluctuations as a function of cantilever height and voltage over polymer of various compositions and thicknesses [1]. In parallel, we have developed a zero-free parameter linear-response theory of thermally induced dielectric fluctuations [2] that successfully describes our observations. Having understood dielectric fluctuations, we are now investigating fluctuations induced by carrier motion in organic materials in order to extract the local charge mobility.

11:40am **EM-TuM12 High Precision Local Electrical Probing: Potential and Limitations for the Analysis of Nanocontacts and Nanointerconnects***,* ***A. Bettac****, J. Koeble, B. Guenther, M. Maier, A. Feltz,* Omicron NanoTechnology GmbH, Germany*, D. Jie, N. Chandarsekhar,* Institute of Materials Research & Engineering, Singapore*, C. Joachim*, CEMES-CNRS, France

The variety of approaches for individual nanoscale devices is tremendous. In contrast however, comprehensive concepts towards electrically integrated and therefore functional devices are rare. The individual (metallic) contact interface represents one of the main challenges and high precision local electrical probing has the potential to increase efficiency in evaluating different approaches. To meet the involved requirements, we have established and being advancing an approach integrating SPM technology with high resolution electron microscopy: (1) Rapid and simultaneous SEM navigation of four local STM probes; (2) Localization of nanostructures by high resolution SEM; (3) Individual probe fine positioning by atomic scale STM imaging; (4) STM based probe approach for "soft-landing" of sharp and fragile probes and controlled electrical contact for transport measurements; (5) approaches towards sharp and clean STM tips; (6) suitable low noise signal re-routing for transport measurements; and (7) chemical or magnetic analysis by complementary analysis techniques.

We will report on recent technical enhancements and illustrate achievements and limitations along specific applications. As a model system, we have chosen Au islands on MoS_2 [1]. These islands represent contact pads, each electrically connected by an individual STM probe. As good band gap (approx. 1.3eV transverse gap) semiconductor, MoS_2 has the potential to sufficiently decouple nanostructures electrically at low voltage. Those Au triangular islands have a lateral size of typically 10-30nm and form an "atomically" clean and defined metal-semiconductor interface. We will present measurements on (1) probe navigation and electrical contacting with contact distances in the 10nm regime. (2) reproducible Schottky like IV properties for the individual STM tip/Au island/substrate contact; (3) surface conductance measurements with variable inter-island distance down to 17nm; and (4) we also show that the individual STM probe can be employed under SEM to manipulate those Au islands [2] with high precision in order to generate arbitrary multi probe planar contact configurations.

Furthermore, we will present a newly developed probing system. The complete stage including probes is cooled down to LHe temperatures, while each probe is capable of atomic resolution STM. A major challenge is the integration of an high performance UHV Gemini SEM into the thermally shielded probe stage compartment, while maintaining the sample temperature below 10K during SEM operation.

[1] MSM Saifullah et al., Nanotechnology, 13, 659 (2002)

[2] J.S. Yang et al., J. Vac. Sci. Tech. B, 25, 1694 (2007)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Energy Frontiers Topical Conference
Room: Mesilla - Session EN+EM-TuA

Electronic Materials for Energy Conversion & Storage
Moderator: G.W. Rubloff, University of Maryland

2:00pm **EN+EM-TuA1 High-capacity and High-rate Metal Oxide Anodes for Li-ion Batteries**, ***A.C. Dillon****, C. Ban,* National Renewable Energy Laboratory*, L.A. Riley, A.S. Cavanagh, S.M. George,* University of Colorado*, Y.S. Jung, Z. Wu, Y. Yan,* National Renewable Energy Laboratory*, S.-H. Lee*, University of Colorado **INVITED**

Significant advances in both energy density and rate capability for Li-ion batteries will be necessary for implementation in next generation electric vehicles. By employing metal oxide nanostructures, it is possible to achieve Li-ion anodes that have significantly higher capacity than the state-of-the-art graphite technology. For example we have demonstrated that thin film MoO_3 nanoparticle electrodes (~2 μm thick) have a stable reversible capacity of ~630 mAh/g when tested at C/2.[1] By fabricating more conventional electrodes (~35 μm) with a conductive additive and binder, an improved reversible capacity of ~1000 mAh/g is achieved.[2] The increased capacity for the MoO_3 coin cell electrode compared to the thin film electrode may be attributed to improved electronic/ionic mobility with the conductive additive and more complete access to the nanostructures. We have also demonstrated that by applying a thin atomic layer deposition coating of Al_2O_3, improved rate capability for the high volume expansion MoO_3 is achieved for thick more conventional electrodes[3].

More recently we have focused our work on iron oxide nanostructures, as iron is an inexpensive, abundant and a non-toxic material. Furthermore, we have synthesized binder-free, high-rate capability electrodes. The electrodes contain Fe_3O_4 nanorods as the active lithium storage material and carbon single-wall nanotubes (SWNTs) as the conductive additive. The highest reversible capacity is obtained using 5 wt.% SWNTs, reaching 1000 mAh/g (~2000 mAh/cm^3) at C rate when coupled with a lithium metal electrode, and this high capacity is sustained over 100 cycles. Furthermore, the electrodes exhibit high-rate capability and stable capacities of 800 mAh/g at 5C and ~600 mAh/g at 10C. Scanning electron microscopy indicates that this high-rate capability is achieved because Fe_3O_4 nanorods are uniformly suspended in a conductive matrix of SWNTs. Raman spectroscopy is employed to understand how the SWNTs function as a highly flexible conductive additive. We expect that this method can be used to achieve other binder-free anodes as well as cathodes with similar high-rate capability[4].

(1) Lee, S.-H.; Kim, Y.-H.; Deshpande, R.; Parilla, P. A.; Whitney, E.; Gillaspie, D. T.; Jones, K. M.; Mahan, A. H.; Zhang, S. B.; Dillon, A. C. Adv. Mat. 2008, 20, 3627-3632.

(2) Riley, L. A.; Lee, S.-H.; Gedvilias, L.; Dillon, A. C. Journal of Power Sources 2010, 195, 588-592.

(3) Riley, L. A.; Cavanagh, A. S.; George, S. M.; Jung, Y.-S.; Yan, Y.; Lee, S.-H.; Dillon, A. C. ChemPhysChem 2010, *in press*.

(4) Ban, C.; Wu, Z.; Gillaspie, D. T.; Chen, L.; Yan, Y.; Blackburn, J. L.; Dillon, A. C. Advanced Materials 2010, *in press*.

2:40pm **EN+EM-TuA3 Engineering $Li_xAl_ySi_zO$ Thin Films as a Solid Electrolyte for 3D Microbatteries**, ***Y.-C. Perng****, J. Cho, D. Membreno, B. Dunn, J.P. Chang*, UCLA

The development of secondary lithium-ion batteries has been directed primarily at portable electronics applications. However, these batteries also have the potential to function as a power source for micro-systems through engineering of electrodes into 3D architectures based on high aspect ratio pillars. In order to utilize this potential, an ultra-thin and highly conformal solid electrolyte layer is required to coat the 3D electrode array. The solid electrolyte lithium aluminosilicate ($LiAlSiO_4$), is a promising candidate for this application due to high ionic conductivity along its c-axis resulting from channels formed by the alternating tetrahedra of aluminum-oxygen (Al-O) and silicon-oxygen (Si-O). The length of c-axis of lithium aluminosilicate can be adjusted by changing the crystallization temperature for desired conductivity characteristics.

Atomic layer deposition (ALD) was employed in this work to synthesize thin film lithium aluminosilicate. The self-limiting characteristic of ALD allows for precise control of thickness and composition of complex oxides and results in a highly conformal and pinhole-free coating suitable in 3D micro-battery applications. The metal precursors used in this work are tetraethyl orthosilicate (TEOS), trimethylaluminum (TMA) and lithium t-butoxide (LTB). We also investigated the use of tri-t-butoxy-hydroaluminate (LTBA) but found that the metal composition was difficult to control and high carbon contents. Using the three precursors mentioned above with water vapor as the oxidant, we deposited SiO_2, Al_2O_3 and Li_2O,

at deposition rates in the range of 0.8~2Å/cycle. The overall deposition rate of stoichiometric $LiAlSiO_4$ was ~5Å/cycle using a chamber base pressure of 10^{-2} Torr and substrate temperature of 300°C. The concentration of each metal element in $Li_xAl_ySi_zO$ thin films is found to correlate closely to ALD cycles and the associated incubation times. The crystalline structures as well as the local environment of the Li-conducting channels are also affected by the ALD cycles and sequences, as indicated by ultraviolet photoelectron spectroscopy (UPS), transmission electron microscopy (TEM) imaging and nuclear magnetic resonance (NMR) analyses. The Li-ion conductivities of ALD $Li_xAl_ySi_zO$ thin films were determined by impedance measurements using a four-point probe setup with contacts made to the film surface. The films have high ion conductivity and low electronic conductivity, the values of which are strongly influenced by the lithium content and distribution in the synthesized thin films.

3:00pm **EN+EM-TuA4 Laser-Deposition and Characterization of Amorphous Thermoelectric Films**, ***G.B. Wilks***, Air Force Research Laboratory, *P.T. Murray,* University of Dayton, *S.B. Fairchild, N.W. Gothard, J.E. Spowart*, Air Force Research Laboratory

From the Efficient Cluster Packing model describing the topology of metallic glasses, it is understood that certain compositions are favored for glass-formability based on the ratio of atomic sizes between constituents. In this regard, the half-Heusler composition $Zr_{0.5}Hf_{0.5}NiSn$ is nearly ideal. Although the crystallized form of this material has been widely studied because of its high thermoelectric power factor, it has been suggested that partial vitrification may enhance the thermoelectric figure of merit by preserving the favorable aspects of electronic structure while significantly disrupting thermal transport. Capitalizing on the high quench rates possible during pulsed laser deposition, a spectrum of thin films including amorphous and partially-amorphous duplex microstructures has been grown under various conditions. Transport characteristics relevant to the thermoelectric effect are rationalized in light of accompanying microstructure characterization.

4:00pm **EN+EM-TuA7 Probing Charge Transport in Exploratory Nanocrystal-Based Devices**, ***P. Nagpal***, *V.I. Klimov*, Los Alamos National Laboratory **INVITED**

Colloidally synthesized semiconductor nanocrystals offer the exciting opportunity to exploit unique physical properties, such as size tunable band gap, in low-cost, solution-processed thin film devices. However, charge transport in as-deposited thin films of colloidal nanocrystals is hindered by organic ligands. At the Center for Advanced Solar Photophysics (CASP), a DOE Energy Frontier Research Center, we are investigating the mechanism of charge transport in nanocrystal films by employing them in a range of simple device architectures, with the goal of optimizing them for photovoltaic application. As an example, I will present recent work in nanocrystal-based optical field effect transistors specifically designed to study electron transport and the dynamics of the photogenerated carriers in these semiconductor thin films. These devices offer invaluable information regarding field dependant mobility, optical gating and changes in the Fermi-level at the nanocrystal film interface. I will then discuss other exploratory device efforts at CASP, and how the information generated will be used collectively for the development of solar cells and other energy-related applications.

4:40pm **EN+EM-TuA9 Investigation of GaTlP for Use in Multijunction Photovoltaics**, ***C. Downs***, *T. Vandervelde*, Tufts University

To achieve the highest possible conversion efficiencies in multijunction photovoltaics, the individual layers of the device must both be lattice-matched and have optimal band-gap spacing. Lattice-matched or strain-compensated epitaxy is required for the growth of junctions thick enough to elicit high quantum efficiency. Ideally, for spectral matching, one would have an infinite number of junctions that are current-matched; however, fabrication of a large number of junctions is neither easy nor desirable because of problems that arise from series resistance. In the end, it becomes a balancing act where the optimal number of junctions for a high efficiency concentrator cell is 3-6 junctions, with the conversion efficiency directly linked to how well spacing of the band gaps of the cell are optimized for absorption of the solar spectrum. Unfortunately, many of the optimal lower band-gaps for these multijunction cells do not occur in the dominant materials system (i.e. Ge and mixtures of In, Ga, Al, As, and P). As such, of late there has been a strong push to characterize new materials in hopes of providing more design options for photovoltaic cells. GaTlP is one such material, theorized to be useful as one of the lower junctions of 3+-junction cells while still being lattice-matched to GaAs and Ge. In this research, the change in lattice constant and band gap of GaTlP with varying compositions are investigated first by computational simulation and then with physical devices. New efficiency records should be achievable by incorporating these new optimal junction materials into the design for multijunction cells. This development will help solar concentrator cells achieve grid parity, thereby becoming a viable renewable energy choice.

5:00pm **EN+EM-TuA10 Photo Induced Ferroelectric Properties of $Pb_{0.95}La_{0.05}Zr_{0.54}Ti_{0.46}$ Thin Films**, ***H.V. Nampoori***, *S. Kotru*, University of Alabama

Thin films of lanthanum doped lead zirconate titatante (PLZT) have gained attention due to the large photostrictive response, and their possible use for contact less actuators and sensors. Variation in composition and doping are known to influence the photostrictive responses as well as ferroelectric behavior of these materials. PLZT is also a potential material for photovoltaic devices due to its high electro-optic coefficient and optical transparency.

In this work, thin films of $Pb_{0.95}La_{0.05}(Zr_{0.54}Ti_{0.46})O_3$ (PLZT) were prepared using Metal-Organic Decomposition technique (MOD). The films are deposited by spin coating. Sputter deposited Pt electrodes serve as top contacts for the films. Thickness of the grown films varied from 70-350 nm and the growth temperature was chosen in the range of 550-700ºC. Details of the film growth process including effects of temperature, thickness and annealing, and electrical and optical characterization will be presented. In addition parameters which affect the electrical properties like ferroelectric hysteresis and leakage behavior mechanisms will be discussed. The photo induced effects on the ferroelectric and the leakage properties, giving insight to the photovoltaic properties of ferroelectric thin films would be presented

Magnetic Interfaces and Nanostructures
Room: Zuni - Session MI+EM-TuA

Spintronics
Moderator: S.-W. Hla, Ohio University

2:00pm **MI+EM-TuA1 All-Electric Spintronics with Quantum Point Contacts: From Spin Physics to Spin Electronics**, ***P. Debray***, University of Cincinnati **INVITED**

The controlled creation, manipulation, and detection of spin-polarized currents by purely electrical means remains a central challenge and objective of spintronics. One approach to meet this challenge has been to rely on coupling of the electron orbital motion to its spin. Attempts have been made to use the Rashba spin-orbit coupling as a tool to achieve this objective. Despite intense effort there has so far been no report of any success. In this talk, I will present experimental evidence that a quantum point contact made from a semiconductor with intrinsic spin-orbit coupling can generate completely spin-polarized current when its lateral confinement is made highly asymmetric by tuning the bias voltages of the side gates that create it. Such quantum point contacts can be used as all-electric spin polarizer or detector. I will discuss how they can replace the ferromagnetic electrodes of conventional spin valves to yield all-electric spin valves with very high On/Off values. By avoiding the use of ferromagnetic contacts or external magnetic fields, the use of such quantum point contacts will make feasible the development of a variety of semiconductor spintronic devices.

2:40pm **MI+EM-TuA3 Incorporation of Mn Atoms into N-polar Wurtzite GaN(000-1) Surface Studied using Scanning Tunneling Microscopy**, ***A.V. Chinchore***, *K. Wang, M. Shih, A.R. Smith*, Ohio University Nanoscale and Quantum Phenomena Institute

There has been much interest in dilute magnetic semiconductors. Mn-doped gallium nitride was proposed as a possible dilute magnetic semiconductor with Curie temperature above room temperature [1]. Consequently, many studies have been carried out to investigate the growth and properties of Mn-doped GaN. Despite much work however, not much is known about the location of Mn atoms in the GaN surface. We present in this new study evidence for the precise position of Mn atoms in the nitrogen polar wurtzite GaN (000-1) surface.

The N-polar GaN (000-1) surface is prepared by molecular beam epitaxy using a Ga effusion cell and a rf N-plasma source on sapphire substrates. The growth is monitored in-situ using reflection high energy electron diffraction. The as-grown GaN surface shows a smooth 3×3 reconstruction. The sample is transferred in-situ to the analysis chamber where it is imaged using room-temperature scanning tunneling microscopy (STM). The as-grown sample surface shows large terraces of 3×3 reconstruction. Transferring the sample back to the growth chamber, Mn is then deposited onto the 3×3 surface at a rate of about 0.01 monolayers (ML's) per second for a total of about 0.3 ML, at a sample temperature of 250 ˚C. After this, the surface remains in a 3×3 structure.

STM images of the surface after Mn deposition show a modified 3×3 reconstruction including almost uni-axial trench-like structures over large areas which are not seen on the clean GaN surface. The closely-spaced trenches run along [11-20], and they are separated by an even number of gallium adlayer rows. The position of these features also coincides precisely with Ga adlayer row positions. A model for this structure involving Mn atoms within the GaN(000-1) adlayer has been developed. Additional work exploring the coverage dependence of this structure is also underway. This work has been supported by DOE (Grant No.DE-FG02-06ER46317) and NSF (Grant No.0304314). Equipment support from ONR is also acknowledged.

[1] T. Dietl, H. Ohno, F. Matsukura, J. Cibert, and D. Ferrand, Science 287, 1019 (2000).

3:00pm **MI+EM-TuA4 Formation of Ferromagnetic MnGa Monolayers on GaN(0001) Studied by STM**, ***K. Wang***, *A.V. Chinchore, M. Shi, A.R. Smith*, Ohio University Nanoscale and Quantum Phenomena Institute

Ferromagnetic (FM) metal/semiconductor bilayers are of great interest due to their importance in novel spintronics applications, such as spin injection and spin light-emitting diodes[1]. It has been shown[2] that δ-MnGa, a FM alloy with T_C higher than room temperature (RT), can be grown epitaxial on top of w-GaN(0001) with sharp interface and controllable magnetism. Here we report detailed studies on the formation of the first few MnGa monolayers formed by depositing up to 3 monolayers (ML's) of Mn onto w-GaN(0001) "1x1" surface at elevated substrate temperature. Mn-induced surface reconstructions and formation of smooth Mn_xGa_{1-x} crystalline monolayer films are observed by reflection high-energy electron diffraction (RHEED), Auger electron spectroscopy as well as in-situ RT-scanning tunneling microscopy (RT-STM). RHEED data showed well-ordered surface reconstructions exhibiting mainly 1/3rd and 2/3rd order streaks along [1-100] directions at lower than around 0.5 ML of Mn coverage, while two different sets of reconstruction streaks could be identified depending upon the Mn coverage. Two different types of atomic row-like features both running along close-packing direction of GaN, but having different row-row spacings, are observed with STM at room temperature. The unit-cells derived are consistent with RHEED observation. At higher than around 0.5 ML, atomically smooth MnGa layers start to cover up the surface as shown by both RHEED and STM; the epitaxial relationship is derived as d-MnGa[011]//GaN[0001] and d-MnGa[001]//GaN[11-20]. Structural and electronic properties at representative stages will be presented, as well as possible magnetic properties of MnGa ML's. This work has been supported by DOE (Grant No.DE-FG02-06ER46317) and NSF (Grant No. 0730257). Equipment support from ONR is also acknowledged.

[1] S.A. Wolf *et al*, Science **294**, 1488 (2001).

[2] E. Lu *et al*, Phys. Rev. Lett. **97**, 146101 (2006); K.K. Wang *et al,* Mater. Res. Soc. Symp. Proc. 1118-K06-06 (2009).

4:40pm **MI+EM-TuA9 Chemical Switching of Coupled Molecular Spins: On and Off**, *C. Waeckerlin, D. Chylarecka, A. Kleibert, K. Mueller,* Paul Scherrer Institute, Switzerland*, C. Iacovita,* University of Basel, Switzerland*, F. Nolting, T.A. Jung,* ***N. Ballav***, Paul Scherrer Institute, Switzerland

Herein we present a unique approach to reversibly control between the *on* and *off* state of the spin of an organometallic molecule coupled to a ferromagnetic substrate by a chemical switch. Such an ultimate degree of control was achieved via modification of the coordination strength of the central metal ion of the organometallic molecule by an external ligand. Thus the regulation of oxygen affinity in hemoglobin by iron-porphyrin moiety as shown in nature has been used as a designed concept to perform the switching event of single molecular spin. Use of external stimuli to control single molecular spins at magnetic-interfaces is of potential interest for spintronics and quantum information.

5:00pm **MI+EM-TuA10 The Spin-Resolved Electronic Structure of the Strongly Correlated $M^{II}[TCNE]^{\bullet-}$ Magnets**, *S.J. Janjua,* University of Missouri-Kansas City*, K.I. Pokhodnya,* North Dakota State University*, J. Trunk,* Brookhaven National Laboratory*, C.S. Olson,* North Dakota State University*, J.C. Sutherland, E. Vescovo,* Brookhaven National Laboratory*,* ***A.N. Caruso***, University of Missouri-Kansas City

$M^{II}[TCNE]^{\bullet-}$ organic-based magnets are an important class of solids for both application and magnetic exchange and correlation study. The detailed spin polarized occupied electronic structure of $M^{II}[TCNE]^{\bullet-}$ magnets has eluded description from conventional ligand field theory, the results of elementally- or spin-sensitive photon and electron spectroscopies as well as spin resolved density functional calculations. This talk will present heuristic models for M=V, Fe and Ni in the context of the local physical structure and recent less conventional electronic structure studies (UV/Vis MCD), but with a new twist to the onsite and nearest neighbor Coulomb repulsion based correlation.

