Electronic Materials and Processing
Room 2003 - Session EM-MoA

Contacts, Interfaces and Defects in Semiconductors
Moderator: F. Ren, University of Florida

2:00pm **EM-MoA1 Metals are not Created Equal: Metal Barrier-layer Dependent Ohmic Performance of Ti/Al/Metal/Au Schemes on AlGaN/GaN Heterostructures***, **F.M. Mohammed**, L. Wang, I. Adesida,* University of Illinois at Urbana-Champaign

AlGaN/GaN HEMTs are useful for application in microwave power amplification. Low-resistance ohmic contacts are required for enhanced performance of these devices. To this end, Ti/Al/MetalAu schemes, where Metal layer is a high melting-point element such as Ni, Ti, Mo, etc. have been investigated. In such a design, Ti participates in interfacial reactions yielding TiN and rendering the contact/GaN interface n-type doped. Coupling it with metals of high conductivity, such as Al, can enable direct Ohmic contact formation. However, the propensity of Al to easily oxidize upon annealing poses major reliability challenges. To solve this problem a Metal/Au bilayer cap is deposited. The Metal layer is believed to act as a barrier against the outdiffusion of Al and the indiffusion of Au. However, microstructural characterizations of Ti/Al/Mo/Au and Ta/Al/Mo/Au indicate that the Mo layer is not effective as a diffusion barrier. Therefore, a critical assessment of the presumed role of the Metal-layer acting as a diffusion barrier is needed. Here, we present the study of Ohmic performance and surface morphology of Ti/Al/Metal/Au schemes, where Metal is Ti, Mo, Pt, Ir, Ni, Ta, or Nb, carried out to identify the role of the barrier layer on contact formation and reliability of the metallizations. A strong dependence of contact resistance and specific contact resistivity, as well as surface morphology, on the type of Metal layer used was found. SEM/EDS characterization has shown evidence for alloy segregation, Metal layer fragmentation, Al-Au solid solution formation, and possible Au and/or Al reaction with Metal layer. The observed variations in Ohmic performance and surface morphology did not correlate with the properties of elemental Metal-layers. Contrary to the generally accepted opinion of the layer acting as a mere diffusion barrier layer, results from the present study provide new insights on the active role this layer plays on the characteristics of metallizations.

2:20pm **EM-MoA2 Tailoring the Interfacial Reactions between Ti/Al/Mo/Au Ohmic Contacts and AlGaN/GaN by Si lAyers: An Investigation by Cross-Sectional TEM***, **L. Wang**, F.M. Mohammed, I. Adesida,* University of Illinois at Urbana-Champaign

The interfacial reactions activated during annealing between Ti-containing metallizations and GaN or AlGaN are believed to be the ohmic contact formation mechanism. During annealing, Ti extracts N from the nitride layers and forms Ti-nitrides, such as TiN, AlTi2N, etc, triggered by their low enthalpies of formation as compared to that of GaN or AlGaN. It is believed this reaction generates a highly n-type layer in GaN or AlGaN which facilitates carrier tunneling. It was widely observed that the resulting Ti-nitride layers are continuous. However, our observation of the Ti/Al/Mo/Au contacts on AlGaN/GaN indicated that TiN did not always form as a continuous layer. Discrete TiN islands were observed to grow preferentially along dislocations and penetrate through AlGaN. The TiN islands, having an electrical resistivity as low as 13 Î¼Î©-cm depending on N content being smaller than Ti, electrically link the metal layer with the 2DEG at the AlGaN/GaN interface and make direct transport of carriers possible. This mechanism is also observed in the contacts to GaAs-based devices. In this paper, we demonstrate, with the aid of analytical TEM, that the interfacial reaction of Ti/Al/Mo/Au contacts on AlGaN/GaN heterostructures could be tailored by adding Si layers. Of particular importance is the Si/Al ratio. At low Si/Al ratio [0.138 and 0.276 (atomic ratio)], discrete metal islands rich in Al and Au form along dislocations and penetrate through the AlGaN layer. At medium ratio of 0.415, no island formation along dislocation is observed, rather a continuous layer of AlN forms at the interface. In both low and medium Si/Al ratio cases, Si dissolves in the metal and no silicide is perceived. At high Si/Al ratio (0.829), silicides, such as TiSi and MoSi2, are observed to precipitate. The observed reaction pathways are discussed in light of the Al-Si phase diagram. Meanwhile, the effects of the reactions on ohmic characteristics of different contacts are also presented.

2:40pm **EM-MoA3 2006 AVS Gaede-Langmuir Award Lecture - Interface Bonding, Reactions and Defect Formation at Semiconductor Interfaces***, **L.J. Brillson**[1],* The Ohio State University **INVITED**

The formation of barriers to charge transfer at semiconductor interfaces has been a focus of considerable research, much of it led by AVS scientists, for over fifty years. While early work centered on the intrinsic physical properties of the semiconductor, ultrahigh vacuum surface studies revealed the importance of extrinsic, interface-specific effects in understanding the systematic behavior of these Schottky barriers. Without intervening adsorbate layers, chemical reactions and interdiffusion can occur, even near room temperature, which alter the interface region, introducing new phases, crystal defects, and localized electronic states. Surface science techniques display local atomic bonding that depends systematically on thermodynamics and a qualitative transition between reactive and unreactive interfaces. Indeed, atomic-scale interlayers that change such chemistry introduce macro-scale electronic effects. These effects increase in importance as electronic structures shrink to nanoscale dimensions and interfaces constitute much of the entire structure. Detecting these states at or near interfaces requires techniques orders of magnitude more sensitive than conventional surface science provides. Low energy, nanoscale depth-resolved cathodoluminescence spectroscopy (NDRCLS) yields this capability, revealing states at the surface as well as tens to hundreds of nanometers below. DRCLS studies show the importance not only of interface chemistry but also crystal defects. Defects both resident in the semiconductor as well as created by interface reaction and diffusion can impact Schottky barrier formation. GaN, AlGaN, SiC and ZnO - metal junctions provide representative examples of chemically-induced defects near interfaces. Indeed, such defects appear to play a role in limiting Schottky barrier heights for semiconductors in general. These systematics suggest new ways to predict and control Schottky barriers in the nanoscale regime.

3:20pm **EM-MoA5 Inhomogeneous Schottky Contacts on Silicon Carbide: Localized Fermi Level Pinning by Defects***, D.J. Ewing,* Carnegie Mellon University*; Q. Wahab, M. Syväjärvi, R. Yakimova,* Linköping University, Sweden*; S. Tumakha, M. Gao, L.J. Brillson,* The Ohio State University*; **L.M. Porter**,* Carnegie Mellon University

Schottky barrier inhomogeneities, apparent as a knee in the low-voltage (Log I)-V characteristics, were present in a significant percentage of 4H-SiC diodes prepared from a variety of methods, sources, and contact materials. More than 500 Ni, Pt, or Ti diodes were characterized by a variety of techniques. Both commercially-produced chemical vapor deposited (CVD) epilayers and noncommercially-produced CVD and sublimation epilayers were used. The combined results from current-voltage measurements and modeling, electron beam induced current (EBIC), and site-specific and depth-resolved cathodoluminescence were used to develop a model to describe the relationship between specific defect states and the inhomogeneous behavior. By modeling the inhomogeneities as two Schottky barriers in parallel, high and low Schottky barriers were calculated for the non-ideal diodes. The high-barrier (ideal) barrier-heights for Pt, Ni, and Ti increased with metal workfunction with a slope parameter of 0.44, whereas the low barriers were predominantly centered at one of three values: 0.6, 0.85, and 1.05 eV. The site-specific and depth-resolved CL measurements of non-ideal diodes also revealed three different emission peaks (at 2.2, 2.4, and/or 2.65 eV), with the 2.4 eV peak originating from stacking faults observed in EBIC images; these peaks are the complements of the low barrier height values. Based on the results, the low-barrier barrier-heights can be explained by localized Fermi level pinning by specific material defects within the SiC epilayers. This model will be presented in terms of the defect level positions in the bandgap and their correspondence with the low barriers.