Electronic Materials and Processing
Room: Southwest Exhibit Hall - Session EM-TuP

Electronic Materials and Processing Poster Session

EM-TuP1 Indium Nitride Epilayer Prepared by UHV- Plasma-Assisted Metalorganic Molecule Beam Epitaxy, ***W.-C. Chen,*** National Applied Research Laboratories, Taiwan, *S.-Y. Kuo,* Chang Gung University, Taiwan, *F.-I. Lai, H.-Y. Wang, W.-T. Lin,* Yuan-Ze University, Taiwan, *C.N. Hsiao*, National Applied Research Laboratories, Taiwan

Indium nitride films grown at various growth temperatures were prepared on GaN buffer layer using self-designed plasma-assisted metal-organic molecule beam epitaxy. The influence of substrate temperature on film crystal structure, surface morphology, optical and electrical properties is studied using x-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM), X-ray diffraction, Hall effect, and photoluminescence (PL) measurements. The results show that all InN films grown on the GaN template have good quality and the full width at half maximum is around 1000 arcsec. At 500ºC, the optical measurements on the films revealed a luminescence feature in the vicinity of 0.7 eV. Also, TEM images of the films exhibit better structural properties indicated by a sharper InN/GaN interface. SEM images determine the growth rate of about 14 nm/min. These results indicate that the optoelectronic properties and crystalline quality can be improved significantly by increasing the growth temperature.

EM-TuP2 The Relationship between Surface Termination and Crystal Structure for HPCVD-grown InN Layers, ***A.R. Acharya***, *M. Buegler, S. Gamage,* Georgia State University, *J.S. Tweedie, R. Collazo,* North Carolina State University, *N. Dietz, B.D. Thoms*, Georgia State University

The surface structure and termination of semiconductor thin films are important factors during epitaxial growth and may affect the interfacial properties of devices. The structure and surface bonding configuration of indium nitride layers grown by high pressure chemical vapor deposition (HPCVD) have been studied using high resolution electron energy loss spectroscopy (HREELS) and X-ray diffraction (XRD). HREELS analysis of InN layers suggests that the surface is primarily terminated with NH2 species. This result is consistent with XRD, which shows the co-existence of different surface orientations. The observed termination by NH2 is in contrast to previous HREELS work on HPCVD-grown InN layers, which showed only NH species on the nitrogen-terminated surface.

EM-TuP3 Rapid Thermal Ex-Situ Activation and Effect on Contacts to p-type GaN, ***J.H. Melby***, *L. Huang, R.F. Davis, L.M. Porter*, Carnegie Mellon University

The difficulty of achieving ohmic contacts to p-type GaN is associated with the inherent difficulties involved in acceptor doping with Mg. Poor doping efficiency results in high contact resistance and high semiconductor sheet resistance. In GaN based devices, these issues lead to parasitic voltage drops and associated Joule heating. When grown via CVD methods a significant amount of Mg forms a complex with hydrogen. This complex prevents Mg from participating in active doping. The challenge is to achieve large concentrations of free Mg in the films. In-situ post-growth annealing has been found to enhance p-type conductivity, but there is a large disparity in activated Mg acceptors versus incorporated Mg atoms. Furthermore, we know of no reports in the literature regarding optimization of the annealing conditions. In this study we have conducted I-V, C-V, Hall, and contact resistance measurements of Ni/Au contacts on Mg-doped GaN films grown on AlN/SiC (0001) substrates as a function of annealing temperature and time, and nitrogen or oxygen concentration for in-situ and ex-situ anneals. We found that in-situ cooling in nitrogen after growth is important for initial activation of Mg dopants; however, additional in-situ annealing in nitrogen after growth had little effect on the electrical properties. We also found that the electrical characteristics are particularly sensitive to the presence of oxygen and temperature during ex-situ annealing; > 200% improvements in hole concentration were observed for annealing in 1:1 N_2:O_2 at 800°C. The electrical data will be correlated with SIMS data of the hydrogen concentration as a function of annealing conditions.

EM-TuP4 Investigation of Crystal Structure and Optical Properties of $Cd_{1-x}Mn_xS$ Epilayers, ***D.J. Kim***, *Y.D. Choi,* Mokwon University, Republic of Korea, *J.W. Lee*, Hanbat University, Republic of Korea

High quality $Cd_{1-x}Mn_xS$ epilayers were grown with changing source temperature on GaAs (111) substrates by the hot-wall epitaxy method. The crystal structure of the grown $Cd_{1-x}Mn_xS$ epilayers was confirmed to be the hexagonal structure by X-ray diffraction pattern (XRD) and scanning electron microscopy (SEM) image. To explore binding states and their potential applications, the hexagonal structured $Cd_{1-x}Mn_xS$ epilayers have been characterized using x-ray photoelectron spectroscopy (XPS). The optical properties of the $Cd_{1-x}Mn_xS$ epilayers were investigated in a wide photon energy range between 2.0-8.5 eV using spectroscopic ellipsometry (SE) at room temperature. The data obtained by SE were analyzed to find the critical points of the pseudodielectric function spectra, $<\varepsilon(E)>=<\varepsilon_1(E)>+i<\varepsilon_2(E)>$, such as E_0, E_{1A}, E_{1B}, E_0', F_1, and E_2 structures. In addition, the second derivative spectra, $d^2\varepsilon(E)/dE^2$, of the pseudodielectric function of $Cd_{1-x}Mn_xS$ epilayers were numerically calculated to determine the critical structures. Four structures, such as E_0', F_1, and two E_2 structures, from 6.0 eV to 8.0 eV were observed with changing Mn composition, for the first time, at 300 K by ellipsometric measurements for the $Cd_{1-x}Mn_xS$ epilayers.

EM-TuP5 Photovoltaic Characteristics of Sputtering-Deposited CdTe Thin Film Solar Cell by Hydrogen Doping Treatment, ***C.-H. Lim***, *S.-H. Ryu, J.-S. Park,* Chosun University, Republic of Korea, *N.-H. Kim,* Chonnam National University, Republic of Korea, *G.-B. Cho, W.-S. Lee*, Chosun University, Republic of Korea

CdTe thin film has the near ideal band gap energy of 1.45 eV for the achievement of the theoretical maximum photovoltaic conversion efficiency of 31%. CdTe thin film also has a high optical absorption coefficient of over 99% of the incident sunlight with only about 2 µm of active thickness. However, the highest conversion efficiency of 16.5% was recorded in the CdTe/CdS heterostructured thin film solar cell . Therefore, the investigations would be strongly required to improve the conversion efficiency with the sufficiently absorbed light. In this study, hydrogen doping treatment was performed with the various hydrogen gas levels and doping temperature in the vacuum desiccator at the fixed doping time in order to improve the efficiency of CdTe/CdS heterostructured cell because the hydrogen affects the electrical properties of CdTe through the fast diffusion of the interstitial hydrogen. The effects of hydrogen doping treatment on the electrical and optical properties of CdTe thin film were investigated by UV-Visible spectrophotometer and Hall effect measurement. The role of hydrogen was examined by some analytical methods including photoluminescence (PL) spectra. The improved cell parameters of CdTe/CdS thin film solar cell were successfully obtained at the optimum condition including short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF), and efficiency. Acknowledgement: This work was supported by National Research Foundation of Korea(NRF) grant funded by the Korean Government(MEST) (20 10-0016048).

EM-TuP6 Crystal Structure Analyses of Bis(triisopropylsilylethynyl)-Pentacene Nanofilms Deposited on OTS-SAM and Poly(3,4-ethylenedioxythiophene) Surfaces, ***S. Kim***, *S. Choi,* Paichai University, Republic of Korea, *C. Yu,* Pohang Accelerator Laboratory, Republic of Korea, *T. Kim,* Paichai University, Republic of Korea, *J.-H. Boo*, Sungkyunkwan University, Republic of Korea

Highly pure 6,13-bis(triisopropylsilylethynyl)pentacene (TIPS-PEN) nanofilms were deposited on a very high quality OTS-SAM surface at two different substrate temperatures (70°C and 90°C) via the vacuum thermal evaporation (VTE) method. X-ray reflectivity (XRR) and grazing angle incidence x-ray diffraction (GID) measurements over a wide temperature range (30°C-284°C) revealed that out-of-plane crystallinity of the film (~10 nm) remains intact but in-plane crystallinity starts to become poor from ~100°C, and to become much worser from 260°C. Atomic force microscope images showed that TIPS-PEN films (~55 nm) prepared at the substrate temperature of 90°C or above commonly have a number of huge cracks between enormous crystal domains (up to 3mm) whereas the films didn't form such morphology below Ts=90°C. These results clearly suggest that an optimum substrate temperature of TIPS-PEN nanofilms on OTS-SAM surface must be somewhere between 70°C and 90°C, and the process temperature must be kept below 90°C in order to form and maintain a highly crystalline film for an organic thin film transistor device since in-plane crystallinity of a semiconductor channel deeply affects the performance of a transistor.

EM-TuP7 Atomic Imaging of Monolayer Nucleation of Atomic Layer Deposition Precursors, *W. Melitz,* ***J. Shen****, J. Clemens, E. Chagarov, A.C. Kummel*, University of California at San Diego

For highly scaled atomic layer deposition (ALD) of gate oxides (EOT < 1nm) on III-V semiconductors, the general requirements for an unpinned, high mobility oxide/III-V interface are as follows: (a) The metal precursor cannot disrupt the substrate during deposition; (b) The metal precursor must form a monolayer of nucleation sites in order for aggressive scaling of the

equivalent oxide thickness (EOT); (c) The oxide has to be resistant to atom donation to/from the substrate; (d) The oxide needs to bond weakly to the interface or to form nearly covalent bonds to the interface to balance polarity. The nucleation/passivation layer has to enable all four requirements. Half cycle room temperature ALD of trimethylaluminum (TMA) and dimethylaluminium ethoxide (DEAE) have been performed on InAs and InGaAs surface to compare two precursors for the same oxide one of which is oxygen-free and one which contains oxygen. The electronic properties of the clean and deposited surfaces are probed via scanning tunneling spectroscopy and microscopy (STS and STM), and Kelvin probe force microscopy (KPFM). Previous STS and KPFM studies for both clean InAs and InGaAs (4×2) surfaces determined the Fermi level is pinned 0.3eV above the valance band; DFT studies show that the surface are pinned by homodimers in the trough. STM and STS show that TMA forms an ordered monolayer of absorbates which unpin the Fermi level suggesting that an ordered monolayer layer might be a requirement for unpinning. However, STM of DEAE reacted InGaAs(001)-(4x2) shows a nearly amorphous monolayer layer while STS shows even this amorphous layer unpins the interface. The influence of larger ligands on the DEAE might account for more degeneracy in bonding configurations making order structures less probable. The results are consistent with a multitude of bonding configuration being able to unpin the Fermi level as long as the pining sites are removed and the presence of oxygen in the precursor not being an impediment to passivation as long as there is still attractive interactions between the absorbates which promote monolayer formation.

EM-TuP8 Synthesis and Magnetic Properties of $Zn_{1-x}Mn_xO$ Hollow Nanospheres,
***D.R. Liu**, T.C. Wu, Y.C. Yeh, W.H. Cho*, National Applied Research Laboratories, Taiwan

ZnMnO is one of the most promising diluted magnetic semiconductors (DMS) materials due to its predicted above room temperature ferromagnetism. In this study, Al_2O_3 layer was conformally deposited on the surface of polystyrene (PS) nanoshpere with different diameter (100nm~800nm) by atomic layer deposition (ALD). After removal of PS nanosphere by heating, Al_2O_3 hollow nanospheres were formed. Then the $Zn_{1-x}Mn_xO$ (x=0.03, 0.05, 0.07) coatings were grown on Al_2O_3 hollow nanospheres by pulsed laser deposition(PLD). According to the results of high-resolution x-ray diffraction, the $Zn_{1-x}Mn_xO$ hollow nanospheres are polycrystalline with a preferential growth direction of (002). The surface and cross-section morphologies of the hollow nanospheres were analyzed using a field-emission scanning electron microscope (FE-SEM). Photoluminescence spectra in applied magnetic field demonstrate ultraviolet emission peaks which have shift with the increase of Mn ion concentration. The magnetic properties of the nanospheres were measured by a superconducting quantum interference device (SQUID) magnetometer and x-ray magnetic circular dichroism (XMCD) spectroscopy. The results show the magnetic properties of $Zn_{1-x}Mn_xO$ hollow nanospheres strongly depend on the Mn composition fraction and the size of nanospheres.

EM-TuP9 Fringing Field effects of Different Size Indium Gallium Zinc Oxide (IGZO) Active Layers Thin Film Transistors,
***J. Noh**, S. Kwon, J.H. Noh,* University of Tennessee, *P.D. Rack*, University of Tennessee at Knoxville; Oak Ridge National Laboratory

To realize the high performance-thin film transistors (TFTs) using amorphous indium gallium zinc oxide (a-IGZO) as the semiconducting active layer, we will present the how the a-IGZO with different active sizes affects the electrical characteristics of TFTs. The TFTs are fabricated with a bottom-gate staggered structure and the a-IGZO active size is photolithgraphically patterned to different lateral dimensions. A Cr gate is deposited on buffered silicon dioxide on a silicon substrate and SiN_x is thegate dielectric which is deposited via plasma enhanced chemical vapor deposition (PECVD). The a-IGZO semiconducting active layers are deposited using rf magnetron sputtering in a reactive Ar-O2 atmosphere which controls the carrier concentration which can be metallic at low oxygen flow rates and insulating at high (>20% O2) flow rates. The a-IGZO layer is patterned with different size by wet etch process with diluted HF. Finally, source and drain electrodes are formed and the device is annealed for activation. We will discuss the TFT characteristics based on fringing electric field effects in which the fringing electric field around the periphery of the patterned source and drain electrodes can induce electrical conduction as current paths in the semiconductor layer, changing electrical properties in the device, especially increasing the leakage current through the backchannel on IGZO. Furthermore, we will correlate the different pattern size of IGZO to the electrical properties of the TFT devices . Finally, we will present a new application for our a-IGZO TFTs: an addressable microfluidic electrowetting channel device.

EM-TuP10 Optical Constant Measurements and Relation to Substrate Currents of Dielectric Layers under Vacuum Ultraviolet Irradiation*,*
D.B. Straight, H. Sinha, J. Lauer, University of Wisconsin-Madison*, N.C. Fuller, S.U. Engelmann, Y. Zhang,* IBM Research*, G.A. Antonelli,* Novellus Systems, Inc.*, Y. Nishi,* Stanford University*, **J.L. Shohet***, University of Wisconsin-Madison

We report an inexpensive and rapid method to measure the reflectance of dielectrics in the vacuum ultraviolet (VUV) range of the spectrum using synchrotron radiation. Porous low-*k* organosilicate (SiCOH) dielectrics deposited on silicon were irradiated with VUV photons of various energies. Reflectance is calculated from ratio of the measured reflected photon flux to the measured incident photon flux. A 90% transmitting nickel mesh connected to a picoammeter was used to measure the incident and reflected photon flux. When the sample is absent from the path of the VUV photons, a photon dump is used to minimize any possible reflectance. Thus, the net photon flux incident on the nickel mesh is the synchrotron flux. Under these circumstances the reading from the picoammeter is proportional to the synchrotron flux. When the sample is present some of the photons are reflected from the sample. Since the sample is placed normal to the VUV photon flux, the reflected photons can travel back to the nickel mesh. Thus, under these conditions, the nickel mesh current is sum of the incident synchrotron photon flux and the reflected photon flux. The reflectance is calculated from the two current measurements. The reflectances of SiCOH of different porosities were compared. By using the Kramers-Kronig algorithm, [1] the index of refraction and the extinction coefficient as a function of energy can be obtained from the reflectance. We also find that during VUV irradiation, the reflectance of a dielectric and the substrate current are inversely correlated. Thus, the reflectance can be obtained from the substrate current and vice versa. We conclude that reflectance or substrate current measurements can determine which photon energies are more likely to be absorbed and can therefore cause dielectric damage during processing. [2] Reducing the flux of deleterious photon energies in processing systems can minimize dielectric damage.

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EM-TuP11 Resistive Switching in Big Band Gap Material- beta - Ga_2O_3,
***S.X. Zheng**, T.C. Lovejoy,* University of Washington*, V. Garcia, S. Ueda,* NIMS, Japan*, A. Pakhomov, M.A. Olmstead, F.S. Ohuchi*, University of Washington

Gallium oxide has a unique combination of properties that hold significant promise for variety applications. Pure beta-Ga2O3 has band gap of 4.8 eV which has potentials as UV-transparant optics material. Recent findings suggest its n-type semiconducting behavior after treating it in reducing atmospheres, which place it in the group of new generation transparent conductive oxides. On the other hand, its conductivity change after gases like CO and NO2 makes it a potential gas sensing material. Despite its unique optic/optoelectronic properties, incomplete mechanistic understanding of the origins of conductivity becomes a barrier to device development. According to recent findings, oxygen vacancy contribution to the conductivity is widely accepted due to inverse correlation of conductivity and oxygen partial pressure during material growth. However, other models were also proposed, e.g, experimental results show trace amount of impurities can enhance the conductivity of Ga2O3 without changing its crystal structure. On the other hand, formation energy calculation suggests possible vacancy alignment along conducting direction can also improve the electron hopping, thus enhance the conductivity. Unfortunately, most of the conclusions were either lack of experimental support, or based on samples prepared from different synthesizing techniques, whose properties can be substantially changed.

In this report, Single crystal beta-Ga2O3 prepared by float zone technique was used to investigate the electrical property change after heating under different atmospheres. It is discovered that by passing direct current through the material in the ultra high vacuum, resistivity of beta-Ga2O3 along [010] direction can have significant increase, which contradicts to the oxygen vacancies model. A detailed investigation using X-ray Photoemission Spectroscopy (XPS), Scanning Tunneling Microscopy (STM), Physical Property Measurement System(PPMS) reveals the change in stoichiometry, work function, surface morphology and polaron hopping dimensions, which bring insight to the origins of conductivity in Ga2O3 along different crystal

orientations. Based on the understanding on the single crystal conductivity, epitaxial Ga2O3 thin film with designated resistive switching properties using Pulse laser deposition can also be prepared.

EM-TuP12 Mass Fabrication of TiO_2-based Resistive Switching Arrays by Step and Flash Imprint Lithography,
***K.D. Kim**, D.K. Yun,* Korea Institute of Machinery and Materials, Republic of Korea*, H.Y. Jeong,* ETRI, Republic of Korea*, J.H. Lee, J.H. Jeong,* Korea Institute of Machinery and Materials, Republic of Korea*, S.Y. Choi,* ETRI, Republic of Korea*, H.H. Park,* KANC, Republic of Korea*, J.H. Choi*, Korea Institute of Machinery and Materials, Republic of Korea

Nanoimprint lithography is a low-cost method of fabricating nanoscale patterns as small as 6 nm. It has been emerged as a key technology for the fabrication of devices with nanoscale patterns, such as polarizer, optical devices, bio devices, and patterned media. The ultraviolet nanoimprint lithography (UV-NIL) process is also a promising alternative to the expensive conventional optical lithographic process for producing non-volatile memory. Resistive random access memory (RRAM), which utilizes the resistance change effect of oxide material, has attracted considerable attention and been widely investigated due to its potential application in memory devices.

In this study, identical patterns and characteristics of sub-100nm TiO_2-based resistive switching systems on 4 inch silicon substrates are demonstrated using Step and flash imprint lithography (SFIL). SFIL is a nanoimprint lithography technique, offering the advantages of a high aspect-ratio, reliable nano-patterns and a transparent stamp that can be used to facilitate overlay techniques. The overlay process from the alignment system in IMPRIO 100 was appropriate for the fabrication of nanoscaled crossbar arrays in this work. Crossbar arrays consisting of TiO_2 resistive switching material sandwiched between Pt and Al electrodes with a width of 80 nm and a half-pitch of 100 nm are in turn replicated through successive imprinting and etching processes. Use of a direct metal etching process enhances the uniformity of the TiO_2/electrodes interface. The electrical property of the crossbar arrays showed the reproducible resistive switching behavior resulting in the application of the nonvolatile resistive memory.

EM-TuP13 Fabrication of Heavy Capacitive Organic Capacitor using All Ink Jet Process,
***I.J. Bae**, J.J. Han, I.S. Chung*, Sungkyunkwan University, Republic of Korea

We attempted to fabricate an organic capacitor on polyethersulphone (PES) substrate using ink jet printing. The capacitor cell was designed for the storage capacitor in E-paper backbone panel. Two different materials like Poly-4-vinylphenol (PVP) and Poly Methyl Methacrylate (PMMA) were examined by varying thickness and w%. The Area of the capacitor was 100 um x 100um. Silver was used as a metal electrode. All the processes were done using ink-jet printer. The dielectric properties were analyzed by measuring C-V, and the physical properties including the morphologies of the ink jet films were analyzed using optical microscope, SPM and SEM.

EM-TuP14 Copper-Electrochemical Mechanical Planarization (Cu-ECMP) Characteristics with a Change of Electrical Variables,
***K.D. Myung**, W.-S. Lee,* Chosun University, Republic of Korea*, N.-H. Kim*, Chonnam National University, Republic of Korea

Electrochemical mechanical planarization (ECMP) process for copper interconnects is an alternative process of the conventional chemical mechanical polishing (CMP) process due to its critical limitation in the recent industrial standards by the high pressure and abrasive. ECMP process dissolved the copper to copper ions for the generation of copper complex layer on the surface electrochemically by applying in an aqueous electrolyte with the electrical source, and then removed the copper complex layer by polishing with the lower pressure. In this study, ECMP was performed with changes of electrical variables including current, voltage, immersing time, size of electrodes, electrode materials, and distance between each electrode. ECMP characteristics such as removal rate, WIWNU%, RMS roughness, and peak-to-valley roughness were measured. The properties of electrolyte were examined as functions of the upper electrical variables in order to estimate the influences of the changed electrolyte on the ECMP characteristics in Cu-ECMP process. The surface of copper was also analyzed with various electrical variables by using XPS and nanoindentation to investigate the surface behaviors with chemical and mechanical properties. Acknowledgement: This work was supported by National Research Foundation of Korea(NRF) grant funded by the Korean Government(MEST) (2010-0016609).

EM-TuP15 Nanoparticle-enhanced Multilayered Thin Film Cooling Devices,
***M. Hines**, C. Cochran, Z. Xiao*, Alabama A&M University

We report the fabrication of solid-state cooling devices using the nanoparticle and Bi_2Te_3 and Sb_2Te_3 multilayered thermoelectric thin films. The multilayer thin films have a periodic structure consisting of alternating Bi_2Te_3 and nanoparticle layeres or Sb_2Te_3 and nanoparticle layers. The Bi_2Te_3 and Sb_2Te_3 thin films were deposited using e-beam evaporation. PbS Nanoparticle thin film was prepared to form the multilayered film using spin coating. The multilayer structure of films and the interface of layers were analyzed by X-ray diffraction and reflection. The multilayer thin films-based cooling devices were fabricated using the microfabrication process. The thermal and electrical properties of the nanoparticle-enhanced multilayered thin films and the cooling temperature difference of the fabricated devices were measured. The measurement results on the nanoparticle-enhanced material systems and the fabricated cooling devices will be reported in the conference.

Graphene Focus Topic
Room: Brazos - Session GR+EM+MS+TF+MI-WeM

Graphene and Carbon-based Devices
Moderator: N.P. Guisinger, Argonne National Laboratory

8:00am **GR+EM+MS+TF+MI-WeM1 Epitaxial Graphene: Effects of Dielectric Overlayers and Device Design on FET Performance**, ***M.J. Hollander***, *R. Cavalero, D. Snyder, M. LaBella, K. Trumbull, Z. Hughes, J. Robinson*, The Pennsylvania State University

The realization of a graphene-based electronic technology necessitates large-area graphene production, as well as the ability to integrate graphene with highly insulating films that act as the gate dielectric in field effect transistors (FETs). Graphene's two dimensional nature allows for phenomenal electronic properties and ultimate scalability, but also makes it susceptible to doping and scattering by charged impurities, dangling bonds, and other defects that may derive directly from choice in gate dielectric and deposition technique. The nature and extent of the effect of the dielectric over-layer on conduction within the graphene channel is of fundamental interest in designing and producing graphene based FETs. Atomic layer deposition (ALD) has proven to be an excellent technique toward the integration of dielectrics with graphene and provides a means to produce high quality films for gate dielectrics at temperatures below 300C, but requires the use of a thin nucleation layer to promote complete coverage and to protect the graphene.

We present results on graphene FETs utilizing various gate dielectrics and various nucleation layers. Graphene was grown epitaxially on 100 mm SiC wafers and processed using standard photolithographic techniques. Al_2O_3 and HfO_2 gate dielectrics were investigated using SiO_2, TiO_2, and Al_2O_3 nucleation layers in various combinations. We show that choice of gate dielectric and nucleation layer can have a dramatic effect on transistor performance and charge carrier mobility. Saturation current, transconductance, and device hysteresis were examined in the fabricated FETs while charge carrier mobility and charge carrier density within the epitaxial graphene were evaluated using Van der Pauw structures. Graphene FETs utilizing Al_2O_3 and SiO_2 seeded dielectrics exhibit the best performance while TiO_2 seeded and unseeded devices exhibit large gate leakage currents resulting in non-functioning FETs. Additionally we provide evidence that the choice of dielectric and seed can significantly impact the Dirac point (minimum conduction), amount of hysteresis, and on/off ratio of the graphene FETs. Trends in saturation current, and transconductance appear be independent of nucleation layer and gate dielectric choice, indicating that conduction through the channel may be limited by mechanisms independent of the nucleation layer and gate dielectric.

In addition to the aforementioned performance metrics, FET performance after continued application of high electric fields across the channel will be reported. Finally, we examine how choice of channel length and width, along with transistor design, effect performance.

8:20am **GR+EM+MS+TF+MI-WeM2 Graphene Oxide on Patterned Self-Assembly Monolayer for Cancer Marker Detection**, ***D.-J. Kim***, *C.Y. Jung, O.J. Yoon, N.-E. Lee*, Sungkyunkwan University, Republic of Korea, *J.-S. Park*, Korea Electronics Technology Institute, Republic of Korea

Graphene, two-dimensional sheet of sp^2-hybridized carbon atom, has received much attention in recent years for many applications such as energy storage and conversion, batteries, fuel cells, optoelectronic device, field-effect transistors, electromechanical resonators, chemical sensors, and biotechnologies. Oxidized form of graphene, graphene oxide, which has functional groups of epoxide, carbonyls, hydroxide, and phenol groups at both sides can also provide various functionalities for biomedical applications because the high densities of defective sites can provide many active sites for electron transfer to biological species, similarly to graphene. In this study, we demonstrate the graphene oxide based immunosensor for cancer marker detection. Graphene oxide pattern was formed selectively on self-assembly monolayer (SAM) pattern formed by using inkjet printing. The hydroxyl terminated ITO electrode was first selectively functionalized by the amine ($-NH_2$) group by inkjet printing of SAM, and the graphene oxide flakes were adsorbed selectively on the SAM pattern. After immobilization of monoclonal antibody to PSA (prostate specific antigen) which is the biomarker in prostate cancer, the electrochemical performance of immunosensor was evaluated by varying the concentration of PSA-ACT (prostate specific antigen/α1-antichymotrypsin) complex. And the PSA polyclonal antibody conjugated with gold nanoparticles was applied to amplification of electrochemical signal because the attachment of nanoparticles onto electrodes drastically enhances the conductivity and electron transfer from the redox analytes. The results showed that graphene oxide based immunosensor can be possibly applied to the delicate diagnosis of various disease markers as well as PSA at the extremely low level and with ultra-high sensitivity.

8:40am **GR+EM+MS+TF+MI-WeM3 Spintronics in Graphene Based Nanostructures**, ***J. Fernández-Rossier***, Universidad de Alicante, Spain **INVITED**

Spintronics in graphene has received attention from two complementary points of view. On one side, the small spin orbit coupling and nuclear spin density suggest that graphene should have very long spin relaxation and decoherence times, which would make it suitable for long distance spin transport and, eventually, for spin-based quantum computing. Although small, spin orbit interaction turns graphene into a spin hall insulator, at very small temperatures, so that the edges of graphene should carry spontaneous spin currents. Independently of the above, the zigzag edges of graphene nanostructures, like graphene ribbons and islands, are predicted to present ferromagnetic spin order due to electron electron coupling. In this talk I will discuss the properties of graphene nanostructures when both the spin-orbit coupling and the Coulomb interactions are included. I will show how the combined action of spontaneous spin order and spin orbit coupling results in persistent charge currents flow in the edges of a variety of graphene nanostructures.

9:20am **GR+EM+MS+TF+MI-WeM5 CVD Gate Dielectrics and Bandgap Engineering of Graphene Layers**, ***W.J. Zhu***, *D. Neumayer, V. Perebeinos, P. Avouris*, IBM T.J. Watson Research Center

Graphene is very promising for electronic devices, particularly for analogue high frequency devices due to its high intrinsic mobility. One challenge in graphene devices is the formation of gate dielectrics on graphene due to its hydrophobic nature. We found a new CVD gate insulator that provides uniform coverage on graphene while preserving the channel mobility, thus making it a very promising gate dielectric for graphene devices. We also studied the channel resistance and the modification of the band structure as a function of the vertical electric field near the Dirac (neutrality) points in the fabricated top-gated graphene devices. We found that as the vertical field increases, in bi-and tri-layer graphenes, the band-gap increases, while in multi-layer graphene, the band-overlap increases. The values of band-gap/overlap in bi-, tri- and multi-layer graphenes were estimated using a simple model which takes into account the variations of the surface electrostatic potential at the Dirac/neutrality point.

9:40am **GR+EM+MS+TF+MI-WeM6 Characterization of Devices Fabricated from Electrostatically Transferred Graphene: Comparison with Epitaxial based Devices**, ***S.W. Howell***, *L.B. Biedermann, T. Ohta, T.E. Beechem, W. Pan, A.J. Ross, D.C. Trotter*, Sandia National Laboratories

In this paper, we present our recent advancements in electrostatically transferring epitaxial graphene (EG) from SiC(0001) and SiC(000-1) to arbitrary glass substrates (including Pyrex). We will compare the electronic properties of electrostatically transferred EG and nominally-equivalent as-grown EG on SiC. These properties are measured using magnetoresistive, four-probe, and field effect transistor geometries. We feel this is a potential enabling technology for integration of graphene with structured and electronically-active substrates, such as MEMS and CMOS.

CVD-grown graphene on Cu has attracted wide interest since it can be readily transferred to arbitrary substrates. However, CVD-grown graphene has been shown to have lower mobilities and smaller domain sizes than EG. EG is difficult to transfer to arbitrary substrates. Currently two techniques exist to transfer EG – a gold/polymer film handle and thermal tape exfoliation [1,2]. While transfer is possible with these techniques, problems exist including contamination and damage, as measured by Raman spectroscopy.

To overcome the issues with the above mentioned transfer techniques, we have developed a technique capable of electrostatically transferring both patterned and chip-scale regions of EG to arbitrary glass substrates. We start with high-quality graphene (mobility 14,000 cm^2/Vs and domains >100 um^2) grown using an Ar-mediated approach [3,4]. In electrostatic graphene transfer, a large electric field is applied between the donor graphene sample (anode) and the acceptor insulating substrate (cathode). This strong electrostatic force deposits graphene on the insulating surface. Electrostatic transfer of EG is a clean technique which, unlike other EG transfer methods, does not contaminate the graphene with adhesive residue or gold contaminates. Both few-layer graphene from SiC(000-1) and monolayer graphene from SiC(0001) have been transferred using this technique.

Our initial attempts at EG transfer have been extensively characterized with Raman spectroscopy and atomic force microscopy. Raman spectroscopy shows that the inherent strain in EG has been partially relaxed. Furthermore, a defect peak (D peak) is frequently not seen in the transferred graphene indicating that the procedure does not significantly damage the graphene film.

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.

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[2] S. Unarunotai *et al. APL* **95**, 202101 (2009)

[3] W. Pan *et al.* submitted to APL (2010)

[4] K. Emtsev *et al. Nature Mat.* **8**, 203 (2009)

10:40am **GR+EM+MS+TF+MI-WeM9 Electron Transport in Dual-Gated Mono- and Bilayer Graphene Devices with High-k Dielectrics**, ***E. Tutuc****, S. Kim, B. Fallah, K. Lee, J. Nah, S.K. Banerjee,* The University of Texas at Austin*, L. Colombo*, Texas Instruments, Inc. **INVITED**

A key issue for graphene-based devices is the deposition of thin high-k dielectric layers combined with a minimum electron mobility degradation. Here we examine the carrier transport in mono and bilayer graphene field-effect transistors with top Al_2O_3 and HfO_2 dielectrics. The high-k dielectric films are grown by atomic layer deposition (ALD), and using a 1nm-thick Al interfacial layer in order to create intentional nucleation centers for the ALD. We show that this deposition technique allows the realization of high mobility graphene devices with aggressively scaled top dielectrics. We investigate the carrier mobility dependence on dielectric thickness and temperature in mono-layer graphene field-effect transistors with high-k dielectrics. The electron transport in dual-gated graphene bilayers with Al_2O_3 top dielectric reveals an interesting band-gap energy dependence on transverse electric field and perpendicular magnetic field in this system.

11:20am **GR+EM+MS+TF+MI-WeM11 In-situ X-ray Photoelectron Spectroscopy Studies of Ozone-based ALD Al_2O_3 Dielectrics on Graphite and Graphene**, ***A. Pirkle****, S. McDonnell,* University of Texas at Dallas*, L. Colombo,* Texas Instruments, Inc.*, R.M. Wallace*, University of Texas at Dallas

We present a study of ozone-based atomic layer deposition (ALD) of Al_2O_3 films on graphene and bulk graphite. Uniform deposition of scalable device-quality high-k dielectrics on graphene is a substantial hurdle for the implementation of conventional FET devices as well as novel device structures exploiting the unique transport properties of graphene. Trimethylaluminum (TMA) / O_3 processes are found to result in uniform Al_2O_3 depositions on graphite and graphene surfaces (1), in contrast to common TMA / H_2O-based processes which result in nonuniform nucleation at defects and step edges.

In order to further examine the nature of interactions between TMA / O_3 and graphene, we utilize *in-situ* x-ray photoelectron spectroscopy (XPS) coupled via a UHV transfer line to an ALD reactor. Morphology of deposited films is also examined *ex-situ* using atomic force microscopy (AFM). We examine the impact of several parameters on Al_2O_3 deposition. Choice of deposition temperature is critical, as etching of graphene by O_3 is observed at elevated temperatures (2) but dielectric quality is degraded at low temperature (3). We also examine the impact of surface condition on Al_2O_3 composition particularly with regard to partially reacted TMA precursor molecules; various surface treatments are employed to approximate realistic device processing conditions. Finally, the effect of variations in purge time between ALD precursor pulses is studied; a reduction in deposition with increased purge time indicates that weakly bonded precursor molecules (TMA and O_3) are easily desorbed from the graphene surface.

This work is supported by the NRI SWAN and MIND centers.

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Thin Film
Room: Dona Ana - Session TF+EM-WeM

High K Dielectrics for Si Electronics
Moderator: S. Gupta, University of Alabama

8:00am **TF+EM-WeM1 Moore's Law - From Simple Scaling to Integrating New Materials and Introducing New Device Architectures**, ***R. Hendel***, Periodic Structures Inc. **INVITED**

Moore's Law has been the driver for semiconductor integrated circuits over more than 40 years. Relentless scaling of dimensions switching provided increasing functionality and performance, resulting in leading edge single chips today that incorporate more than 1 Billion transistors.

All attempts on predicting the end of Moore's Law have been futile – innovations have always allowed continued scaling at reduced cost. However, while Moore's Law appears to be a continuous curve, we rarely reflect on the underlying changes that had to occur to enable this rate of progress. These changes comprised device architecture, the introduction of new materials and break-through processes.

Since Moore's Law describes a learning curve for which cost reduction is central, process simplicity frequently won out over performance advantages if the latter came at high cost. Self-aligned implanted poly-gate over the early metal gate structures is a prime example. Aggressive reduction in the cost per function also provided performance benefits: Smaller transistors switched faster and used less power to do so – truly a win-win situation.

Key innovations along this path were:

· The switch from thermal diffusion doping to implant

· The introduction of CMP, which was key in increasing the number of metal layers that could be integrated.

· The introduction of high-k dielectrics in conjunction with metal gates which addressed the critical gate leakage problem and will allow the introduction of new and better performing channel materials.

Compared to the past, the future will require even more innovation along three potential directions:

· Continuous improvements of current methodologies along existing technologies, consisting of solid engineering and hard work.

Innovations pursued in this category are: highly regular layouts, new channel materials in conjunction with modified hi-k/MG (yet planar) structures.

· Significant changes to traditional device structures and processes.

An example of innovations pursued in this category is the FinFET, which presents significant challenges in materials and processes that must be resolved before introduction into the manufacturing cycle.

· Radical new structures and approaches resulting in major deviation from today's mainstream technologies.

An example is new fundamental circuit components such as the Memristor or new approaches available if considering device operations at cryogenic temperatures (which may be feasible for server farms), allowing the exploration of concepts such as superinsulators.

This presentation will highlight the state-of-the-art in process technology and discuss challenges that require attention and timely solutions.

8:40am **TF+EM-WeM3 Non-destructive Depth Profiles of Hafnium Silicate Films by Angle-Resolved and Variable-Kinetic Energy XPS**, ***C. Weiland****, N. Lorenz, R. Opila*, University of Delaware

High dielectric constant, or high-k films are currently being employed in semiconductor devices. Hafnium silicate ($Hf_xSi_{(1-x)}O_2$) films are a promising material system for such applications, as they combine the high dielectric constant of HfO_2 with the high stability against crystallization of SiO_2. The $Hf_xSi_{(1-x)}O_2$/Si interface must be defect free as defects at this interface can create charge centers which decrease channel mobility. Atomic layer deposition (ALD) is frequently used to deposit high-k films, and provides excellent thickness control and conformality by reacting only one saturating layer of reactant at a time. This work focuses on studying the composition and interface quality of $Hf_xSi_{(1-x)}O_2$ films deposited by ALD using novel silicon precursors and water as the oxidizer. Films are analyzed using non-destructive depth profiles by angle-resolved and variable-kinetic energy X-ray photoelectron spectroscopy (ARXPS, VKE-XPS). In ARXPS, the effective probe depth is varied by changing the takeoff angle between surface and detector. As a complementary technique, VKE-XPS provides depth profiles by adjusting the incident X-ray energy, and thus the corresponding inelastic mean free path of the photoemitted electrons. VKE-XPS also allows the ability to probe deeper into films than conventional lab-based sources, providing the possibility of analyzing thicker films or

entire gate stacks. Using these techniques, we have studied the composition and interface quality of $Hf_xSi_{(1-x)}O_2$ films deposited using various Si precursors. The presence of charge at the interface manifests itself as shifts in the energy of the photoelectron peaks. Using this data, we can determine charge at the high-k/silicon interface as well as measure band offsets.

9:20am **TF+EM-WeM5 Study of SiO_2 and SiN_x Passivation of HfInZnO Oxide Semiconductor Thin Film Transistor**, ***J.C. Lee****, E.H. Lee, J.G. Chung, B. Anass, J.H. Lee, J.S. Park, M.K. Ryu*, Samsung Advanced Institute of Technology, Korea

ZnO based oxide semiconductor is a promising material for thin film transistor which has transparent, high electric mobility, and the advantage of low temperature process. Several kinds of ZnO based oxide semiconductors (InZnO, GaInZnO, HfInZnO, etc.) have been adapted to the active material of thin film transistor. However most of ZnO based oxide semiconductors have very sensitive property to ambient environment. It is essential to prevent the penetration of moisture into ZnO based oxide thin film transistor (TFT). In the purpose of preventing moisture penetration and/or protecting damage from TFT processes, SiN_x or SiO_2 passivation layer is used frequently.

In this study, we investigated the interface reactions between amorphous HfInZnO (Hf:In:Zn= 10:35:55, 40nm thickness) oxide semiconductor active layer and the passivation layer of SiN_x or SiO_2 (20 nm thickness). TEM, XPS and SIMS were used to investigate the interface reactions such as atomic diffusion, reduction of HfInZnO, chemical state, microstructure.

According to experimental results, a SiO_2 phase and Indium metallic state were observed at the interface between SiNx and HfInZnO active layer. On the other hand, there was not observed Indium metallic state at the interfaces between SiO_2 and HaInZnO layers. In the case of SiN_x passivation, it is considered that some Si took oxygen from Indium oxide in HfInZnO and oxidized to SiO_2. And some of Indium oxide reduced to metallic Indium at the interface. Indium diffusions from HfInZnO layers into passivation layers were observed at the both of SiNx and SiO_2 samples. In the case of SiN_x passivation, it was a little bit higher diffusion than that of SiO_2 passivation. The low binding energy shift was observed at the Zn_{2p} XPS spectra at the both samples. However, there was no distinct difference at the Hf_{4d} spectra.

If there is metallic Indium between passivation and HfInZnO active layers, the metallic Indium may influence the conductance of active layer. The threshold voltage (V_{th}) shift of thin film transistor (TFT) could be affected by the change of conductance of active layer.

We observed that the V_{th} negative shift of the TFT used SiN_x passivation was higher than that of SiO_2 passivation. It may be due to the existence of metallic Indium at the interface.

In this report, it will be described the relationships between interface reactions and the property of HfInZnO oxide TFT in detail.

9:40am **TF+EM-WeM6 Capacitance-Voltage (C-V) and X-ray Photoelectron Spectroscopy (XPS) Study of the Effect of a La_2O_3 Layer in the TiN/HfO_2/SiO_2/p-Si Stack**, ***E.J. Bersch****, M. Di,* University at Albany*, S.A. Consiglio, R.D. Clark, G.J. Leusink,* Tokyo Electron America Inc.*, A.C. Diebold*, University at Albany

There has been much attention paid recently to the lowering of the threshold voltage (V_t) that is accomplished by including an additional ultrathin (~5-10 Å) oxide layer in the high-k/metal gate metal oxide semiconductor field effect transistor (MOSFET) gate stack. We have investigated the TiN/HfO_2/La_2O_3/SiO_2/p-Si stack, where the La_2O_3 layer is the so-called V_t-shift layer. For several variations of this stack, where both the thickness and the position of the La_2O_3 layer were systematically varied, we measured two quantities directly related to the V_t, the flatband voltage (V_{fb}) and the Si band bending. The V_{fb} was measured using capacitance-voltage (C-V) measurements on stacks with 500 Å TiN layers, and the Si band bending was measured on sister wafers with 30 Å TiN layers. For a set of samples where the thickness of the La_2O_3 between the HfO_2 and SiO_2 layers was varied, we observed that the V_{fb} and Si band bending both become more negative as the thickness of the La_2O_3 was increased. For a set of samples where position of the La_2O_3 within the HfO_2 layer was varied, we observed that the V_{fb} and Si band bending became less negative as the amount of HfO_2 between the La_2O_3 and the SiO_2 was increased. These observations support the proposition that there is a dipole at the La_2O_3/SiO_2 interface which affects the Si band bending, as has been reported in the literature.[1,2] We have also observed that there is a difference in the V_{fb} and Si band bending in TiN/HfO_2/La_2O_3/SiO_2/p-Si stacks with thermally grown and chemically grown SiO_2 layers. Results of this study as well as one where the thickness of thermally grown SiO_2 layers was varied will be presented, and it implications on the theory of the interface dipole with be discussed.

1. K. Kita, et al., *Appl. Phys. Lett*, 94, 132902 (2009).

2. P.D. Kirsch, et al., *Appl. Phys. Lett*., 92, 092901 (2008).

10:40am **TF+EM-WeM9 Modification of Defect-State Concentrations with Vacuum Ultraviolet and Ultraviolet Irradiation of Hafnium-Oxide Dielectric Layers***,* ***H. Ren****,* University of Wisconsin-Madison*, S.-L. Cheng, Y. Nishi,* Stanford University*, J.L. Shohet*, University of Wisconsin-Madison

The effects of 7.2 eV vacuum ultraviolet (VUV) and 4.9 eV ultraviolet (UV) irradiation on a 20 nm HfO2 layer atomic layer deposited (ALD) on (100) Si substrate are explored with electron-spin resonance (ESR). Silicon dangling-bond defect concentrations (*Pb* centers) and positively charged oxygen vacancies (*E*' centers) were measured with *g*-factor fitting. The concentrations of the defect states are presented. VUV irradiation increases the level of *Pb0* and *Pb1* states, while UV decreases the level of *Pb0* and *Pb1* states, but increases the level of *E*' states significantly. [i] [#_edn1] In addition, rapid thermal annealing (RTA) mitigates the effects of both VUV and UV irradiation. Surface-potential measurements with a Kelvin probe show that electron photoemission process dominate VUV irradiation. On the other hand, electrons are transferred from *E*' states to the silicon substrate during UV irradiation. At the same time, electrons are photo-injected into the dielectric layer from the substrate. Furthermore, VUV spectroscopy measurements show that the Fermi level for *E*' defect states is around 4.7 eV, which is within the bandgap of the dielectric layer. Also, previous work [ii] [#_edn2] shows that the E' states, as oxygen-interstitial defects (OID), are located within the HfO2 layer. We conclude that VUV irradiation modifies the concentrations of the silicon dangling-bond defect states and UV irradiation can be a potential source for positively charge oxygen vacancies during the processing.