3:40pm **EM-MoA6 Carbon Nanotube Based Transparent Contacts for Photovoltaics***, **T.M. Barnes**, J. van de Lagemaat, M. Contreras, G. Rumbles, S.E. Shaheen, T.J. Coutts,* National Renewable Energy Lab*; C.L. Weeks, I.A. Levitsky, J.A. Peltola, P.J. Glatkowski, D.A. Britz,* EIKOS, Inc

Transparent electrodes are an integral part of photovoltaic (PV) devices, and the transparent conducting oxide (TCO) films currently in use are not ideal for all PV applications. Nanostructured bundles of single wall carbon nanotubes (SWCNT) can be solution-deposited to form highly conductive and transparent thin films. The films consist of entangled bundles of SWCNTs with a large fraction of void space. The optoelectronic properties of the SWCNT films approach those of commonly used TCO films. Unlike

[1] **Gaede Langmuir Award Winner**

ZnO and other traditional TCOs, however, the SWCNT film has little absorption in the visible or near infrared. Furthermore, in stark contrast to other available TCO materials, the SWCNT films are essentially hole conductors due to the intrinsic p-type conductivity of the SWCNTs. In this paper, we demonstrate the utility of SWCNT-based transparent contacts on several different types of thin-film solar cells. First, they were successfully used to replace ZnO in high-efficiency CIGS devices. Second, the SWCNT coating was used to replace ITO and PEDOT:PSS in excitonic, bulk heterojunction devices, resulting in an exceptionally high efficiency for a device without indium or PEDOT:PSS. These coatings work well in excitonic devices because the large void fraction allows for interpenetration of the active polymer at the nanoscale. They are also highly amenable to use on flexible substrates. This abstract is subject to government rights.

4:00pm **EM-MoA7 Tuning the Schottky Barrier Height in Mg/Si Diodes***, **H. Nienhaus**, S. Glass,* University of Duisburg-Essen, Germany

Thin metal film Mg/p-Si(111) Schottky diodes have been successfully used for sensing of chemically induced electron-hole pairs.@footnote 1@ Controlled variation of the homogeneous Schottky barrier height allows to probe the energy distribution of hot charge carriers. Different types of Mg/p-Si diodes were prepared by thermal evaporation of thin Mg layers on H-passivated Si(111) surfaces at low temperatures followed by various annealing procedures. After deposition at 190 K, the current-voltage characteristics of the diodes are typical for interfaces with lateral inhomogeneity and high ideality factors. The homogeneous barrier height is measured as 0.8 eV. This value is much larger than expected from theory of metal-induced gap states. The deviation is explained by interface dipoles due to the monatomic hydrogen layer between Mg and Si. The hydrogen is removed by annealing the diodes to room temperature. This procedure leads to the formation of an intermediate Mg silicide layer and to a significant reduction of the barrier height. The annealed diodes exhibit excellent current-voltage properties. Applications of the diodes for chemical sensing (chemicurrents) and for internal photoemission are discussed. @FootnoteText@ @footnote 1@ S. Glass, H. Nienhaus, Phys. Rev. Lett. 93 (2004) 168302.

4:20pm **EM-MoA8 High-Resolution Depth Profiling of Implanted As and Sb in Si(001) with Excess Vacancy Concentration***, M. Dalponte, H. Boudinov,* Universidade Federal do Rio Grande do Sul, Brazil*; **L.V. Goncharova**, T. Feng, T. Gustafsson, E. Garfunkel,* Rutgers University

Medium energy ion scattering (MEIS) was used to investigate the near-surface defect distribution and As and Sb redistribution in silicon substrates with excess vacancy concentration and separation by implantation of oxygen (SIMOX) substrates, and also the effects of post-implantation annealing. As and Sb are the preferred n-type dopant for Si due to their small depth penetration during implantation and low diffusivity during annealing. Also, Sb requires a lower thermal budget to achieve the desired junction parameters, compared to As. A 150 nm deep vacancy-rich layer was formed by O@sub 2@@super +@ or N@sub 2@@super +@ implantation at 240keV, using a dose of 2.5x10@super 16@cm@super -2@ at 400°C. As and Sb were then implanted at 20keV to a dose of 5x10@super 14@ cm@super -2@ at room temperature. Dopant segregation to the SiO@sub 2@/Si interface and some dopant loss was observed in all samples. Several effects related to the nature of the defects present in the sample as well as to the pre-implantation species were observed after longer annealing. The amount of dopant loss appears to be correlated with the structure of the defects. The highest dopant losses were observed in the N and O pre-implanted samples, where the vacancies had point defect character. In Si (no excess vacancies) and SIMOX (vacancies in the form of stable complexes) the dopant loss was much lower than in the N and O samples. Effects due to the different chemical nature of pre-implanted species were also observed. The N pre-implanted samples had the lowest segregated Sb percentage and uniform dopant distribution. The nitrogen accumulation at the SiO@sub 2@/Si interface appears to reduce dopant losses, compared to the O pre-implanted samples with the same vacancy structure. CNPq, CAPES, NSF and SRC/Sematech are gratefully acknowledged for their financial support.

4:40pm **EM-MoA9 Mechanism of Initial Oxidation of Hydrogen and Halogen Passivated Ge Surfaces***, **S. Sun**,* Stanford University*; Y. Sun, Z. Liu, D. Lee, P. Pianetta,* Stanford Synchrotron Radiation Laboratory

In order to keep scaling down the CMOS, new semiconductor materials are needed. Germanium (Ge) is one of the good candidates, because of its high intrinsic low field carrier mobilities. Research shows that Ge surface can be cleaned by HX (X = F, Cl, Br, I) and passivated by hydrogen or halogen. However, our experimental results show that neither hydrogen nor halogen passivated surfaces are stable in the room air. To be more specific, oxide will grow on these passivated surfaces in the room air. In order to probe the mechanism of the initial surface oxidation, systematic study is performed by synchrotron radiation photoelectron spectroscopy (SR-PES) at Stanford Synchrotron Radiation Laboratory (SSRL). Experimental results for samples with different passivation (hydrogen and halogen) and under various oxidation conditions (dry oxygen, moisture, and mixture of oxygen and moisture) will be shown, respectively. Then, results for different sample orientations, i.e. (111), (100) and (110), will be compared. Finally, the oxidation mechanism will be discussed in detail.

Electronic Materials and Processing
Room 2003 - Session EM-TuM

Zinc Oxide

Moderator: S.M. Durbin, University of Canterbury, New Zealand

8:00am **EM-TuM1 Impact of Subsurface Defects in Metal-ZnO(000-1) Schottky Barrier Formation***, **H.L. Mosbacker**, M.J. Hetzer,* The Ohio State University*; Y.M. Strzhemechny,* Texas Christian University*; M. Gonzalez, S.A. Ringel,* The Ohio State University*; D.C. Look,* Wright State University*; G. Cantwell,* ZN Technology, Inc.*; L.J. Brillson,* The Ohio State University