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[i] [#_ednref] H. Ren, S.L. Cheng, Y. Nishi and J.L. Shohet, *Applied Physics Letters* (to be published)

[ii] [#_ednref][ii] J.L. Lauer, J.L. Shohet and Y.Nishi, *Applied Physics Letters* **94**, 162907 (2009)

11:00am **TF+EM-WeM10 Plasma Enhanced Atomic Layer Deposition of Ruthenium Ultra-Thin Films for Advanced Metallization***,* ***J. Swerts****, S. Armini, L. Carbonell, D.A. Annelies, F.A. Alexis, S. Mertens, T. Witters, M. Schaekers, Z. Tőkei, G. Beyer,* IMEC, Belgium*, V. Gravey, A. Cockburn, K. Shah, J. Aubuchon,* Applied Materials Inc.*, S. Van Elshocht*, IMEC, Belgium

Electrochemical deposition of Cu for interconnect metallization traditionally uses Physical Vapor Deposition (PVD) of a Cu seed layer on top of a PVD Ta/TaN barrier to conduct the current. However, the limitations of PVD in respect of step coverage compromise its use in future technology nodes. Atomic Layer Deposition (ALD) for barrier deposition combined with seedless Cu electroplating is one of the metallization routes explored for sub-25 nm line widths. However, compatibility with seedless electroplating seriously limits the choice of materials. Among the different candidates, Ru-based layers have been identified as very promising.

We report the growth and scalability of Ru films by plasma-enhanced ALD (PE-ALD) from MethylCyclopentadienylPyrrolylRuthenium (MeCpPyRu) and N_2/NH_3 plasma. The layers were deposited using a 300 mm showerhead type reactor (AMAT) with direct plasma capability. The substrate temperature during deposition was 330C. The Ru growth per cycle was 0.04 nm. As substrates we used Si wafers with 100-300 nm SiO_2 on which a thin TaN or TiN layer was deposited by ALD or PVD.

The metal nitride is needed as a growth enabler since Rutherford backscattering spectrometry (RBS) showed that only 1E14 Ru atoms/cm^2, i.e. less than a monolayer, were deposited on SiO_2 after 120 PE-ALD cycles. The minimal thickness of the metal nitride to enable Ru growth has been determined to be as low as 0.7-0.8 nm which is promising for scaling. Growth studies on scaled and thick ALD TiN or TaN still showed a limited growth inhibition during the first 40 cycles followed by a linear growth behavior. Static time-of-flight secondary ion mass spectroscopy (TOFSIMS) suggests Ru layer closure for a film thickness around 2 nm.

Atomic force microscopy revealed that the root mean square roughness values were below 0.4 nm for film thicknesses up to 20 nm. X-ray diffraction showed that the Ru layers have a hexagonal structure. The density of the Ru layer was 11.75 g/cm^3 as derived from X-ray reflectivity and RBS. Elastic recoil detection analysis and TOFSIMS indicate that the N, O, C-levels in the bulk Ru layers were << 1%. Surface analysis by static TOFSIMS showed the presence of organic contamination identified as MeCp ligands from the Ru precursor. In contrast, the Pyrrolyl ligand was not observed. A post deposition thermal treatment of the Ru film removes the ligand organic contamination. The impact of this surface contamination on the seedless Cu electroplating efficiency will be discussed. Finally, the

step coverage of TiN/Ru and TaN/Ru stacks in narrow lines (65-15 nm width) was evaluated by transmission electron microscopy.

11:20am **TF+EM-WeM11 Effects of Hydrogen Plasma Pretreatment on Superconformal Gap-Filling of Cu-Al Alloy**, ***H.K. Moon***, *N.-E. Lee*, Sungkyunkwan University, Republic of Korea

As the feature of microelectronic interconnects has continued to shrink, Cu resistivity is expected to increase at the nanoscale due to increased surface and grain boundary scattering of electrons. To prevent increase of the resistivity in nanoscale interconnects, alloying Cu with other metal elements such as Al, Mn, and Ag is being considered to increase the mean free path of the drifting electrons. The formation of Al alloy with a slight amount of Cu broadly studied in the past. The investigation of Cu alloy with a very small Al fraction, by contrast, recently started. The formation of Cu-Al alloy is limited in wet chemical bath and was mainly conducted for fundamental studies by sputtering or evaporation system. However, these deposition methods have a limitation in production environment due to poor step coverage in nanoscale Cu metallization. In this work, gap-filling of Cu-Al alloy was conducted by cyclic MOCVD (metal organic chemical vapor deposition), followed by thermal annealing for alloying, which prevented an unwanted chemical reaction between Cu and Al precursors and hydrogen in the gas phase. To fill the Cu-Al alloy into sub-100nm trench without overhang and void formation, furthermore, hydrogen plasma pretreatment of the trench pattern with Ru barrier layer was introduced in order to suppress of Cu nucleation and growth near the entrance area of the nano-scale trench by minimizing adsorption of metal precursors. As a result, superconformal gap-fill of Cu-Al alloy could be achieved successfully in the 40-nm trench with an aspect ratio of 4. Examined morphology, microstructure, chemical composition, and electrical properties of superfilled Cu-Al alloy will be discussed in detail.

11:40am **TF+EM-WeM12 Depth Resolved Cathodoluminescence Spectroscopy of Amorphous High-*k* Dielectric $LaLuO_3$**, ***S. Shen***, Ohio State University, *Y. Liu*, *R.G. Gordon*, Harvard University, *L.J. Brillson*, Ohio State University

We have used depth-resolved cathodoluminescence spectroscopy (DRCLS) to measure the native point defects and reaction-induced defects within ultrathin $LaLuO_3$ dielectric films. The rare earth oxide $LaLuO_3$ is gaining much attention because of its high dielectric constant (28 ~ 32) and its potential application to replace SiO2 as a gate dielectric for Si microelectronics, requiring both sub-nanometer thick gate oxide layers and low leakage currents. $LaLuO_3$ deposited by atomic layer deposition (ALD) provides films with high crystallization temperature and relatively high conduction band offset, but they have non-negligible leakage currents that are attributed to electronic trap states in the band gap. Annealing can partially reduce these traps but can also induce diffusion/reaction at the $LaLuO_3$ interfaces. We used DRCLS to determine the changes in defect levels of WN/20 nm $LaLuO_3$/Si gate structures as a function of annealing and the introduction of an Al_2O_3 diffusion barrier at the Si interface. A 10 nm WN/20nm $LaLuO_3$/Si structure as-grown exhibits defect emissions at 2.4, 3.2, 3.8, 4.2 and 4.7 eV as well as a 5.48 eV band gap. With 300ºC cyclic annealing, 10 nm WN/20nm $LaLuO_3$/Si, the band gap emission is absent and high energy emissions at 4.2 and 4.7 eV shift to 3.8 eV. A 10 nm WN/20nm $LaLuO_3$/0.4 nm Al_2O_3/Si interlayer structure exhibits negligible difference from the interlayer-free stack without anneal. However, with annealing, the WN/20nm $LaLuO_3$/0.4 nm Al_2O_3/Si defects at high energy and the band gap remain unchanged while the lower energy defects are suppressed. The 5.48 eV band gap emission agrees with an internal photoemission gap of 5.3 eV measured previously. The 4.2 and 4.7 eV emissions are consistent with weighted density function approximation calculations showing two oxygen-vacancy-related states at similar energies near the $LaLuO_3$ conduction band edge. The DRCLS–measured degradation of optical features with annealing of the interlayer-free structure is attributed to Si diffusion and reaction with $LaLuO_3$ as observed by cross sectional TEM. This degradation is suppressed with the Al_2O_3 barrier layer. Furthermore, the annealing of the interlayer structure reduces all the low energy defect emissions. Finally, the highest lying state at 4.7 eV above the valence band (0.78 eV below the conduction band) agrees reasonably well with the 0.6-0.7 eV electrical measurements of leakage current. These results highlight the importance of annealing with a diffusion barrier at the Si interface to suppress defects within $LaLuO_3$ without Si reaction at the $LaLuO_3$ interface.

Electronic Materials and Processing
Room: Dona Ana - Session EM+SS-WeA

High-k Dielectrics for III-V Electronics
Moderator: A.C. Kummel, University of California at San Diego

2:00pm **EM+SS-WeA1 High-k III-V MOSFETs Enabled by Atomic Layer Deposition**, ***P. Ye***, Purdue University **INVITED**

2:40pm **EM+SS-WeA3 Passivation of Al_2O_3/InGaAs(100) Interfaces by Atomic Layer Deposition and Annealing**, ***F.L. Lie***, *B. Imangholi*, University of Arizona, *W. Rachmady*, Intel Corp., *A.J. Muscat*, University of Arizona

Identification of the source of interfacial defects between high-k films and III-V substrates is crucial for developing passivation methods. Efforts have been made to isolate defects based on a specific chemical moiety at an interface. A study reported that doubly-O coordinated Ga and displaced As formed when GaAs is exposed to oxygen, induces mid-gap states[1]. Another study suggested that high activity interface defects originate from structural disorder instead of specific chemical moieties[2]. This project aims to understand the nature of Al_2O_3/InGaAs interface defects by relating composition to electrical performance. The modification of InGaAs(100) surfaces due to surface cleaning, Al_2O_3 deposition, and post deposition annealing (PDA) was investigated using capacitance-voltage (CV) curves, large AC signal conductance (LSC), and x-ray photoelectron spectroscopy (XPS). Al_2O_3 films were deposited by atomic layer deposition (ALD) using trimethylaluminum (TMA) and water precursors on native oxide covered and aqueous HF etched InGaAs(100) surfaces. XPS analysis on a native oxide sample revealed ~8Å oxide (52% As, 29% Ga, and 21% In) and a monolayer excess of As on an As-terminated substrate. TMA reacted on this surface during ALD, thinning the oxide to ~4.2 Å (45% As, 29% Ga, and 27% In). Aqueous HF treatment removed the native oxide and produced an As-rich surface, which re-oxidized in air. Surfaces consisted of ~4.2 Å oxide (91% As) and 1.5 monolayer excess As on an As-terminated surface. ALD Al_2O_3 on the liquid-cleaned surface produced a chemically sharp Al_2O_3/InGaAs interface with less than a monolayer of As oxide. CV and LSC measurements were performed on Au/Ni/10 nm Al_2O_3/InGaAs stacks. The deep-level surface recombination velocity (SRV) values extracted represent the net effect of interface defects, which includes the defect density and capture cross section. The similar SRV values obtained for native oxide (34$\pm$6 cm/s) and aqueous HF (29$\pm$13 cm/s) prepared surfaces suggest that the presence or absence of oxides was not the only determining factor. PDA in forming gas and NH_3 ambients significantly improved the electrical quality, as reflected in SRV values of 1 to 5 cm/s for both surfaces. XPS analysis showed increased excess As and Ga_2O_3 at the interface of both surfaces, likely due to thermally or H-induced reactions between interfacial As oxide and Ga atoms in the substrate. These results suggest that high activity defects in III-V's could be associated with interfacial dangling bonds and are amenable to standard passivation methods used in Si technology.

[1]Hale M. J. et al, J. Chem. Phys. 119(13), 2003

[2]Caymax M. et al, Microelectron. Eng. 86, 2009

3:00pm **EM+SS-WeA4 An In Situ Examination of Atomic Layer Deposited Al_2O_3/InAs(100) Interfaces**, ***A.P. Kirk***, *M. Milojevic, D.M. Zhernokletov, J. Kim, R.M. Wallace*, University of Texas, Dallas

An in situ half-cycle atomic layer deposition/X-ray photoelectron spectroscopy (ALD/XPS) procedure was conducted in order to learn more about the evolution of the Al_2O_3 dielectric interface with undoped InAs(100). Without breaking vacuum, monochromatic XPS was used to examine the InAs(100) surface following ammonium sulfide passivation or ammonium hydroxide etching and then after each individual ALD pulse of trimethyl aluminum (TMA) and deionized water (DIW) precursors (e.g. single TMA pulse/XPS scan; single DIW/XPS scan; etc.). Ammonium sulfide was more effective at minimizing native oxides than ammonium hydroxide. Regardless of chemical cleaning technique, after depositing up to 1 nm of Al_2O_3, elemental arsenic (As^o or As-As bonds) remained at the interface which may have adverse implications for devices such as metal oxide semiconductor field effect transistors (MOSFET). After heating to 300 °C (typical ALD reactor temperature), As-S bonding was reduced below the XPS detection limit. The In^{1+} chemical state (e.g. In_2O) was preserved while trivalent In and As oxidation states were minimized following exposure to TMA. The chemical reaction pathways appear to be similar to that observed for GaAs and InGaAs. We will also present electrical characterization studies and examine the correlation to the in situ interface analysis.

4:00pm **EM+SS-WeA7 Fermi-level Unpinning of $HfO_2/In_{0.53}Ga_{0.47}As$ Gate Stacks using Hydrogen Anneals**, ***R. Engel-Herbert***, *Y. Hwang, N.G. Rudawski, S. Stemmer*, University of California, Santa Barbara

Compound (III-V) semiconductors are currently being investigated to replace Si as channel material in metal oxide semiconductor field effect transistors. A significant challenge is the high trap density (D_{it}) at the dielectric/III-V semiconductor interface, causing Fermi level pinning. Recently, it has been reported that the D_{it} can be reduced by sulfur passivation and hydrogen annealing for $Al_2O_3/In_{0.53}Ga_{0.47}As$ interfaces.

In this presentation, we will present our studies of the effect of forming gas anneals on the electrical properties of $HfO_2/In_{0.53}Ga_{0.47}As$ metal oxide semiconductor capacitors . HfO_2 films with thicknesses between 9 and 18 nm were deposited in-situ on As-decapped n-type $In_{0.53}Ga_{0.47}As$ channels by chemical beam deposition using hafnium *tert*-butoxide (HTB) as the source. Samples were post-deposition annealed in forming gas. For comparison samples annealed in nitrogen were also studied. Capacitance-voltage (CV) and conductance-voltage (GV) curves were measured at room temperature. The interface trap density D_{it} was quantified using both the Terman and the conductance methods. The conductance method showed that the D_{it} was reduced from $1.3X10^{13}cm^{-2}eV^{-1}$ to $8X10^{12}cm^{-2}eV^{-1}$ near midgap. The conductance peak shifted in frequency with a change in negative gate voltage, consistent with an unpinned Fermi level. The 1 MHz CV curve reached the calculated minimum capacitance value, indicating Fermi level unpinning. The nitrogen annealed control sample did not reach the minimum capacitance and the conductance peak shift at negative bias was moderate, indicating Fermi level pinning at midgap. We will also present comparisons of the extracted band bending for both nitrogen and forming gas annealed stacks and discuss the mechanisms by which forming gas anneals can reduce the midgap D_{it}.

4:20pm **EM+SS-WeA8 Valence Band Alignment in low-k Dielectric/Cu Interconnects as Determined by X-ray Photoelectron Spectroscopy**, ***S. King***, *M. French, M. Jaehnig, M. Kuhn*, Intel Corp.

Electrical leakage in low-k/Cu interconnect structures is becoming a growing vital concern as the nano-electronics industry moves to increasingly tighter metal spacing's for sub 22 nm technology nodes and continues to replace dense SiO2 dielectrics with low density / porous SiOC:H "low-k" dielectric materials. In order to understand the various possible leakage mechanisms in low-k/Cu interconnects, a knowledge of the basic band alignment between Cu and low-k dielectric materials is needed but has gone largely unreported. In this regard, we have utilized X-ray Photoelectron Spectroscopy (XPS) to measure the Valence Band Alignment and Schottky Barrier at interfaces of importance to Cu/low-k interconnects. XPS has been used extensively for determining the band alignment of numerous semiconductors to other semiconductors, metals, and dielectrics. In this paper, we demonstrate that XPS can also be utilized to determine the band alignment at interfaces between amorphous dielectrics and metals of interest to the low-k/Cu interconnects industry. Specifically, we have utilized XPS to determine the Schottky Barrier between Cu and low-k dielectric SiC and SiCN capping layers deposited on Cu via Plasma Enhanced Chemical Vapor Deposition (PECVD). We have also utilized XPS to determine the valence band alignment at SiCN:H/SiOC:H interfaces. Lastly, the impact of various plasma surface treatments on the band alignment at these interfaces was also investigated.

4:40pm **EM+SS-WeA9 III-V CMOS: A sub-10 nm Electronics Technology?**, ***J.A. del Alamo***, Massachusetts Institute of Technology **INVITED**

CMOS scaling is at the heart of the microelectronics revolution. The ability of Si CMOS to continue to scale down transistor size while delivering enhanced performance is becoming increasingly difficult with every generation of technology. For Moore's law to reach beyond the limits of Si, a new channel material with a high carrier velocity is required. A promising family of materials for this is III-V compound semiconductors.

III-Vs are well known for their unique suitability for high frequency electronics. III-V-based integrated circuits are currently in use in a variety of communications and defense applications. The prospect of III-Vs entering the logic roadmap is tantalizing. This work reviews some of the critical issues.

The barrier for insertion of a new channel material into the CMOS roadmap is huge. Any new technology has to beat Si designs in performance at

device footprints that allow the integration of billions of transistors on the same chip. In addition, cost-effective manufacturing must be realized.

To make this work, a III-V CMOS technology has to solve a number of challenging technical problems. The development of a gate stack that includes a high-K dielectric and yields a high-quality semiconductor interface with a III-V compound semiconductor is up there as one of the greatest and most fascinating problems in modern semiconductor technology. Recent research suggests that this is an eminently attainable goal. Transistor size scalability is also a major worry. Will it be possible to scale future III-V transistors to the required dimensions while preventing excessive short-channel effects and attaining the demanding parasitic resistance objective? This is a topic that will call for extensive experimental and simulation research. Fortunately, calibrated simulators today reproduce quite well the characteristics of 30 nm gate length III-V FETs and should be valuable in projecting to devices in the 10 nm range. If planar device designs are unsuitable, 3D designs might offer a viable path. Recent 3D device demonstrations with impressive characteristics give hope that this is a promising strategy. A future III-V CMOS technology will also have to "look and feel" as much as Si as possible. This calls for the formation of thin high-quality III-V layers on top of large Si wafers. In fact, depending on what emerges as the best option for the p-channel device, a major challenge in itself, two dissimilar materials might need to be integrated side by side in very close proximity on top of a Si wafer. These are all great problems that will require the coordinated attention of scientists and technologists with expertise in many different domains.

5:20pm **EM+SS-WeA11 Potential Profiles of III-V MOSCAPs with Kelvin Probe Force Microscopy *In Situ*, *W. Melitz*,** *J. Shen, S. Lee, J.S. Lee, A.C. Kummel,* University of California at San Diego*, S. Bentley, D. Macintyre, M. Holland, I. Thayne*, University of Glasgow, UK

Cross-sectional scanning probe microscopy (SPM) is an imaging technique which can map the potentials inside an operational MOSCAP or MOSFET device. Kelvin probe force microscopy (KPFM) measures the contact potential difference (CPD) of a conductive cantilever and a sample surface with a precision of better than 10 meV. In cross-sectional KPFM, (X-KPFM) a fully functional MOSFET or MOSCAP is cleaved in UHV, and the potential inside the working device is measured in two-dimensions; UHV cleaving is critical to preserve an oxide-free surface so the unperturbed potentials can be measured. Cross-sectional KPFM can determine the effect of surface passivation of the gate oxide in operational devices, influence of the fixed charge in the gate oxide with semiconductor channel material, structural features and their effects on the potential distribution, and even work function offsets of the gate and semiconductor. The biggest challenges in imaging cleaved devices is obtaining good cleaves and finding the structure of interest while maintaining good tip conditions for high resolution. Using a comb structure for the electrodes increases the density of the devices on the cleave face to increase the number of working devices. The cleave edge of the sample drastically affects the stability of the cantilever. In order to increase the stability, the devices were embedded in a >300nm insulator; therefore, the device of interest in not located directly on the edge face. Using this capping technique, high spatial resolution in a UHV cleaved MOSCAP with KPFM shows the amount of band bending in the semiconductor channel caused by the fixed charge in the oxide. High resolution KPFM has also been demonstrated for a range of external gate biases, illustrating the flexibility of KPFM for investigating MOS devices. Current efforts focus on implementing KPFM into patterned scaled MOSCAP and MOSFET devices.

Nanometer-scale Science and Technology
Room: La Cienega - Session NS+EM+EN-WeA

Photonic and Plasmonic Materials and Devices
Moderator: P. Cheng, Cornell University

2:00pm **NS+EM+EN-WeA1 Spatially-Resolved Study of Luminescence and Composition in III-Nitride Nanowires*, G.T. Wang*,** *Q. Li*, Sandia National Laboratories

Given the strong interest in III-nitride-based nanowires for optoelectronic and energy applications, a better understanding of their optical properties and structure-composition is required, particularly at nanoscale spatial resolutions, which could shed light into issues such as the nature and distribution of radiative defects and alloy compositional variations. Here, we present a spatially-resolved, correlated study of luminescence and composition in GaN, Al(Ga)N/GaN, and InGaN/GaN core-shell nanowires grown by metal-organic chemical vapor deposition. For GaN nanowires, a surface layer exhibiting strong yellow luminescence (YL) near 566 nm in the nanowires was directly revealed by high resolution, cross-sectional cathodoluminescence (CL) imaging, compared to weak YL in the bulk. In contrast, other defect related luminescence near 428 nm (blue luminescence) and 734 nm (red luminescence), in addition to band-edge luminescence (BEL) at 366 nm, were observed in the bulk of the GaN nanowires but were largely absent at the surface. As the nanowire width approaches a critical dimension, the surface YL layer completely quenches the BEL. The surface YL is attributed to the diffusion and piling up of mobile point defects, likely isolated gallium vacancies, at the surface during growth. AlGaN/GaN and AlN/GaN core-shell nanowires were observed to exhibit stronger BEL and weaker YL as compared with bare GaN nanowires, which may relate to the passivation of nanowire surface states. InGaN/GaN core-shell nanowires were also investigated by correlated CL and cross-sectional scanning TEM (STEM). Dislocation-free InGaN layers with up to ~40% indium incorporation were achieved on GaN nanowires. The indium composition distribution in the InGaN layers were qualitatively correlated to the strain energy density distribution as calculated by finite element analysis models. The observed high indium incorporation and high crystalline quality in the heteroepitaxial InGaN layers is attributed to strain-relaxed growth on the nanowires. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

2:20pm **NS+EM+EN-WeA2 Photonic Crystal Cavities and Vertical Confinement to Increase the Conversion Efficiency of a Thermophotovoltaic Cell*, C. Shemelya*,** *T. Vandervelde*, Tufts University

For many years researchers have attempted to efficiently harvest waste heat and transform it into a usable energy via thermophotovoltics (TPVs). The low quantum efficiency (QE; i.e. the probability that a photon will be absorbed) in most TPV cells is probably the biggest limiting factor in achieving an economically viable device and directly affects the conversion efficiency (CE; i.e. the probability that a photon will be converted into a carrier that is collected). In many cases, top of the line TPV cells might only have a CE of 20%. Recent advances in micro-/nano-fabrication techniques have enabled the creation of novel structures to enhance the absorption and, therefore, the conversion of the incident thermal photons. In particular, photonic crystals (PhC) interface enhancements have been shown to increase the efficiency of photon to current conversions for infrared photodetectors. The addiction of a back reflecting layer, or vertical confinement layer can further increase conversion efficiencies. Here, we report on the enhancement of photon conversion by integration of PhC structures and vertical confinement layers into the TPV cells. To this end, photonic crystals consisting of rods of either air or dielectric surface-passivation material are placed into the base semiconductor TPV cells to increase duration of thermal photon absorption, resulting in significantly enhanced QE and CE. The use of photonic crystals and vertical confinement in augmenting the conversion efficiency of TPV cells is applicable for most IR wavelengths, making this a widely useful technology. The ability to harvest waste heat for energy will help make many processes and/or systems more energy efficient, which will be a critical component in ushering in an era of energy independence.

2:40pm **NS+EM+EN-WeA3 Unconventional and Broadband Plasmonics*, T.W. Odom*,** Northwestern University **INVITED**

Breakthroughs in photonics and optoelectronics demand actively controlled materials that are inexpensive, robust, and scalable. The interaction of light with surface plasmons—collective oscillations of free electrons—in metal nanostructures has resulted in exceptional displays of enhanced optical transmission, collimation of light through a subwavelength aperture, and negative permeability and refraction at visible wavelengths. The structures that display these phenomena typically consist of ordered arrays of particles or holes with sizes of the order 100 nm. Surface plasmons can interact with each other over much longer distances, however, and thus the ability to organize nanoscale materials over multiple length scales could lead to new plasmonic metamaterials with novel optical properties.

This talk will describe how superlattices and low symmetry plasmonic lattices provide an important first step to meet these goals. We will introduce new soft nanolithography tools for creating new plasmonic structures, including PEEL (a procedure combining **P**hase-shifting photolithography, **E**tching, **E**lectron-beam deposition, and **L**ift-off) and solvent assisted nanoscale embossing (SANE). These methods can achieve arrays of 50-nm features simultaneously over 6-in2 areas without needing electron, ion, or photon-based lithographies. We will then discuss how the optical properties of the plasmonic crystals and the nanoparticle arrays can be engineered and then manipulated by external factors to produce large optical responses.

4:00pm **NS+EM+EN-WeA7 Controlling Plasmon Enhanced Photoconduction in Porphyrin-Gold Nanoparticle Assemblies**, ***D.J. Conklin***, *S.U. Nanayakkara, T.-H. Park,* University of Pennsylvania*, J.T. Stecher, M.J. Therien,* Duke University*, D.A. Bonnell*, University of Pennsylvania

Recently we demonstrate plasmon-induced electronic transport in hybrid metal nanoparticle-molecular devices that realized enhancements of up to a factor of 200. This was realized in a hybrid structure that consists of an array of gold nanoparticles linked by (porphinato)zinc(II) oligomers. Here we examine the role of metal particle size, spacing, molecular length and radiation power on the photoconductive properties. Controlling these parameters allows the relative roles of nano antennae focus increasing effective photon flux and hot electron distribution to the current enhancement to be compared.

This phenomenon offers a pathway to selectively enhance specific optical energies or to design a hybrid structure that can simultaneously enhance a range of optical wavelengths. Applications in optical devices and a range of photovoltaics could exploit this new phenomenon [ACS Nano, 2010, 4 (2), pp 1019-1025] .

4:20pm **NS+EM+EN-WeA8 From Red-Coloured Coatings to Light Trapping in Solar Cells: on the Tunability and Control of the Surface Plasmon Resonance Behaviour**, ***M. Creatore***, *H. Takeke Beyene, M. Ponomarev, M.C.M. van de Sanden*, Eindhoven University of Technology, Netherlands

The combination of (noble) metal nanoparticles (NPs) with dielectrics is an on-going research subject, due to the generated surface plasmon reasonance (SPR) effect, relevant in several technological applications such as color filters, optical switching devices and sensors, to name a few.

In this contribution, we report on the tunability and control of the surface plasmon resonance behaviour through the engineering of metal NP/dielectric interfaces for two applications, i.e. thickness- and viewing angle- independent red- coloured decorative coatings and light trapping enhancement in silicon- based tandem thin film solar cells. Both studies have been carried out by making use of a vacuum chamber where plasma-enhanced chemical vapour deposition for the dielectric layer and magnetron sputtering for the metal NP deposition are combined.

Multilayer structures composed of gold NPs sandwiched between SiO_2 layers represent a valid solution for the independent control of NP size and density: while a constant NP size guarantees a narrow surface plasmon frequency, an increased NP density leads to an enhancement in the absorption [1]. A multi-diagnostic approach consisting of spectroscopic ellipsometry, transmission electron microscopy and Rutherford backscattering analysis has allowed the characterization of the deposited coatings: gold NPs (diameter 10-15 nm) with a surface area coverage of 26% and sandwiched between 40 nm- thick SiO_2 layers, exhibit a red colour, whereas the color intensity (i.e. from cool to warm deep red) increases with the layer number, i.e. NP density.

While in this first application the main mechanism contributing to extinction is *absorption*, for an efficient sun light management/ trapping within a solar cell, *scattering* plays a dominant role. In particular, for amorphous (a-Si:H)/microcrystalline (μc-Si:H) silicon tandem solar cells a promising approach consists in the incorporation of an intermediate layer (e.g. ZnO) sandwiched between the top a-Si:H and the bottom μc-Si:H cell, able to efficiently scatter photons of a specific frequency range back to the top cell or forward to the bottom cell. In this respect, copper NPs (30-150 nm diameter) when coupled to ZnO layers, are responsible for the generation of a plasmon peak at 700 nm, which shifts towards higher wavelengths with an increase in NP size, therefore showing its potential towards low energy photon forward scattering into the bottom μc-Si:H cell.

[1] H. T. Beyene, F.D. Tichelaar, P. Peeters, I. Kolev, M.C.M. van de Sanden, M. Creatore, accepted for publication in Plasma Processes and Polymers (2010).

4:40pm **NS+EM+EN-WeA9 Index-Matching at the Nanometer Scale**, ***G. Broenstrup***, *C. Leiterer, N. Jahr, B. Hoffmann, F. Talkenberg,* Institute of Photonic Technology, Germany*, S.H. Christiansen*, Max Planck Institute for the Science of Light, Germany

Silicon nanowires (SiNW) show high potential as future building blocks for photonic devices. They show strong resonant enhancement effects resulting in high absorption efficiencies and even higher scattering efficiencies. Since both effects are based on the same underlying physical principles the resonant enhancement of the absorption as well the resonant enhancement of the scattering of light occurs at the same wavelength. These large scattering efficiencies could result in an increased reflectivity of structures based on these SiNWs.

To overcome the increased scattering efficiencies we show an index matching core-shell approach.

The SiNWs are wrapped with a thin oxide layer with a refractive index smaller than the refractive index of silicon. The thickness of the wrapping layer is formed using atomic layer deposition (ALD), which allows to control the thickness of the layer at the Angstrom scale. The microstructure is analyzed using transmission electron microscopy (TEM).

The scattering behavior of these individual SiNWs with an oxide layer are measured using an optical microscope with a coupled spectrometer. The experimental data is analyzed using an extended Mie theory.

It will be shown, that this method can be used to tune the absorption efficiencies and the scattering separately to different wavelengths.

5:00pm **NS+EM+EN-WeA10 20 μs Photocurrent Response from Lithographically Patterned Nanocrystalline Cadmium Selenide Nanowires**, ***S.-C. Kung***, *W.E. van der Veer, F. Yang, K.C. Donavan, R.M. Penner*, University of California, Irvine

Lithographically patterned nanowire electrodeposition (LPNE) provides a method for patterning nanowires composed of nanocrystalline cadmium selenide (*nc*-CdSe) over wafer-scale areas. We assess the properties of (*nc*-CdSe) nanowires for detecting light as photoconductors. Structural characterization of these nanowires by X-ray diffraction and transmission electron microscopy reveals they are composed of stoichiometric, single phase, cubic CdSe with a mean grain diameter of 10 nm. For *nc*-CdSe nanowires with lengths of many millimeters, the width and height dimensions could be varied over the range from 60 to 350 nm (w) and 20 to 80 nm (h). Optical absorption and photoluminescence spectra for nc-CdSe nanowires were both dominated by band-edge transitions. The photoconductivity properties of nc-CdSe nanowire arrays containing ~350 nanowires were evaluated by electrically isolating 5 μm nanowire lengths using evaporated gold electrodes. Photocurrents, i_{photo}, of 10-100× (i_{dark}) were observed with a spectral response characterized by an onset at 1.75 eV. iphoto response and recovery times were virtually identical and in the range from 20 to 40 μs for 60 × 200 nm nanowires.

5:20pm **NS+EM+EN-WeA11 Efficient, Single Layer Organic Light-Emitting Devices Based on a Graded Composition Emissive Layer**, ***N.C. Erickson***, *R.J. Holmes*, University of Minnesota

We demonstrate efficient electrophosphorescence from devices comprised of a single organic active layer. High efficiency is realized by combining both hole- and electron-transporting host materials (HTM and ETM, respectively) into a single, graded composition emissive layer with the green emitter, *fac*-tris(2-phenylpyridine) iridium (III). The composition of the host-material is continuously graded to realize 100% HTM at the anode, and 100% ETM at the cathode. A peak external quantum efficiency of η_{EQE}=(19.3 ± 0.4) % is realized in the forward-viewing direction at a luminance level of 600 cd/m^2, corresponding to a power efficiency of η_P =(66.5 ± 1.3) lm/W. This performance is similar to that realized in more conventional and complex, multi-layered structures. The graded composition of the structure balances electron and hole injection and transport leading to efficient exciton formation, permitting high efficiency using a single active layer. The graded composition architecture may be further utilized to realize simple, efficient organic light-emitting devices for use in display and lighting applications.

Electronic Materials and Processing
Room: Dona Ana - Session EM+SS-ThM

Nitride Surfaces and Interfaces
Moderator: Engel-Herbert, Penn State University

8:00am **EM+SS-ThM1 Recent Advances in the MOCVD Growth of III-N Light Emitting Diodes**, ***R.D. Dupuis***, *J.-H. Ryou, H.-J. Kim, J. Liu, Z.M. Lochner, J. Kim, S. Choi, S.-S. Kim*, Georgia Institute of Technology **INVITED**

Group III-nitride-based green light-emitting diodes (LEDs) are increasingly used in applications for full-color displays, back-lighting, and color-mixing-based general illumination lighting systems. Recently, the potential for III-N LEDs to replace all forms of conventional lighting sources has been discussed and advanced white-light LEDs have entered the market place for general consumer use. However, significant fundamental and technical challenges remain for III-N LEDs to achieve their full potential, such as the improvement of the peak internal quantum efficiency (IQE) and the minimization of the efficiency droop with increasing injection current density. For full-color lighting based upon III-N RGB LEDs, other impediments remain. The peak IQE of green LEDs are significantly lower than shorter-wavelength InAlGaN-based blue and longer-wavelength InAlGaP-based red LEDs, a feature referred to as a "*green gap*". In addition, the efficiency of green LEDs at high drive currents decreases with increasing injection current more significantly than in blue LEDs. In this paper, we will review some of the recent work and advances in the area of improving the high-current-density performance of III-N LEDs.

8:40am **EM+SS-ThM3 Microstructural Comparison of InGaN/GaN Multi Quantum Wells Grown on SiC and GaN Substrates**, ***F. Liu***, *L. Huang,* Carnegie Mellon University, *E.A. Preble, T. Paskova, K. Evans,* Kyma Technologies, Inc., *R.F. Davis, L.M. Porter*, Carnegie Mellon University

Light emitting diodes (LED) with InGaN/GaN multi-quantum wells (MQW) as the active region are now being widely investigated for blue and green light sources. However, InGaN/GaN MQWs grown on sapphire or SiC substrates commonly contain V-shaped defects with densities as high as 10^9cm^{-2}. These V-defects, which are believed to degrade the internal quantum efficiency of the LED, are remarkably reduced via growth on GaN substrates. In this study, we present a detailed microstructural comparison between $In_{0.2}Ga_{0.8}N$ (3nm)/GaN (8nm) MQWs grown on AlGaN/ SiC (0001) and GaN (0001) substrates via metalorganic chemical vapor deposition at 790ºC. The composition was determined by analyses of x-ray diffraction (XRD) and photoluminescence measurements. The microstructure was characterized using a variety of techniques, including transmission electron microscopy (TEM), scanning electron microscopy (SEM), electron channeling contrast imaging (ECCI), and photoelectrochemical (PEC) etching. SEM images revealed that the V-defect density decreased from1 x 10^{10} cm^{-2} to 7 x 10^6 cm^{-2} in MQWs grown on SiC and GaN substrates, respectively. Cross-sectional TEM images on MQWs grown on SiC substrates indicated that V-defects invariably originated from threading dislocations. To test this hypothesis, we investigated the threading dislocation densities prior to the growth of the MQWs (i.e., in (300-500 nm) GaN films grown on SiC and GaN substrates) via PEC etching and ECCI. The dislocation densities observed in these samples (~6 x 10^9 cm^{-2} on SiC; ~4 x 10^6 cm^{-2} on GaN) are close to the respective densities of V-defects observed in samples after growth of the MQWs. These results from multiple techniques provide convincing evidence that the dislocation densities in the GaN layer above the substrate determine the densities of V-defects in the MQW. The introduction of dislocations directly from GaN substrates into the homoepitaxial layers is also under investigation using the techniques described herein.

9:00am **EM+SS-ThM4 Switching GaN Polarity on Homoepitaxial Substrates**, ***J.K. Hite***, *M.E. Twigg, M.A. Mastro, F.J. Kub, C.R. Eddy, Jr.*, Naval Research Laboratory

Gallium nitride (GaN), a highly advantageous material for both optical and electronic devices, can be grown in the (+/-) c-direction of its lattice with two different polar faces, nitrogen- (N-) or gallium- (Ga-) polar. The face or polar orientation of the material establishes many quite varied properties of the material, from chemical reactivity to dopant incorporation to spontaneous and piezoelectric-induced electric field directions in the crystal. Control of the polarization fields and, thus, polarization induced doping is the basis of Ga-polar and N-polar GaN-based high electron mobility transistor operation. On heterogeneous substrates, such as silicon carbide (SiC) and sapphire (Al_2O_3), the growth conditions, doping levels, and buffer or nucleation layer properties are used to control the polarity of resulting GaN epilayers. Further, in the case of heavily doped p-type layers, spontaneous polarity inversion has been demonstrated even on GaN epilayers, switching from Ga-polar to N-polar in the doped layer.[1] However, this approach leads to uncontrolled inversion domain boundaries and often results in dopant clustering[2] in the film, impacting film quality and resultant device performance.

In contrast, this new approach enables the controlled formation of Ga-polar GaN from a N-polar crystal. Instead of using concentrated doping, the polarity switch in this case hinges on both surface treatment and the addition of an optimized polarity inversion layer. Initial material characterization verified that the film was without N-polar inclusions or inversion domain boundaries. Chemical etching of the material in 4M KOH under slightly elevated temperatures (40°C) for 10-40 minutes as well as convergent beam electron diffraction[3] are employed to verify the polarity of the films. The structural quality of the films is ascertained with transmission electron microscopy and x-ray diffraction. In addition, the dislocation density and grain size are determined through the use of electron channeling contrast imaging.[4] While lateral polarity heterostructures have been of interest due to their unique electrical and structural properties,[5] this method offers the promise of engineering both lateral and vertical polarity heterostructures and the potential of novel variable polarity-based devices.

[1]V. Ramachandran et al., Appl. Phys. Lett. **75,** 808, 1999.

[2]M. Hansen et al., Appl. Phys. Lett. **80**, 2469, 2002.

[3]F.A. Ponce et al., Appl. Phys. Lett. **69**, 337, 1996.

[4]Y.N. Picard et al., Appl. Phys. Lett. **91**, 094106, 2007.

[5] M. Stutzmann et al., Phys. Status Solidi b **288,** 505, 2001.

9:20am **EM+SS-ThM5 Studies of InGaN Growth Morphology and Its Relationship to Multiple Quantum Well Luminescence**, ***D. Koleske***, *S.R. Lee, M.H. Crawford, M.E. Coltrin, J.M. Kempisty, K.C. Cross*, Sandia National Laboratories

It has been suggested that InGaN quantum well (QW) thickness fluctuations, acting in conjunction with piezoelectric fields, are sufficient to cause exciton localization and reduce non-radiative recombination at dislocations [1]. Consequently, the study of InGaN step morphology and the control of InGaN/GaN interfaces may be crucial for understanding and improving blue and green LED quantum efficiency. To this end, a variety of InGaN QW and thin film structures have been grown to determine how the surface roughens when GaN is alloyed with InN. Statistical analysis of the step-height distributions from AFM images shows that the nominally single-layer step heights transition to multiple-layer step heights as InGaN is grown on GaN. Further analysis of the surface-roughness power spectral density suggests that the main smoothing mechanism changes from an evaporation/recondensation mechanism to a surface diffusion mechanism as the growth temperature is lowered to incorporate indium into GaN. Exploiting these two smoothing mechanisms allows the construction of otherwise identical MQW structures with smoother or rougher InGaN QW interfaces. Initial studies of the correlations between QW interface roughness and luminescence intensity suggest that some degree of InGaN QW roughness leads to higher luminescence efficiency, lending credibility to theories that propose a structural-based enhancement of exciton localization. [1] D. M. Graham, *et al.*, J. Appl. Phys. 97 103508 (2005).

This research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:40am **EM+SS-ThM6 High-Quality, Large-Area, and Free-Standing GaN Epilayer Growth and Liftoff using Self-Assembled Interlayer of Silica Microspheres**, ***Q. Li***, *G.T. Wang*, Sandia National Laboratories

We demonstrate that self-assembled monolayers of silica microspheres can be used as inexpensive, selective growth masks for both significant threading dislocation density reduction and laser-free lift-off of GaN epilayers and devices. Silica microspheres self-assemble into close-packed monolayers on the surface of an initial GaN epilayer on sapphire using a Langmuir-Blodgett method. In a subsequent GaN regrowth, the silica microspheres effectively terminate the propagation of threading dislocations. As a result, the threading dislocation density, measured by large area AFM and CL scans, is reduced from 3.3 × 10^9 cm^{-2} to 4.0 ×10^7 cm^{-2}. This nearly two orders of magnitude reduction is attributed to a dislocation blocking and bending by the unique interface between GaN and silica microspheres. The sequential wet etching of the samples in HF

solution removes the silica microspheres sandwiched between the GaN epilayers and the growth template. Further wet etching of the samples in KOH solution successfully detaches the GaN epilayers from the growth templates. 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.

10:40am **EM+SS-ThM9 GaN(0001) Surface at Various Conditions: Fundamental Properties and Basic Dynamic Processes - Ab Initio Study**, ***S.K. Krukowski***, Polish Academy of Sciences, Poland **INVITED**

Due to its polar nature, gallium nitride, GaN properties strongly depend on its orientation. Therefore various GaN surfaces have different physical properties, which is related to their different atomic structure and also to the different electric fields in the subsurface layers. A new developed procedure allows to simulate these fields exactly, in a controlled fashion, within the slab model, by modification of the termination of the opposite side of the slab. These techniques will be discussed using bare Ga-terminated GaN(0001) surface as a working example. It will be shown that the field causes shift of the energy of the surface and band states, which is known as Surface States Stark Effect (SSSE). This approach will be employed also in the discussion of the hydrogen covered GaN(0001) surface. Both equilibrium properties and dynamic processes will be investigated with the account of the role of electric field, or equivalently doping in the bulk semiconductor, in shaping of the surface electronic and energetic properties. .Equilibrium properties such as hydrogen adsorption sites and energy, and also the thermodynamic and energetic stability will be discussed for various coverage. It will be shown that adsorption of molecular hydrogen on bare GaN(0001) surface leads to its dissociation and location of H atoms in the sites, above the Ga surface atoms. The interaction with adsorbed species leads to strong relaxation of the surface with Ga atoms moving upwards towards H adatoms. Generally, the hydrogen adatoms are strongly confined at the GaN(0001) surface, having their energy 1 eV below that in the GaN bulk. Thus the hydrogen coverage of GaN (0001) surface is stable, and its removal is extremely difficult. The energy of H - induced surface states strongly depend on the doping in the bulk: in p-type GaN the state is close to valence band maximum, but for n-type it is located 2 eV lower. The determined dynamic properties include the adsorption paths showing that the adsorption of molecular hydrogen depends on the coverage: for small coverage, molecular hydrogen is chemically adsorbed at the surface while for 1ML H-coverage it encounters significant energy barriers, drastically lowering the probability of this process. Adsorption of atomic hydrogen does not depend on the coverage, leading at some instances to creation of H_2 admolecules which subsequently could be desorbed form the surface.