ZnO has emerged as a leading candidate for next generation semiconductor electronics due to its superior optoelectronic, microelectronic, and nanoelectronic properties. Central to realizing ZnO device applications are their electrical contacts with metals, yet Schottky barrier studies over the past 4 decades have not taken a comprehensive approach to isolating effects due to surface contamination, lattice defects, impurity dopants, and interface chemical reactions. We have used low energy depth-resolved cathodoluminescence spectroscopy (DRCLS) at 10 K in an ultrahigh vacuum scanning electron microscope and macroscopic current-voltage (I-V) measurements to study Schottky barrier (SB) formation at metal interfaces to clean, ordered ZnO(000-1). We fabricated sets of 30 nm-thick, 0.4 mm diameter Au, Al, Ni, Pt, Pd, Mo, Ta and Ir diodes on the same single crystal surfaces from different vendors. Prior to metallization, DRCLS revealed orders-of-magnitude difference in native bulk defect densities for crystals grown by different techniques, and these defect densities varied substantially between the crystals' bulk and surface. For all crystals, surfaces treated with a remote oxygen (20% O2/80% He) plasma created clean, ordered surfaces and reduced defect emissions in the surface region. Micro-DRCLS taken through the metal diodes revealed defect transitions at 2.1,2.5, and 3.0 eV that change dramatically with process steps and metal. I-V measurements exhibited transitions from Ohmic to SBs and lower idealities for Pt, Au, Ir, and Pd with plasma treatment. Deep-level optical and transient spectroscopies correlated bulk and surface defects, showing deep levels at 2.54 eV and 0.53 eV, while DRCLS shows that these densities can increase by > 100x at the surface. Our results indicate that metals can induce defects at the ZnO surface and impact device performance. The magnitude of the metal's influence directly correlates to the defect densities at the surface and ZnO bulk.

8:20am **EM-TuM2 Surface and Optical Properties of Zn-face versus O-face ZnO***, S. Chevtchenko, J.C. Moore, U. Ozgur, X. Gu, **A.A. Baski**, H. Morkoc,* Virginia Commonwealth University

We have compared the surface and optical properties of Zn-face (0001) and O-face (0001bar) ZnO samples. The samples used in this study were diced from the same bulk crystal prepared by Cermet Inc.@footnote 1@ Each sample had a thickness of ~0.4 mm and carrier concentration of 4.5x10@sup 16@ cm@sup -3@ at room temperature, corresponding to a Fermi level 0.11 eV below the conduction band. For optical characterization, steady-state photoluminescence (PL) using a He-Cd laser was measured at 15 K and 300 K (RT). Low-temperature PL for both surfaces showed the expected main transitions (free exciton, donor bound exciton, donor acceptor pair), with the most intense donor bound exciton transition at 3.359 eV having a FWHM of 1.7 meV, indicating a high quality sample. We did not observe any significant difference in the low-temperature PL spectrum for samples with different polarity. However, at RT the O-face sample demonstrated nearly double the near-band-edge emission intensity as that seen for the Zn-face. Using scanning Kelvin probe microscopy, we have also measured surface contact potentials of 0.39 V (Zn-face) and 0.50 V (O-face), which correspond to an upward band bending of 0.20 eV (Zn-face) and 0.09 eV (O-face), assuming an electron affinity of 4.4 eV. This relatively small difference in band bending for the polar ZnO surfaces indicates that spontaneous polarization is not a dominant contributor. Rather, we attribute band bending to surface states associated with dangling bonds. Also, the lower band bending of the O-face surface is consistent with the higher band-edge emission observed for this surface in room temperature PL studies. Finally, conductive atomic force microscopy studies show enhanced reverse-bias current conduction for the O- versus Zn-face samples. This effect may be due to different interactions of the two surfaces with ambient, in particular with water and hydrogen. @FootnoteText@ @footnote 1@ B. Nemeth and J.E. Nause; http://www.cermetinc.com.