The research was partially supported by the European Union within European Regional Development Fund, through grant Innovative Economy (POIG.01.01.02-00-008/08).

11:20am **EM+SS-ThM11 Surface Photovoltage Behavior for p-type vs. n-type GaN**, ***A.A. Baski***, *M. Foussekis, M.A. Reshchikov*, Virginia Commonwealth

Devices based on wide-bandgap GaN are successfully being used today, but a better understanding of surface effects such as band bending could further improve their performance. Many results have been reported on the upward surface band bending for n-type GaN, but fewer exist on the downward band bending for p-type GaN. Surface photovoltage (SPV) measurements using a Kelvin probe can directly measure the change in surface potential during UV illumination, and thereby indirectly measure the resulting decrease in band bending. We have studied steady-state and transient SPV for band-to-band (365 nm) illumination on a variety of p-type (Mg-doped) and n-type (Si-doped) GaN samples grown by hydride vapor phase epitaxy and metal organic chemical vapor deposition.

For n-type and p-type GaN samples, short (5 s) UV exposures generate an SPV magnitude of about 0.5 eV in both air and vacuum environments. The sign of the SPV signal is positive for n-type GaN and negative for p-type GaN, corresponding to a positive or negative change in surface potential, respectively. This fast component of the SPV corresponds to the accumulation of photo-generated holes (n-type) or electrons (p-type) at the semiconductor/oxide interface and leads to a corresponding decrease in band bending. As expected, this "internal" mechanism does not appear to depend on the sample environment. After ceasing illumination, decay of the SPV in dark and under all environments is slow with a logarithmic time dependence.

It is during longer UV exposures that the SPV behavior becomes noticeably different for n- vs. p-type samples. For n-type GaN, a long UV exposure (1 h) typically causes the SPV to decrease to 0.35 eV in air, but to increase to 0.6 eV in vacuum. This SPV behavior is consistent with the photo-induced adsorption of negatively charged oxygen species in air and their desorption in vacuum. In contrast, long UV exposure for some p-type samples has caused the SPV to reach a surprisingly large value of -1.1 eV in air, but to not change significantly in vacuum. The more negative SPV in air again indicates the adsorption of negative surface species, but the rather large change over extended illumination is not expected, particularly given that a comparable opposite change does not occur in vacuum (as for n-type). Therefore, the charging of the surface layer on p-type GaN and how it affects band bending is still under investigation. We have developed a phenomenological model that is able to distinguish contributions from internal (fast) and external (slow) mechanisms in SPV transients, and have demonstrated that the native oxide layer can play a significant role.

11:40am **EM+SS-ThM12 Investigation of the Structure of GaN(0001) Pseudo-1x1 Structure at Low Temperature**, ***A.R. Smith***, *T. Chen, K. Wang, Y. Liu*, Ohio University Nanoscale and Quantum Phenomena Institute

The wurtzite GaN(0001) surface has previously been determined to be in a pseudo-1x1 structure which includes approximately 2 monolayers (ML's) of Ga sitting atop the last GaN bilayer [1]. This metallic structure, commonly observed, was initially determined using a combination of reflection high energy electron diffraction (RHEED), Auger electron spectroscopy, and scanning tunneling microscopy (STM). In addition, there has been theoretical work performed for this surface. [2,3] In RHEED, the main observation is the appearance of satellite streaks located at 1/6th (or 1/12th) of the primary streak spacing outside of the primary streaks. It was initially modeled as a bi-axially contracted Ga bi-layer, contracted by approximately 16% relative to the GaN bulk. Theoretical calculations found only the top Ga ML to be contracted bi-axially. More recent theory work by Rinehimer et al. suggest that instead it is uniaxially contracted but having a similar structure. [3]

We investigate the pseudo-1x1 structure experimentally using a new growth and analysis system consisting of a molecular beam epitaxy (MBE) chamber for preparation of the surface and a RHEED system to monitor it. The sample growth stage also has the feature of allowing cooling to cryogenic temperatures as well as heating. The pseudo-1x1 structure is prepared by MBE growth on MOCVD-grown GaN substrates. Following this, the sample is cooled down, and the diffraction pattern is monitored. At low temperature, we observe the onset of new diffraction streaks located at approximately 5/12 and 7/12 of the primary streak positions, as well as disappearance of the pseudo-1x1 satellite streaks.

Models for the low-temperature GaN(0001) structure are currently being formulated which may give new insights into the structure of the pseudo-1x1, based on this new low-temperature RHEED data. As one model currently under consideration, a uniaxial, aperiodic superstructure is proposed in which the top Ga layer freezes into a coherent layer but with the resultant extra Ga atoms being displaced vertically. To further probe this model, low-temperature STM experiments are currently being planned, to be conducted in an adjacent in-situ STM system. This work is supported by the National Science Foundation (Grant No. 0730257) and by a grant from Ohio University.

[1] A. R. Smith, R. M. Feenstra, D. W. Greve, M.-S. Shih, M. Skowronski, J. Neugebauer, and J. E. Northrup, J. Vac. Sci. Technol. B **16** (4), 2242 (1998).

[2] J. E. Northrup, J. Neugebauer, R. M. Feenstra, A. R. Smith, Phys. Rev. B **61**, 9932 (2000).

[3] J.A. Rinehimer, M. Widom, J.E. Northrup, and R.M. Feenstra, Phys. Stat. Sol. (b) **245(5)**, 920 (2008).

Thin Film
Room: Ruidoso - Session TF-ThM

Modeling and Analysis of Thin Films
Moderator: S.B. Sinnott, University of Florida

8:00am **TF-ThM1 Thermodynamics of Clustering and Magnetism in $Ti_{1-x}Al_xN$ and $Ti_{1-x}Cr_xN$ Thin Film Materials from First-Principles**, ***B. Alling***, *I.A. Abrikosov, L. Hultman*, Linköping University, Sweden

Multinary nitride materials are widely used as coatings for wear protection of cutting tools, e.g. TiAlN, as well as in thin film electronic applications. One important aspect of the success of TiAlN is a composition dependent thermodynamically driven age-hardening process through spinodal decomposition into TiN and cubic AlN at cutting tool operational temperatures. To understand this phenomena and to be able to tailor optimal compositions for different applications, we perform a thorough theoretical thermodynamics investigation based on first principles calculations.

By mapping the complete quantum mechanical complexity of the system onto a generalizes Ising Hamiltonian for the configuration of Ti and Al

atoms, we are able both to predict thermodynamics using accurate Monte Carlo simulations and achieve a deeper understanding of the interactions governing the system.

One physical property that is difficult to find in nitrides and which disfavors the usage of the materials class in spintronics, is room temperature ferromagnetism. TiCrN is one of the rare nitride systems where strong ferromagnetism is seen. We use our methodological framework to analyze and explain why the magnetic interactions that favor anti-ferromagnetism in pure CrN is changed in the TiCrN solid solution, as well as the intricate dependence of the Curie temperature on the CrN content.

8:20am **TF-ThM2 Electronic Mechanism for Toughness Enhancement in $V_xM_{1-x}N$ Thin Films**, *D.G. Sangiovanni*, ***V. Chirita***, *L. Hultman*, Linköping University, Sweden

We use Density Functional Theory (DFT) calculations in the generalized gradient approximation (GGA) to predict the properties of a number of novel V-M-N thin films in the B1 (NaCl) structure. The new compounds are obtained by alloying VN with Nb, Mo and W, in concentrations of 50 %. We evaluate the elastic moduli and constants of these ternaries and perform a detailed analysis of their electronic structure. These results are compared with the corresponding properties of typical binaries such as TiN and VN. Our calculations show that the new ternaries have hardness comparable with TiN and VN, and significantly, a resolute ductile behavior. This unique combination of hardness/ductility, which is in contrast to the hardness/brittleness relationship typically found in hard coatings, equates to significantly increased toughness, as confirmed by the stress-strain relationship we obtain for all these compounds. The electronic structure results presented herein reveal a layered charge density, consisting in alternating high and low electron density regions, similar to that recently reported for Ti-Mo/W-N thin films [1]. To fully understand the mechanism responsible for this interleaved arrangement of electrons, we carry out crystal orbital overlap population (COOP) and electron localization function (ELF) calculations, and succeed to energetically resolve the bonding/antibonding contributions, of the first and second neighbors, to the chemical bonds in these compounds. Based on the results of this analysis, we find that the electronic mechanism responsible for the observed toughness enhancement in these compounds is rooted in the increased metal-metal (second neighbors) interaction of d-t_{2g} orbitals.

[1] D.G. Sangiovanni, V. Chirita and L. Hultman, Phys. Rev. B **81**, 104107 (2010)

8:40am **TF-ThM3 2010 Gaede-Langmuir Award Lecture- X-ray Absorption Spectroscopy and Many Electron Theory Applied to O-vacancy State Differences between (i) Non-crystalline SiO_2 and (ii) Nano-crystalline HfO_2 Thin Films**, ***G. Lucovsky****, North Carolina State University **INVITED**

Correlated atomic positions of Si-atoms bonded to 2-fold coordinated O-atoms are determined by Si *3d-dervied* T_{2g} states on these atoms [1]. These states constrain dihedral angles contributing to medium range order with *correlation lengths* of ~0.4 and 0.45 nm, and, a *coherence length* of ~1 nm, each obtained from the first sharp diffraction peak in X-ray diffraction [2]. O K edge soft X-ray SiO_2 spectra reveal conduction band edge states with singly degenerate A_1 symmetry, and stronger doubly and triply degenerate E and T_2 *d-state* beginning at energies ~3 eV higher. This difference is smaller in c-Si, ~1 eV. Analysis of O K and $L_{2,3}$ spectra are based on a charge transfer multiplet many electron theory [3]. Energy differences are the same for band edge features obtained from transmission/reflectivity studies in the visible/VUV where the d-state character was not previously recognized [4]. The correspondence derives from O 1s core hole localization, and a coherent process in which 1s core holes are filled by electrons from valence band O 2p p states, accounting for the one-to-one correspondence between sequenced features in the O K edge, and in the Si $L_{2,3}$ spectrum of SiO_2. $L_{2,3}$ spectra, studied by electron energy loss spectroscopy (EELS), have not detected the *weaker* Si A_1 features in the 100 to 104 eV regime of SiO_2, or 98 to 100 eV regime of c-Si. The O K edge X-ray spectra of transition metal elemental and complex oxides are qualitatively different with either doubly or triply degenerate *d-state derived* spectral features at the band edge. This results in significant quantitative differences in (i) the high-spin excited d-states of O-atom vacancy occupied d^2 states, and (ii) the negative ion electronically active d-state traps populated by charge injection. O-vacancy states in SiO_2 are close to mid-gap, and do not contribute to gate stack tunneling processes. This explains the order of magnitude higher interfacial trap densities, d_{it}, and trap-assisted tunneling in HfO_2 gate stacks. It also accounts for significant differences in radiation hardness. XAS spectra are presented for the first time for remote plasma deposited GeO_2. These deposited films display significantly different O K edge spectra than those obtained by oxidation of Ge; more importantly A_1, and E and T_{2g} features *stronger and narrower* than those of SiO_2. Electrical data for deposited GeO_2 dielectrics on Si and Ge substrates are compared for the first time with SiO_2 test devices on the same substrates.

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9:20am **TF-ThM5 New Parameterization of the Modified Embedded Atom Potential for Large Scale Simulations of TiN Thin Films Growth**, ***D.G. Sangiovanni***, *V. Chirita, L. Hultman*, Linköping University, Sweden

Classical Molecular Dynamics (MD) has become an indispensable tool in thin films modeling, as it allows the study of systems and phenomena reaching far beyond the inherent limitations of ab-initio and/or Density Functional Theory (DFT) methods. Generally, the range of systems to which the method can be applied has typically been limited to materials characterized by single-type bonding, such as ionic, covalent or metallic. This situation has been considerably improved in the last decade within the formalism of the Modified Embedded Atom Method (MEAM), which allows the treatment of mixed-type bonding materials, and in recent years, a number of studies have been devoted to MD simulations of important model systems such as TiN. Nevertheless, the very few MEAM parameterizations for TiN reported thus far are able to reasonably reproduce bulk, as well as some surface properties of this material. However, if meaningful MD simulations of TiN thin films growth are to be performed, a number of critical nucleation and diffusion phenomena have to be accounted for besides basic bulk/surface properties. Herein, we propose a new parameterization of the MEAM interaction potential for TiN, which in addition to correctly predicting bulk and surface properties, reproduces the experimentally observed trends in the diffusion of single species (Ti, N) and Ti-N dimers, on the most representative steps/surfaces for TiN growth, the (100) and (111) respectively. Our estimations of activation energies for diffusion and Ehrlich-Schwoebel (ES) step-edge barriers are in good agreement with previous ab-initio calculations and experimental observations. Consequently, this new MEAM parameterization has the potential to adequately account for most essential processes during the initial stages of TiN nucleation, which, as it is well known, dramatically affect the growth mode and properties of thin films in laboratory and computer experiments.

9:40am **TF-ThM6 DSMC Modeling of Metal Vapor Flow in Vacuum in Application to Thin-Film Depositions**, ***V. Ayyaswamy***, *A. Alexeenko*, Purdue University

Electron beam assisted physical vapor deposition (EBPVD) is widely used in a number of vacuum material processing applications for deposition of thin films of metals. The properties of these thin films including thickness uniformity, growth rates and other material properties are dependent, to a great extent, on the geometric configuration of the deposition source and electron gun power. A complete understanding of the deposition process requires the ability to accurately simulate the vapor flow that varies from highly collisional in regions near the source to being free-molecular near the substrate location. The direct simulation Monte Carlo technique, which is by far the most powerful technique to simulate such flows rapidly expanding into vacuum, requires an accurate molecular model for the interaction between the metal vapor atoms. A molecular model has been formulated [1] for the interaction of Cu atoms and validated with experimental data for electron-beam deposition of copper. The main goal of this work is to formulate molecular models for common metal vapors including Gold, Titanium, Nickel, and Aluminium and validate them with experimental data[2,3] for thin-film growth rates at various evaporation rates. The ability to accurately model deposition processes of thin films of metals would greatly assist in the design and control of such vacuum deposition systems and processes.

References

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* Gaede Langmuir Award Winner

Spectroscopic Ellipsometry Focus Topic
Room: Cochiti - Session EL+AS+EM+MS+TF-ThA

Spectroscopic Ellipsometry
Moderator: A.M. Creatore, Eindhoven University of Technology, the Netherlands

2:00pm **EL+AS+EM+MS+TF-ThA1 Developments in Spectroscopic Ellipsometry for Characterization of Organic and Inorganic Surfaces, Interfaces and Complex Layered Materials**, ***M. Schubert***, University of Nebraska - Lincoln **INVITED**

In this paper we will review new developments in Spectroscopic Ellipsometry for characterization of organic and inorganic surfaces, interfaces and complex layered materials. Ellipsometry has matured over the past two decades with instrumentation and methodology capable of addressing today's and tomorrow's challenges in materials characterization and metrology. Ellipsometry measures the general state of polarization of light reflected or transmitted from samples. Owing to its nondestructive and generally applicable concept of investigating light emerging from specimens under investigations, and owing to its extreme accuracy and precision, ellipsometry has paved the way for almost all our modern technologies, continues to enable next-generation devices in electronics and optoelectronics, and emerges into fields of chemical, biochemical and biological platform technologies. Originating from the identification that the information carried upon the polarization within a light beam emerging from surfaces is extremely sensitive to mono and submonolayer characteristics, ellipsometry started decades ago pioneering development of microprocessors and electronic devices, which still today are based on planar thin film technology. Without ellipsometry, today's computation and information technology would be still in its infancy. In this paper, emerging developments and applications for metrology of optical and electrical properties of semiconductors and nanostructures by Terahertz Magnetooptic generalized ellipsometry, also referred to as the Optical Hall effect, will be highlighted. Examples will include state-of-the-art nitride semiconductor device structures and epitaxial graphene, candidates for tomorrow's next-generation devices. Likewise, new approaches for characterizing precise structural, magnetic and optical properties of three-dimensional nanostructure hybrid materials will be discussed. Examples will describe how ellipsometry characterization enables understanding and tailoring of electromagnetic properties of materials created by human intelligence, rather than by nature. New horizons are being explored currently by combining ellipsometry with independent surface sensitive techniques, such as acoustic Quartz-Crystal microbalance techniques. Combinations allow for identification of new information not accessible otherwise. Examples include observation of in-situ formation of self-assembled monolayers, protein adsorption onto sensitized surfaces, and formation of micelle-assisted bilayer configurations. Prospects, challenges and future developments will be reviewed from today's perspective.

2:40pm **EL+AS+EM+MS+TF-ThA3 Characterizing the Adsorption – Desorption Behavior of Organic Molecules Within Thin Mesoporous Carbon Composite Films using Spectroscopic Ellipsometry**, ***B.D. Vogt***, *L.Y. Song, M.Z. Dai*, Arizona State University

Porous carbon materials are commonly utilized as adsorbants (i.e. activated carbon) and as catalyst supports. Direct templated synthetic routes to form ordered mesoporous carbons have recently been developed. By utilizing these concepts, mesoporous carbon composite films containing metal oxides can be synthesized. As a wide range of metal oxides can be utilized, these materials could be utilized in chemical sensing applications or as catalysts in fuel cell membranes. For both of these applications, the porous material will be exposed to organic vapors (such as ethanol in fuel cells). The condensation and evaporation of organic vapors from these materials is therefore an important consideration for their ultimate utilization in these applications. In-situ spectroscopic ellipsometry measurements of the mesoporous films exposed to controlled vapor pressures of organic vapors such as toluene, hexane and ethanol are utilized to understand the adsorption-desorption behavior of these films. Activated desorption of all three compounds is observed for pure carbon films, but addition of a small fraction of metal oxide enables the organics to be desorbed for the porous framework. These adsorption-desorption isotherms can also be utilized to estimate the pore size distribution and porosity of these films.

3:00pm **EL+AS+EM+MS+TF-ThA4 Mueller-Matrix Ellipsometry Studies of Chirality in Chitin-Based Structures and Thin Films of $Al_{1-x}In_xN$**, ***K. Järrendahl***, *H. Arwin, R. Magnusson, P. Sandström, C.-L. Hsiao, J. Landin, S. Valyukh, J. Birch*, Linköping University, Sweden

3:40pm **EL+AS+EM+MS+TF-ThA6 Mueller Polarimetry as a Tool for the Evaluation of the Diffraction Grating Profile Asymmetry**, ***T. Novikova***, *P. Bulkin*, LPICM, CNRS, Ecole Polytechnique, France, *V. Popov*, Moscow State University, Russia, *A. De Martino*, LPICM, CNRS, Ecole Polytechnique, France

4:00pm **EL+AS+EM+MS+TF-ThA7 Monitoring Ultra-Thin Organic Film Growth, *In-Situ*, with Combined Quartz Crystal Microbalance and Spectroscopic Ellipsometry**, ***K.B. Rodenhausen***, *B.A. Duensing, A.K. Pannier, M. Schubert,* University of Nebraska-Lincoln, *M. Solinsky,* The Procter & Gamble Company, *T.E. Tiwald*, J. A. Woollam Co., Inc.

4:20pm **EL+AS+EM+MS+TF-ThA8 Ellipsometric Studies of Electronically Coupled PbSe and PbS Quantum Dot Thin Films**, ***S.G. Choi***, National Renewable Energy Laboratory, *O.E. Semonin,* University of Colorado, *J.M. Luther, M.C. Beard, A.G. Norman,* National Renewable Energy Laboratory, *Z. Lin,* Colorado School of Mines, *A. Franceschetti,* National Renewable Energy Laboratory, *M.T. Lusk,* Colorado School of Mines, *A.J. Nozik*, National Renewable Energy Laboratory

Discovery of multiple exciton generation from colloidal suspensions of semiconductor quantum dots (QDs) has generated growing interests in realization of high-efficiency QD-based solar cells. Among a number of semiconductor QDs explored up to date, lead chalcogenides such as PbSe and PbS have been of great interest as a result of their wide tuning range of bandgap energy, abundance of materials, and large exciton Bohr radius.

In this presentation, I discuss optical properties of electronically coupled PbSe and PbS QD thin films. A series of QD multilayer thin films were prepared by a layer-by-layer dip-coating method onto glass substrates. Diameter of the QDs varies from 3.2 to 7.2 nm and from 3.5 to 8.3 nm for PbSe and PbS, respectively. Room-temperature pseudo-optical functions of the samples were measured by a rotating compensator-type, variable-angle spectroscopic ellipsometer. Transmittance data were also acquired in a normal-incidence configuration.

First, I determined refractive index $N = n + ik$ of the QD films using the B-spline basis functions within the multilayer model (ambient/surface roughness/QD film/substrate). We use the N obtained as the input parameters for modeling the internal quantum efficiency of the QD-based solar cell devices. Then, I extracted dielectric function $\varepsilon = \varepsilon_1 + i\varepsilon_2$ for the ensemble of electronically coupled QDs using the Maxwell-Garnett effective medium approximations. The ε spectra show the first exciton peaks, and the E_1 and E_2 critical-point (CP) structures whose energies are higher than the corresponding bulk values probably due to the quantum confinement effects. This abstract is subject to government rights.

4:40pm **EL+AS+EM+MS+TF-ThA9 In-situ Temperature Measurements by Spectroscopic Ellipsometry: Application to a-Si based Thin Films**, ***D. Daineka,*** LPICM, CNRS, Ecole Polytechnique, France, *V. Suendo,* Institut Teknologi Bandung, Indonesia, *P. Roca i Cabarrocas*, LPICM, CNRS, Ecole Polytechnique, France

Accurate measurement of the substrate temperature is of crucial importance in many semiconductor technologies such as plasma enhanced chemical vapor deposition (PECVD). Traditional tools, both thermocouples and pyrometers, are not always reliable for in situ measurements in vacuum when the substrate can be out of thermal equilibrium. On the other hand, non-contacting optical methods allow to determine the surface temperature with great accuracy, provided the temperature dependence of optical constants for the studied material is known. Since recently, spectroscopic ellipsometers are widely available and often installed on the research deposition systems, which provides an opportunity to use them for temperature monitoring. We have studied the optical functions of amorphous silicon based thin films with spectroscopic ellipsometry in the temperature range from 290 to 520 K. The experimental data were modeled using Tauc-Lorentz dispersion law for amorphous materials. We have found that the temperature coefficients of Tauc-Lorentz parameters, such as the optical gap, are rather close for a few different materials. That similarity suggests that these values can be used to determine the surface temperature for a broad range of amorphous silicon based materials with a good accuracy. Practical examples of using spectroscopic ellipsometry for temperature measurements in the low pressure PECVD environment are given.

5:00pm **EL+AS+EM+MS+TF-ThA10 Real Time Spectroscopic Ellipsometry Studies of Amorphous and Nanocrystalline $Si_{1-x}Ge_x$:H Thin Films for Microbolometer Applications**, ***D.B. Saint John**, H.-B. Shin, M.-Y. Lee, E.C. Dickey, T.N. Jackson, N.J. Podraza*, Penn State University

Hydrogenated amorphous and nanocrystalline silicon (a/nc-Si:H), germanium (a/nc-Ge:H), and their alloys have been used and continue to be assessed for use in uncooled infrared microbolometer applications. These materials may be deposited as uniform layers using equipment common to the manufacturing of displays and photovoltaics and are thus more amenable to manufacturing considerations than the ion beam deposited vanadium oxide films used in most commercial microbolometers. Real optimization of material in the a/nc-$Si_{1-x}Ge_x$:H system for use in these devices requires a better understanding of the relationship between the key electrical properties of interest including resistivity (r), temperature coefficient of resistance (TCR), and the 1/f noise character as a function of the degree of order and composition of the films. $Si_{1-x}Ge_x$:H thin films were deposited using plasma enhanced chemical vapor deposition using SiH_4, GeH_4, and H_2 at variable H_2- dilution. These films have been monitored using in situ real time spectroscopic ellipsometry (RTSE) over a spectral range from 0.75 to 5.15 eV during deposition to detect changes in the film thickness and optical properties in the form of the complex dielectric function spectra ($e = e_1 + ie_2$) as a function of deposition time. From the RTSE measurements and analysis it is possible determine the structure of the material as amorphous, nanocrystalline, or mixed-phase and track the evolution of nanocrystallinity as a depth profile into the film. Ex situ Fourier transform infrared spectroscopic ellipsometry measurements over a spectral range from 0.05 to 0.75 eV were also performed to augment the complex dielectric function spectra and study absorption features relating to bonding. For electrical measurements, contacts were deposited in an isolated transfer length pattern for measurement of resistivity and TCR, while resistors with different volumes were made for volume normalization of the 1/f noise measurements. The TCR was measured from 20°C to 55°C. This study explores to correlations between the electrical and optical properties of a-$Si_{1-x}Ge_x$:H and nc-$Si_{1-x}Ge_x$:H as functions of film processing conditions, resultant composition, and order. a-$Si_{1-x}Ge_x$:H films were prepared as a function of germanium content and hydrogen dilution to identify the impact that germanium and improved order at higher hydrogen dilution conditions have on the electrical properties (r, TCR, 1/f noise). The impact on the electrical properties due to the incorporation of small fractions of nanocrystallites are explored using mixed-phase (a+nc)-Ge:H films with nanocrystallite profiles guided by depth profile studies.

5:20pm **EL+AS+EM+MS+TF-ThA11 Roll-to-Roll Fabrication of Thin Film Si:H Solar Cells: Real Time Monitoring and Post Deposition Mapping by Spectroscopic Ellipsometry**, ***L.R. Dahal**, Z. Huang, D. Attygalle, M.N. Sestak, C. Salupo, S.X. Marsillac, R.W. Collins*, University of Toledo

Real time spectroscopic ellipsometry (RTSE) has been used to monitor the roll-to-roll deposition of thin film Si:H n-i-p solar cells on flexible plastic substrates coated with a Ag/ZnO back-reflector. In this process, the RTSE monitoring position is located directly above the ZnO sputtering target (i.e., at the closest target-substrate separation). RTSE data collection is initiated before the plasma is ignited so that ZnO nucleation can be observed. The film thickness increases with time until a steady state is reached, after which the bulk layer thickness at the monitoring point is constant with time. This occurs when the elapsed deposition time equals the time required for the moving substrate to travel from the leading edge of the deposition zone to the monitoring point. Although a constant substrate speed is selected such that the final film thickness is achieved in the time required to move through the entire deposition zone, this speed does not allow study of film growth that occurs after the substrate passes the monitoring point. To solve this problem, the substrate speed is reduced only in the early stage of growth such that the final film thickness of interest is reached at the monitoring point. In this way, RTSE can be used to analyze the entire layer on an initial length of the roll before the full length of the roll is processed. The thickness evolution of ZnO in the case of both normal and reduced speeds shows good agreement with a simple inverse square variation of the deposition flux from the target to the flexible substrate.

After cell deposition, spectroscopic ellipsometry (SE) has also been applied for large area mapping of the completed 15 cm wide roll, at up to 1.5 m long sections at a time. Key information such as critical point, oscillator amplitudes, band gap energies, and widths have been extracted from which material density, composition, grain structure, disorder, and defect density can be determined. In this paper, optical mapping was applied for the intrinsic absorber layer in a full device a-Si:H solar cell structure. The results clearly show the degree to which thickness uniformity of the absorber layer depends on the gas flow and the electrode configuration. Also, by parameterizing the optical functions of the intrinsic absorber layer using single Lorentz oscillator modified by a low energy absorption cut-off, a map of its band gap and oscillator width can be deduced. Such an SE application is ideal for evaluation of uniformity in bulk thickness db, surface roughness thickness ds, index of refraction, and extinction coefficient (n, k); the critical parameters for fabricating uniform and high efficiency solar modules.

Thin Film
Room: Ruidoso - Session TF-ThA

Multifunctional Thin Films and Characterization
Moderator: J.M. Fitz-Gerald, University of Virginia

2:00pm **TF-ThA1 Structural and Dielectric Properties of Epitaxial $BiFeO_3$:$BiMnO_3$ Nanocomposite Films on Flexible Hastelloy**, ***J. Xiong**, J. Zhai, V. Matias, G. Zou, M. Zhuo, Y. Zhang, D.T. Trugman,* Los Alamos National Laboratory*, B. Tao, Y. Li,* University of Electronic Science and Technology of China*, J. Driscoll,* University of Cambridge, UK*, Q. Jia*, Los Alamos National Laboratory

Growth of multifunctional thin films on flexible substrates is of great technological significance since such a platform is needed for the fabrication of flexible electronics. In this study, we report the growth of nanocomposite $(BiFeO_3)_{0.5}$:$(BiMnO_3)_{0.5}$ [BFO:BMO] films on polycrystalline hastelloy. To grow epitaxial BFO:BMO films on polycrystal substrates, we have used a template consisting of biaxially aligned TiN seed layer deposited by ion-beam-assisted deposited (IBAD) and a $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) buffer layer deposited by pulsed laser deposition. It should be noted that LSMO is used not only as a buffer layer but also as the bottom electrode of the nanocomposite dielectric films. Microstructural characterization by X-ray diffraction and transmission electron microscopy showed that the nanocomposite thin films were epitaxy with orientation relations of $(001)_{BFO:BMO}||(001)_{LSMO}||(001)_{TiN}$ and $[100]_{BFO:BMO}||[100]_{LSMO}||[100]_{TiN}$. Electrical measurements indicated good dielectric and ferroelectric properties which are comparable to that reported for ferroelectric films on single crystal substrates.

2:20pm **TF-ThA2 Comparison of Ion Beam and Magnetron Sputtered Vanadium Oxide Thin Films**, ***O.M. Cabarcos**, B.D. Gauntt, J. Li,* The Pennsylvania State University*, S. Antrazi,* 4Wave Inc.*, E.C. Dickey, D.L. Allara, M.W. Horn*, The Pennsylvania State University

Uncooled Infrared (IR) focal plane arrays are an enabling technology for both military and commercial high sensitivity night vision cameras. The IR imaging is accomplished using MEMS microbolometers fabricated on read-out integrated circuits (ROIC's) and depends critically on the material used to absorb the incoming IR radiation. A typical detector works by monitoring changes in the electrical resistance of the detector material as it absorbs the radiation. Thus, suitable detector materials must exhibit a large temperature coefficient of resistance (TCR) and low noise characteristics to efficiently detect IR photons while also maintaining compatibility with standard IC processing. The most commonly used material in uncooled infrared imaging detectors is vanadium oxide deposited by reactive ion beam sputtering. Here we present a comparison of vanadium oxide thin films grown via reactive ion beam sputtering to films grown using reactive pulsed DC magnetron sputtering. Films deposited using both methods were optically and structurally characterized using Raman spectroscopy, transmission electron microscopy, atomic force microscopy, grazing incidence X-ray diffraction and Rutherford backscattering spectroscopy. Electrical properties of the films were also measured and were found to be very sensitive to the deposition conditions used. The ion beam sputtered films were determined to contain twinned FCC VOx nanocrystals with sub-nanometer scale twin spacing, in the form of large 10-20 nm wide columnar/conical grains. In contrast, the magnetron sputtered films consisted of equiax grains of FCC VOx (5-10 nm) encapsulated in an amorphous matrix. Subtle differences in composition and structure could also be determined from the Raman spectra of the films. These differences in microstructure and composition were then correlated to the measured resistivities and TCRs of the films.

2:40pm **TF-ThA3 Mapping Li-ion Diffusion on the Nanoscale in Thin Film Battery Materials**, ***S.V. Kalinin***, Oak Ridge National Laboratory **INVITED**

The electrochemical energy storage systems based on Li-based insertion and reconstitution chemistries are a vital aspect of energy technologies. Despite the wealth of device-level and atomistic studies, little is known on the mesoscopic mechanisms of ion diffusion and electronic transport on the level of grain clusters, individual grains, and extended defects.

The development of the capability for probing ion transport on the nanometer scale is a key to deciphering complex interplay between structure, functionality, and performance in these systems. Here we

demonstrate how Scanning Probe Microscopy can be utilized to measure Li-ion mobility based on the strong strain-bias coupling in the system when local Li concentrations are changed by electrical fields. The imaging capability, as well as time- and voltage spectroscopies analogous to traditional current based electrochemical characterization methods are developed. The reversible intercalation of Li and mapping electrochemical activity in LiCoO2 is demonstrated, illustrating higher Li diffusivity at non-basal planes and grain boundaries. In Si-anode device structure, the direct mapping of Li diffusion at extended defects and evolution of Li-activity with charge state is explored. The electrical field-dependence of Li mobility is studied to determine the critical bias required for the onset of electrochemical transformation, potentially allowing reaction and diffusion processes in the battery system to be separated at each location. The Scanning Probe Microscopy measurements are compared with classical characterization methods such as cyclic voltammetry and electrochemical impedance spectroscopy. The prospects of Scanning Probe Microscopy for battery characterization are discussed.

This material is based upon work supported as part of the Fluid Interface Reactions, Structures and Transport (FIRST) Center, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number ERKCC61. Part of worked is performed as a user proposal in the Center for Nanophase Materials Sciences at ORNL.

3:40pm **TF-ThA6 Composition and Intermixing at the $LaAlO_3/SrTiO_3$ Interface by Rutherford Backscattering Spectrometry**, ***S.V. Shutthanandan***, *A. Cohen, L. Qiao, S.A. Chambers*, Pacific Northwest National Laboratory

There is a strong and growing interest in complex oxide interfaces because of the wide range of functional properties exhibited. It is well known that the $LaAlO_3/SrTiO_3$ (LAO)/(STO) interface exhibits novel electronic conductivity when grown in certain ways. LAO and STO are both band insulators in the bulk, but their interface exhibits n-type electrical conductivity when LAO is grown on TiO_2-terminated STO. Rutherford backscattering spectrometry (RBS) was used to determine interface composition in several pulsed laser deposition (PLD) grown LAO/STO samples prepared at leading laboratories. RBS data collected on these samples clearly show that La diffuses deep into the STO substrate. The clear presence of a shoulder between the low energy side of the La peak and the high energy side of the Sr peak suggests La indiffusion, although this shoulder could also be caused by pulse pile up in the detector, straggling, and/or multiple/dual scattering effects. Therefore, RBS data were taken as a function of beam current, incident beam energy, and film thickness to determine if this shoulder is due to these artifacts, or La indiffusion. It was determined that none of the aforementioned artifacts occur, thereby implicating La indiffusion. The presence of substitutional La at Sr sites in the substrate provides a plausible explanation for the observed n-type conductivity, as La is a shallow donor in STO.

4:00pm **TF-ThA7 Low Work Function CsI Coatings for Enhanced Field Emission Properties**, ***P.T. Murray***, University of Dayton, *T.C. Back, S.B. Fairchild*, Air Force Research Laboratory

The use of CsI coatings on graphite fiber cathodes has been shown to reduce the field strength required for field emission from approximately 10^4 V/cm to 250 V/cm. Interestingly, the mechanism for enhanced field emission is poorly understood. We have explored the enhancement mechanism by using simulated cathode structures consisting of CsI films deposited (by thermal evaporation and by pulsed laser deposition) onto graphite and Si surfaces; the films were characterized by x-ray photoelectron, Auger electron, ultraviolet photoelectron, and electron energy loss spectroscopy. Two aspects of the enchantment mechanism have been explored. The first, cathode conditioning, was addressed by characterizing the surfaces of CsI-coated cathodes and (stainless steel) anodes before and after conditioning. The results allow us to assess the change in cathode surface chemistry as well as the extent to which material is transferred between electrodes during conditioning. The second aspect concerns the reported observation that CsI coated cathodes, after use, exhibit the disappearance of I and the appearance of a coating that appears to have wetted the cathode surface. We hypothesize that I depletion leaves behind a film of Cs which, with its low melting point, will flow during cathode operation. To test this hypothesis, we have characterized I depletion from CsI by carrying out electron and photon stimulated desorption from CsI surfaces. The talk will conclude with a discussion of our findings and their relevance to the enhancement mechanism.

4:20pm **TF-ThA8 Characterization of SiO_2 Thin Films Prepared by Pulsed Electron Deposition**, ***V.C. Rincon***, *S. Kotru, H.V. Nampoori, M. Chen, R.M. Frazier*, The University of Alabama

Pulsed Electron Deposition (PED) is an ablation-based physical vapor deposition technique similar to Laser Deposition (PLD), where electrons are used as the ablation source. Silicon dioxide is a material which is extensively used by the microelectronic industry and also finds various applications as insulators, protective layers, antireflection coatings etc. There are many different techniques as thermal oxidation of silicon, low pressure chemical vapor deposition (LPCVD), plasma enhanced chemical vapor deposition (PECVD), to grow SiO_2. This work presents growth of thin films of SiO_2 deposited on Si (100) using PED. Films were deposited at oxygen pressure of 4.1mTorr and a pulse frequency of 3 Hz. Substrate temperature was varied from RT- 850 ºC, along with varying the source's voltage in the range of 18-12 KV. Characterization tools such as ellipsometry, FTIR and AFM were employed to study the dependence of optical constants and roughness on the quality of SiO_2 films.

4:40pm **TF-ThA9 Growth and Characterization Studies of $CdS_{1-X}Se_X$ ($0.0 \leq x \leq 1.0$) Alloy Thin Films by Spray Pyrolysis**, ***E. Masumdar***, Rajarshi Shahu Mahavidyalaya, India

The n-CdS1-XSeX thin films of variable composition have been deposited on amorphous glass and FTO coated glass substrates by simple and cost effective spray pyrolysis technique. The various deposition parameters have been optimized by using photoelectrochemical technique. The structural, surface morphological, compositional, optical and electrical properties have been studied. The X-ray diffraction studies indicated that all the films are polycrystalline in nature with hexagonal structure irrespective of the composition. The lattice parameter 'a' and 'c' varies from 4.1034 to 4.2615A° and 6.6664 to 6.9243 A° respectively with change in composition parameter from x = 0.0 to x = 1.0. Polycrystalline texture with nearly smooth surface and clearly defined grains has been observed for all samples from scanning electron microscopy (SEM). EDAX studies confirmed that CdS1-XSeX films have approximately same stoichiometry both initially and finally. The absorption coefficient 'α' is of the order of 104 cm−1. The optical absorption studies reveal that direct allowed transition with band gap energy between 2.44 and 1.74 eV. It is found that resistivity of the films decreased with increase in 'x' up to 0.8 and further it increases for x = 1.0 . Semi-conducting behavior has been observed from resistivity measurements.

Key words: X-ray diffraction; Cadmium compounds; Semiconducting II-VI materials; Optical Properties; Electrical properties.

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5:00pm **TF-ThA10 *In situ* Stoichiometry Control using Reflection-High-Energy-Electron-Diffraction Generated X-rays**, ***C. Keenan***, *S. Chandril,* West Virginia University, *T.H. Myers,* Texas State University - San Marcos, *D. Lederman*, West Virginia University

One major challenge in the stoichiometric growth of complex oxides, such as YMnO3, is the control of the relative compositions of the constituent materials. Desirable properties of oxide materials, such as ferroelectricity, are highly dependent upon material stoichiometry, making stoichiometry control an important issue. While RHEED (Reflection High Energy Electron Diffraction) analysis is typically used as a qualitative tool, RHEED generated x-rays can be used to give quantitative compositional information. The relative compositions of Y and Mn in MBE grown YMnO3 samples were studied using the grazing exit x-rays generated by RHEED electrons. Comparing the results with RBS characterization suggested that the technique has the potential for real-time compositional analysis.

This work was funded by the Office of Naval Research (Grant N00014-02-1-0974), the Air Force Office of Scientific Research (MURI grant F49620-03-1-0330), and the National Science Foundation (CIAM-DMR grant 0502825).

Spectroscopic Ellipsometry Focus Topic
Room: Southwest Exhibit Hall - Session EL+AS+EM+MS+TF-ThP

Spectroscopic Ellipsometry Focus Topic Poster Session

EL+AS+EM+MS+TF-ThP1 Temperature Dependence of the Dielectric Function of AlSb Measured by Spectroscopic Ellipsometry, ***J.J. Yoon***, *Y.W. Jung, J.S. Byun, S.Y. Hwang, Y.D. Kim,* Kyung Hee University, Republic of Korea*, S.H. Shin, S.Y. Kim, J.D. Song*, Korea Institute of Science and Technology, Republic of Korea

AlSb is a promising material for applications in heterostructure devices such as long-wavelength detectors, quantum-well lasers, and laser diodes. However, to understand and properly design these devices, information about its electronic properties and its dielectric function $\varepsilon = \varepsilon_1 + i\varepsilon_2$ is needed. While room-temperature ε data for AlSb exist, very little information is available about its behavior at elevated temperatures. Here, we report pseudodielectric function data $<\varepsilon>$ from 300 to 800 K and from 0.7 to 5.0 eV, determined by spectroscopic ellipsometry. The samples were 1.5 µm thick layers grown on GaAs (001) substrates by molecular beam epitaxy (MBE). This thickness significantly exceeds the critical value for AlSb, so the layers are fully relaxed. The MBE station features an integrated spectroscopic ellipsometer and strain-free windows, thereby allowing e data to be obtained without exposing the samples to air. For AlSb this is critical, because the removal of its oxides is not feasible owing to its reactivity. As a result of these precautions and the method by which these $<\varepsilon>$ data were obtained, we consider them to be the most accurate representation of ε to date. We also analyzed these data for critical-point (CP) parameters by fitting numerically calculated second energy derivatives of to standard analytic CP lineshape expressions. A parametric model was used, which describes dielectric functions by a combination of energy-bounded polynomials and poles, and encodes information in terms of amplitudes, critical-point energies, and broadening parameters. The reconstructed spectra are in excellent agreement with the data. We use these parameters to obtain information about the individual oscillators, including phonon effects, and interpolate them to obtain an analytic representation of the dielectric response of AlSb as a function of temperature. We expect these results to be an important database supporting engineering design, device technologies, and in-situ monitoring and control of device fabrication.

EL+AS+EM+MS+TF-ThP2 Optical Properties and Humidity Effects on Thin Films of Micro Fibrillated Cellulose Studied by Spectroscopic Ellipsometry, *H. Arwin,* ***E. Antunez de Mayolo,*** Linköping University, Sweden*, M. Eita,* Royal Institute of Technology (KTH), Sweden*, H. Granberg,* Innventia Ab, Sweden*, L. Wågberg*, Royal Institute of Technology (KTH), Sweden

High quality micro fibrillated cellulose (MFC) prepared from wood fibers can be used to prepare thin films on solid substrates by a layer-by-layer deposition technique. In applications MFC layers can be used alone or as a constituent in functional coatings, where the MFC can make a significant contribution to mechanical properties of the coating. Examples of potential applications are sensor layers, decorative coatings or mirrors. Here the optical properties in terms of the refractive index of MFC are studied with *in situ* spectroscopic ellipsometry (SE) and the effects on thickness and index due to humidity are investigated.

Films of MFC and polyethyleneimine (PEI) in the thickness range 30 - 300 nm are deposited on silicon substrates. Such MFC/PEI samples are exposed to water vapor in nitrogen (0-90% RH) and the ellipsometric response are measured *in situ* in the spectral range 245 – 1700 nm at an angle of incidence of 70 degrees using a dual-rotating compensator ellipsometer. From the SE-data the MFC/PEI film thickness and layer index are modeled.