8:40am **EM-TuM3 Synthesis and Characterization of ZnO Thin Films***, **T.J. Coutts**, X. Li, T.M. Barnes, J.N. Duenow, C.L. Perkins, S.E. Asher, B.M. Keyes, T.A. Gessert, S. Zhang,* National Renewable Energy Laboratory **INVITED**

N-type ZnO has great promise as a transparent conducting oxide and possibly has the potential to replace indium tin oxide for some applications. The high cost of indium may make it vital to find a replacement for indium tin oxide. ZnO is commonly used as an n-type material but vigorous efforts have also been made in recent years to fabricate p-type thin films. As an n-type material, it already plays an important role in some thin-film solar cells and it may also have the potential to be valuable in flat-panel displays. P-ZnO may have a role to play in solid-state lighting, UV/blue LEDs and lasers, novel solar cell designs and the generation of hydrogen by the splitting of water using light. However, p-type thin films, with relatively high hole concentrations, have been difficult to fabricate, are irreproducible, have low hole mobilities, and tend to be unstable. Nevertheless, efforts continue because of the potential commercial importance. In this paper, we discuss our work on the development of n-ZnO films, fabricated by sputtering, using aluminum, hydrogen and other, less familiar, dopants. The need for high mobility, via higher quality films, remains vital and is being explored using alternative dopants, by alternative growth methods and by optimizing the growth conditions. In addition, we discuss our work on the fabrication of p-ZnO, for which we used both low-pressure metal organic chemical vapor deposition and plasma enhanced chemical vapor deposition. We used both nitric and nitrous oxides as dopants. The films were characterized using SIMS, FTIR, XPS and other techniques. We discuss progress and mechanisms of compensation that account for the relatively low hole concentrations observed. @FootnoteText@ This abstract is subject to government rights.

9:20am **EM-TuM5 Low Resistivity Aluminum-Doped Zinc Oxide Grown by Atmospheric Plasma Enhanced Chemical Vapor Deposition***, **M.D. Barankin**, E. Gonzalez II, A.M. Ladwig, R.F. Hicks,* University of California, Los Angeles

Zinc oxide is a promising material for the transparent conducting oxide in thin-film photovoltaic cells. Today there is a strong push towards low-cost photovoltaics that may be fabricated on flexible substrates in a roll-to-roll process. In this presentation we will demonstrate the low temperature growth of Al-doped ZnO using atmospheric pressure plasma deposition with diethyl zinc and carbon dioxide as the oxygen source. Films deposited at a substrate temperature of 225°C exhibited resistivities of 2â?¢10-3 @ohm@â?¢cm, with an average transparency to visible light of at least 90%. It was found that the resistivity decreased with increasing substrate temperature from 100 to 230°C and with decreasing diethyl zinc feed rate. Maximum growth rates were in the range of 50 - 100 nm/min. These results are in contrast to those obtained by thermal CVD of Al/ZnO using molecular oxygen and diethyl zinc. In this case a sheet resistance of 0.2 @ohm@â?¢cm was obtained for deposition at 225°C. The atmospheric pressure plasma deposition process is unique in its capability of generating transparent conductive zinc oxide at low temperature.

9:40am **EM-TuM6 Transparent Conducting Zinc Oxide Thin Films Doped with Aluminum, Molybdenum, and Vanadium***, **J.N. Duenow**,* Colorado School of Mines*; T.A. Gessert, T.M. Barnes, T.J. Coutts,* National Renewable Energy Laboratory