Due to water exposure, the thickness of an MFC/PEI film is found to increase up to 15% or more, whereas the refractive index decreases. The effects are fully reversible and the dynamics of these changes are monitored with SE and are discussed.

EL+AS+EM+MS+TF-ThP3 Spectroscopic Ellipsometry and X-ray Photoelectron Spectroscopy of La_2O_3 Thin Films Deposited by Reactive Magnetron Sputtering, ***V. Atuchin***, Institute of Semiconductor Physics, Russia*, A.V. Kalinkin,* Boreskov Institute of Catalysis, Russia*, V.A. Kochubey, V.N. Kruchinin,* Institute of Semiconductor Physics, Russia*, R.S. Vemuri, C.V. Ramana*, University of Texas at El Paso

Lanthanum trioxide (La2O3) is one among the most promising high-*k* dielectric materials to replace SiO2 and Si3N4 in advanced metal-oxide-semiconductor devices in gate stack. La2O3 can be prepared by various techniques but the film properties are strongly dependent on the fabrication conditions. Reactive magnetron sputtering deposition is widely used for the preparation of high quality transition multivalent metal oxide films with reproducible parameters and controlled thickness. The technique is preferred since it usually offers a high deposition rate for oxide films and a possibility to control the chemical composition of the film by reactive atmosphere in vacuum chamber. The aim of the present study is to understand the surface structure and evaluate the optical parameters of La2O3 films deposited on Si substrates by magnetron sputtering. La2O3 thin films were deposited onto Si(100) substrates in an argon/oxygen atmosphere using a high purity La target (99.9%). Structural parameters of the films were estimated by reflective high energy electron diffraction (RHEED) method at electron energy of 50 keV. All the films show no diffraction pattern indicating their amorphous nature in the near surface layers. Chemical state examined by the X-ray photoelectron spectroscopy (XPS), SPECS device, monochromatic Al Ka radiation (1486.6 eV) before and after Ar+ (2.5 keV, 2 min) sputtering indicates the stoichiometric film formation. Chemical nature of the species was identified with using binding energy (BE) difference parameter DLa = BE (La 3d5/2) - BE (O 1s) [1]. Optical parameters of the films were measured with spectroscopic ellipsometry (SE) using a Spectroscan ellipsometer in the spectral range of 250 nm < l < 1100 nm at the incidence angle of 70°. The La2O3 films with thickness 500-850 nm were transparent over the spectral range and dispersion relations of refractive index *n* were well derived using a model of (air)/(single homogeneous layer)/(Si substrate). The curves *n*(l) were approximated by Caushy polynomials. Good relation between experimental points and theoretical curves confirms applicability of this simple model for the films. The optical parameters of La2O3 defined with SE are related to film bulk and are insensitive to top surface effects induced by hydration or carbonate formation. These parameters will be used as a basis for SE evaluation of nanometric lanthanum oxide films with thickness below 10 nm.

1.V.V. Atuchin, T.A. Gavrilova, J.-C. Grivel, V.G. Kesler, Electronic structure of layered ferroelectric high-k titanate La2Ti2O7, J. Phys. D: Appl. Phys. 42 (2009) 035305.

EL+AS+EM+MS+TF-ThP4 Analysis of Anomalous Film Growth when Yttrium Oxide Thin Films are Exposed to 7.2eV Light, ***D. Mortensen***, *D.D. Allred*, Brigham Young University

We have recently found that exposure of reactively sputtered yttrium oxide thin films to 7.2 eV photons in air produces a dramatic (factor of 4) increase in the films' thickness. This result was completely unexpected, Y2O3 is exceptional stable, and demanded further investigation. This is particularly important since yttria and neighboring metal oxides such as ZrO2 have been considered, and HfO2 is being used, as components in gate oxides for silicon devices. The excimer lamp used for the study was of the type used in cleaning the surfaces of silicon wafers in the semiconductor industry. It is vital to understand how metal oxides might swell during cleaning.

We have experimentally observed the following:

1. The film-thickness increase is linear with exposure time up to a point.

2. Over a factor of four increase in film thicknesses, as measured by spectroscopic ellipsometry, has been observed. E.g., film which was about 20 nm thick as deposited reached a thickness of about 100nm.

3. When the yttrium oxide sample is placed in a furnace the changes rendered to the yttrium oxide sample are reversed.

4. A film placed in a plasma cleaner does not show this increase.

5. These effects are noticeably absent under the same conditions for a silicon wafer.

6. The refractive index of the film decreased with exposure time, suggesting the film could becoming more porous, though effective media optical models were unsuccessful in modeling the optical properties.

In addition to ellipsometry the films were studied by XPS and STEM.

EL+AS+EM+MS+TF-ThP5 In-Situ Spectroscopic Ellipsometry of Lithium Ion Intercalation in GLAD Three-Dimensional Nanostructured Thin Films, ***E. Montgomery***, *M. Schubert, E.B. Schubert, T. Hofmann, D. Schmidt,* University of Nebraska - Lincoln, *R.A. May*, University of Texas at Austin

Lithium intercalation in thin nanostructured and bulk films from metals and semiconductors has been studied using in-situ spectroscopic ellipsometry. Nanostructured thin films have a large surface area, and the stress caused by the intercalation of lithium is reduced in comparison to continuous films. The films are deposited using electron beam evaporation at a glancing angle or Glancing Angle Deposition (GLAD).

The charge capacity of the films can be observed as a change of index of refraction using ellipsometry. We will study intercalation as a function of structure geometry in chiral and achiral 3D GLAD thin films deposited from different metals onto silicon and other dielectric substrates. We report the anisotropic dielectric functions of the 3D nanostructures and their changes as a function of intercalation time and period.

EL+AS+EM+MS+TF-ThP6 Multi Phase Model Generation of Reflection Anisotropy Spectra of Copper Phthalocyanine Films on Vicinal Silicon Substrates, ***F. Seidel***, *L. Ding, O.D. Gordan, D.R.T. Zahn*, Chemnitz University of Technology, Germany

In this work the in-plane anisotropy of copper phthalocyanine (CuPc) thin films grown on vicinal silicon substrates is explained by simulating Reflection Anisotropy Spectroscopy (RAS). In RAS the complex difference in reflection along two perpendicular directions is measured at an incidence angle close to 0°. While RAS has strong similarities with another polarisation related measurement technique, Spectroscopic Ellipsometry (SE), simulations of RA spectra using a similar mathematical formalism like in SE is not common.

One difference is that in SE the measurements are usually performed at an incidence angle close to the Brewster angle, where the difference between s and p reflected polarisation is maximal. However due to the similarities between the two techniques the evaluation of RA spectra can be performed in a similar way like for SE after some simple mathematical transformations. This in particularly useful when thickness induced interference can lead to incorrect interpretations of RA spectra. Therefore in this work we show that the RA spectra evaluation of CuPc layer with increasing thickness is mainly given by the optical interference effect and not by a change in the optical anisotropy of the film.

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Lauer, J.: EM-TuA10, 6; EM-TuP10, 10
Lederman, D.: TF-ThA10, 25
Lee, E.H.: TF+EM-WeM5, 14
Lee, J.C.: TF+EM-WeM5, **14**
Lee, J.H.: EM-TuP12, 11; TF+EM-WeM5, 14
Lee, J.S.: EM+SS-WeA11, 17
Lee, J.W.: EM-TuP4, 9
Lee, K.: GR+EM+MS+TF+MI-WeM9, 13
Lee, M.-Y.: EL+AS+EM+MS+TF-ThA10, 24
Lee, N.-E.: GR+EM+MS+TF+MI-WeM2, 12; TF+EM-WeM11, 15
Lee, S.: EM+SS-WeA11, 17
Lee, S.-H.: EN+EM-TuA1, 6
Lee, S.R.: EM+SS-ThM5, 19
Lee, W.-S.: EM-TuP14, 11; EM-TuP5, 9
Leiterer, C.: NS+EM+EN-WeA9, 18
Leusink, G.J.: TF+EM-WeM6, 14
Li, J.: TF-ThA2, 24
Li, Q.: EM+SS-ThM6, **19**; NS+EM+EN-WeA1, 17
Li, Y.: TF-ThA1, 24
Lie, F.L.: EM+SS-WeA3, **16**
Lim, C.-H.: EM-TuP5, **9**
Lin, W.-T.: EM-TuP1, 9
Lin, Z.: EL+AS+EM+MS+TF-ThA8, 23
Liu, D.R.: EM-TuP8, **10**
Liu, F.: EM+SS-ThM3, **19**
Liu, J.: EM+SS-ThM1, 19
Liu, P.: EM+MI-MoA8, 1
Liu, Y.: EM+SS-ThM12, 20; TF+EM-WeM12, 15
Lochner, Z.M.: EM+SS-ThM1, 19
Lorenz, N.: TF+EM-WeM3, 13
Losovyj, Y.B.: EM+MI-MoA8, 1
Lovejoy, T.C.: EM-TuA7, **5**; EM-TuP11, 10
Lucovsky, G.: TF-ThM3, **21**
Lusk, M.T.: EL+AS+EM+MS+TF-ThA8, 23
Luther, J.M.: EL+AS+EM+MS+TF-ThA8, 23

— M —

Macintyre, D.: EM+SS-WeA11, 17
Magnusson, R.: EL+AS+EM+MS+TF-ThA4, 23
Maier, M.: EM-TuM12, 4
Marsillac, S.X.: EL+AS+EM+MS+TF-ThA11, 24
Mastro, M.A.: EM+SS-ThM4, 19
Masumdar, E.: TF-ThA9, **25**
Matias, V.: TF-ThA1, 24
May, R.A.: EL+AS+EM+MS+TF-ThP5, 27
McDonnell, S.: GR+EM+MS+TF+MI-WeM11, 13
Melby, J.H.: EM-TuP3, **9**
Melitz, W.: EM+SS-WeA11, **17**; EM-TuP7, 9
Membreno, D.: EN+EM-TuA3, 6
Mertens, S.: TF+EM-WeM10, 14
Meyer, T.: EM+MI-MoA4, 1
Milojevic, M.: EM+SS-WeA4, 16
Montgomery, E.: EL+AS+EM+MS+TF-ThP5, **27**
Moon, H.K.: TF+EM-WeM11, **15**
Morris, P.A.: EM+MI-MoA4, 1
Mortensen, D.: EL+AS+EM+MS+TF-ThP4, **26**
Moyer, J.A.: EM+MI-MoA7, **1**
Mueller, K.: MI+EM-TuA9, 8
Murray, P.T.: EN+EM-TuA4, 7; TF-ThA7, **25**
Muscat, A.J.: EM+SS-WeA3, 16
Myers, T.H.: TF-ThA10, 25
Myung, K.D.: EM-TuP14, **11**

— N —

Nagpal, P.: EN+EM-TuA7, **7**
Nah, J.: GR+EM+MS+TF+MI-WeM9, 13
Nampoori, H.V.: EN+EM-TuA10, **7**; TF-ThA8, 25
Nanayakkara, S.U.: NS+EM+EN-WeA7, 18
Neppl, S.: EM-TuM5, 3
Neumayer, D.: GR+EM+MS+TF+MI-WeM5, 12
Nichols, M.: EM-TuA10, **6**
Nishi, Y.: EM-TuA10, 6; EM-TuP10, 10; TF+EM-WeM9, 14
Noh, J.: EM-TuP9, **10**
Noh, J.H.: EM-TuP9, 10
Nolting, F.: MI+EM-TuA9, 8
Norman, A.G.: EL+AS+EM+MS+TF-ThA8, 23
Novikova, T.: EL+AS+EM+MS+TF-ThA6, **23**
Nozik, A.J.: EL+AS+EM+MS+TF-ThA8, 23

— O —

Odom, T.W.: NS+EM+EN-WeA3, **17**
Ohta, T.: GR+EM+MS+TF+MI-WeM6, 12
Ohuchi, F.S.: EM-TuA7, 5; EM-TuP11, 10
Olmstead, M.A.: EM-TuA7, 5; EM-TuP11, 10
Olson, C.S.: MI+EM-TuA10, 8
Opila, R.: TF+EM-WeM3, 13

— P —

Pakhomov, A.: EM-TuP11, 10
Pan, W.: GR+EM+MS+TF+MI-WeM6, 12
Pannier, A.K.: EL+AS+EM+MS+TF-ThA7, 23
Park, H.H.: EM-TuP12, 11
Park, J.S.: TF+EM-WeM5, 14
Park, J.-S.: EM-TuP5, 9; GR+EM+MS+TF+MI-WeM2, 12
Park, T.-H.: NS+EM+EN-WeA7, 18
Paskova, T.: EM+SS-ThM3, 19
Penner, R.M.: NS+EM+EN-WeA10, 18
Perebeinos, V.: GR+EM+MS+TF+MI-WeM5, 12
Perez, L.M.: EM-TuM6, 3
Perng, Y.-C.: EN+EM-TuA3, **6**
Petkovic, L.M.: EM+MI-MoA9, **1**
Pirkle, A.: GR+EM+MS+TF+MI-WeM11, **13**
Podraza, N.J.: EL+AS+EM+MS+TF-ThA10, 24
Pokhodnya, K.I.: MI+EM-TuA10, 8
Ponomarev, M.: NS+EM+EN-WeA8, 18
Popov, V.: EL+AS+EM+MS+TF-ThA6, 23
Porter, L.M.: EM+SS-ThM3, 19; EM-TuP3, 9
Preble, E.A.: EM+SS-ThM3, 19

— Q —

Qiao, L.: TF-ThA6, 25

— R —

Rachmady, W.: EM+SS-WeA3, 16
Rack, P.D.: EM-TuP9, 10
Ramana, C.V.: EL+AS+EM+MS+TF-ThP3, 26
Rashkeev, S.N.: EM+MI-MoA9, 1
Ren, H.: TF+EM-WeM9, **14**
Reshchikov, M.A.: EM+SS-ThM11, 20
Ricciardo, R.: EM+MI-MoA4, 1
Riley, L.A.: EN+EM-TuA1, 6
Rincon, V.C.: TF-ThA8, **25**
Robinson, J.: GR+EM+MS+TF+MI-WeM1, 12
Roca i Cabarrocas, P.: EL+AS+EM+MS+TF-ThA9, 23
Rodenhausen, K.B.: EL+AS+EM+MS+TF-ThA7, **23**
Ross, A.J.: GR+EM+MS+TF+MI-WeM6, 12
Ruda, H.: EM-TuA11, 6
Rudawski, N.G.: EM+SS-WeA7, 16
Russell, N.M.: EM-TuA10, 6
Rutkowski, M.M.: EM+MI-MoA4, **1**
Ryou, J.-H.: EM+SS-ThM1, 19
Ryu, M.K.: TF+EM-WeM5, 14
Ryu, S.-H.: EM-TuP5, 9

— S —

Saint John, D.B.: EL+AS+EM+MS+TF-ThA10, **24**
Salfi, J.: EM-TuA11, 6
Salupo, C.: EL+AS+EM+MS+TF-ThA11, 24
Sandström, P.: EL+AS+EM+MS+TF-ThA4, 23
Sangiovanni, D.G.: TF-ThM2, 21; TF-ThM5, **21**
Saveliev, I.: EM-TuA11, 6
Schaekers, M.: TF+EM-WeM10, 14
Schmidt, D.: EL+AS+EM+MS+TF-ThP5, 27
Schubert, E.B.: EL+AS+EM+MS+TF-ThP5, 27
Schubert, M.: EL+AS+EM+MS+TF-ThA1, **23**; EL+AS+EM+MS+TF-ThA7, 23; EL+AS+EM+MS+TF-ThP5, 27
Schuckman, A.E.: EM-TuM6, **3**
Seebauer, E.G.: EM-TuA9, **5**
Sehgal, A.: EM-TuA10, 6
Seidel, F.: EL+AS+EM+MS+TF-ThP6, **27**
Semonin, O.E.: EL+AS+EM+MS+TF-ThA8, 23
Sestak, M.N.: EL+AS+EM+MS+TF-ThA11, 24
Shah, K.: TF+EM-WeM10, 14
Shemelya, C.: NS+EM+EN-WeA2, **17**
Shen, J.: EM+SS-WeA11, 17; EM-TuP7, **9**
Shen, S.: TF+EM-WeM12, **15**
Shi, M.: MI+EM-TuA4, 8
Shi, Z.: EM-TuM9, 4
Shih, M.: MI+EM-TuA3, 7
Shimamura, K.: EM-TuA7, 5
Shin, H.-B.: EL+AS+EM+MS+TF-ThA10, 24
Shin, S.H.: EL+AS+EM+MS+TF-ThP1, 26
Shohet, J.L.: EM-TuA10, 6; EM-TuP10, **10**; TF+EM-WeM9, 14
Shutthanandan, S.V.: TF-ThA6, **25**
Sinha, H.: EM-TuA10, 6; EM-TuP10, 10
Sitnitsky, I.L.: EM-TuM2, 3
Smith, A.R.: EM+SS-ThM12, **20**; MI+EM-TuA3, 7; MI+EM-TuA4, 8
Snyder, D.: GR+EM+MS+TF+MI-WeM1, 12
Solinsky, M.: EL+AS+EM+MS+TF-ThA7, 23
Song, J.D.: EL+AS+EM+MS+TF-ThP1, 26
Song, L.Y.: EL+AS+EM+MS+TF-ThA3, 23
Spowart, J.E.: EN+EM-TuA4, 7
Stecher, J.T.: NS+EM+EN-WeA7, 18
Stemmer, S.: EM+SS-WeA7, 16
Straight, D.B.: EM-TuP10, 10
Suendo, V.: EL+AS+EM+MS+TF-ThA9, 23
Susac, D.: EM-TuA11, 6
Sutherland, J.C.: MI+EM-TuA10, 8
Swerts, J.: TF+EM-WeM10, **14**

— T —

Takeke Beyene, H.: NS+EM+EN-WeA8, 18
Talkenberg, F.: NS+EM+EN-WeA9, 18
Tang, J.: EM+MI-MoA8, 1
Tao, B.: TF-ThA1, 24
Thayne, I.: EM+SS-WeA11, 17
Therien, M.J.: NS+EM+EN-WeA7, 18
Thoms, B.D.: EM-TuP2, 9
Tiwald, T.E.: EL+AS+EM+MS+TF-ThA7, 23
Tökei, Z.: TF+EM-WeM10, 14
Tomoyasu, M.: EM-TuA10, 6
Trotter, D.C.: GR+EM+MS+TF+MI-WeM6, 12
Trugman, D.T.: TF-ThA1, 24
Trumbull, K.: GR+EM+MS+TF+MI-WeM1, 12
Trunk, J.: MI+EM-TuA10, 8
Tutuc, E.: GR+EM+MS+TF+MI-WeM9, **13**
Tweedie, J.S.: EM-TuP2, 9
Twigg, M.E.: EM+SS-ThM4, 19

— U —

Ueda, S.: EM-TuA7, 5; EM-TuP11, 10

Utgikar, V.: EM+MI-MoA9, 1

— V —

Valyukh, S.: EL+AS+EM+MS+TF-ThA4, 23
van de Sanden, M.C.M.: NS+EM+EN-WeA8, 18
van der Veer, W.E.: NS+EM+EN-WeA10, 18
Van Elshocht, S.: TF+EM-WeM10, 14
Vandervelde, T.: EN+EM-TuA9, 7; NS+EM+EN-WeA2, 17
Vaz, C.A.F.: EM+MI-MoA7, 1
Vemuri, R.S.: EL+AS+EM+MS+TF-ThP3, 26
Vescovo, E.: MI+EM-TuA10, 8
Villora, E.G.: EM-TuA7, 5
Vogt, B.D.: EL+AS+EM+MS+TF-ThA3, **23**

— W —

Waeckerlin, C.: MI+EM-TuA9, 8
Wågberg, L.: EL+AS+EM+MS+TF-ThP2, 26
Walker, A.V.: EM-TuM9, **4**
Wallace, R.M.: EM+SS-WeA4, 16; GR+EM+MS+TF+MI-WeM11, 13
Wang, G.T.: EM+SS-ThM6, 19; NS+EM+EN-WeA1, **17**
Wang, H.-Y.: EM-TuP1, 9
Wang, K.: EM+SS-ThM12, 20; MI+EM-TuA3, 7; MI+EM-TuA4, **8**
Wang, X.J.: EM+MI-MoA8, 1
Webb, K.M.: EM-TuM6, 3
Weiland, C.: TF+EM-WeM3, **13**
Wilks, G.B.: EN+EM-TuA4, **7**
Witters, T.: TF+EM-WeM10, 14
Woodward, P.M.: EM+MI-MoA4, 1
Wu, T.C.: EM-TuP8, 10
Wu, Z.: EN+EM-TuA1, 6

— X —

Xiao, Z.: EM-TuP15, 11
Xiong, J.: TF-ThA1, **24**

— Y —

Yamashita, Y.: EM-TuA7, 5
Yan, Y.: EN+EM-TuA1, 6
Yang, F.: NS+EM+EN-WeA10, 18
Yang, F.Y.: EM+MI-MoA4, 1
Ye, P.: EM+SS-WeA1, **16**
Yeh, Y.C.: EM-TuP8, 10
Yoon, J.J.: EL+AS+EM+MS+TF-ThP1, **26**
Yoon, O.J.: GR+EM+MS+TF+MI-WeM2, 12
Yoshikawa, H.: EM-TuA7, 5
Yu, C.: EM-TuP6, 9
Yu, L.H.: EM-TuM6, 3
Yun, D.K.: EM-TuP12, 11

— Z —

Zahn, D.R.T.: EL+AS+EM+MS+TF-ThP6, 27
Zhai, J.: TF-ThA1, 24
Zhang, Y.: EM-TuP10, 10; TF-ThA1, 24
Zharnikov, M.: EM-TuM5, **3**
Zheng, S.X.: EM-TuA7, 5; EM-TuP11, **10**
Zhernokletov, D.M.: EM+SS-WeA4, 16
Zhu, W.J.: GR+EM+MS+TF+MI-WeM5, **12**
Zhuo, M.: TF-ThA1, 24
Zou, G.: TF-ThA1, 24
Zwolak, M.: EM-TuM10, **4**