Transparent conducting oxide (TCO) thin films are an integral part of photovoltaic cells, flat-panel displays, and electrochromic windows. The most commonly used TCO, tin-doped indium oxide (ITO), offers excellent performance, but in recent years material costs have risen dramatically because of increased demand for limited indium resources. We are investigating alternative TCOs based on zinc oxide (ZnO). As is the case with many TCO materials, investigations by many groups have not provided clear guidance toward significant improvement of ZnO material quality. We have examined whether electron transport can be enhanced by incorporating dopants with multiple valence states into the ZnO matrix--specifically, whether molybdenum (Mo; valence +6, 5, 4, 3, 2) or vanadium (V; +5, 4, 3, 2) can surpass the performance of aluminum (Al; +3). We deposited these ZnO-based materials by radio frequency magnetron sputtering from fully oxidized targets. We evaluated electrical, optical, and structural properties of these films using Hall measurements, spectrophotometry, and X-ray diffraction, respectively. Baseline studies of undoped ZnO revealed surprisingly high mobility values of 48 cm@super 2@/Vs in films deposited with a hydrogen-to-argon partial pressure ratio of 0.3% at a substrate temperature of 200°C; corresponding carrier concentrations were ~3 x 10@super 19@ cm@super -3@. Similar baseline studies with Al-doped ZnO resulted in films with typical mobility values of

25 cm@super 2@/Vs and carrier concentrations of ~6 x 10@super 20@ cm@super -3@ when deposited in 100% argon at 200°C. Initial results for Mo-doped films deposited in a hydrogen partial pressure ambient show that Mo is an effective dopant of ZnO, suggesting that multi-valent dopants may have value in TCO materials beyond that considered previously. We also present studies of V doping. This abstract is subject to government rights.

10:40am **EM-TuM9 Study of Impurities and Dopants in CVD Grown ZnO:N***, **S.E. Asher**, T.M. Barnes, X. Li, C.L. Perkins, M.R. Young, T.J. Coutts,* NREL

ZnO is an attractive material for optoelectronics due to its wide bandgap and use as a transparent conductor in photovoltaic devices. Reported work shows the ability to dope this material both n- and p-type.@footnote 1@ Films grown by metalorganic chemical vapor deposition (MOCVD) and plasma enhanced chemical vapor deposition (PECVD) have demonstrated p-type conductivity when doped with nitrogen, however, hole concentrations and mobilities are low, and films spontaneously type-convert over time.@footnote 2,3@ Compensation and/or passivation of the nitrogen acceptors by impurities such as carbon and hydrogen are thought to contribute to the poor electrical properties. In this work we have used SIMS and XPS to study contaminant and nitrogen doping levels in ZnO and ZnO:N films grown by MOCVD, PECVD and reactive sputtering. The CVD material is found to contain high levels of carbon and hydrogen, while sputter deposited material is considerably cleaner. We find decreasing carbon and hydrogen as a function of growth temperature for undoped MOCVD grown material. However, we find significant differences in the carbon and hydrogen in both CVD processes when nitrogen is present. For N-doped MOCVD films we also find carbon content appears to be linked to the proportion of oxygen in the deposition ambient. A similar relationship is not observed for N-doped PECVD or sputter deposited material. XPS indicates the presence of carbon bound to nitrogen in the MOCVD material. The relationship between carbon and hydrogen impurities, and nitrogen doping will be discussed.@footnote 4@ @FootnoteText@ @footnote 1@S.J. Pearton, et.al., Prog. Mater. Sci., 50, 293 (2005). @footnote 2@X. Li, et.al., J. Vac. Sci. Tech., A.21, 1342 (2003). @footnote 3@T.M. Barnes, et.al., Appl. Phys. Lett., 86, 112112 (2005). @footnote 4@This work was performed with the support of US Department of Energy Contract No. DE-AC36-99GO10337. This abstract is subject to government rights.

11:00am **EM-TuM10 Carrier Dynamics of ZnO Thin Films - Degeneracy, Inhomogeneity and Multiple Carriers***, **W.C.T Lee**, C.H. Swartz,* University of Canterbury, New Zealand*; M. Cheung, A.N. Cartwright,* University at Buffalo*; S. Chandril, T.H. Myers,* West Virginia University*; S.M. Durbin,* University of Canterbury, New Zealand

Though mobility measured by conventional Hall effect systems has long been used as a figure of merit for the electronic quality of semiconductors, many factors such as multiple layers and inhomogeneity can affect the accuracy and validity of the technique. This is particularly true for ZnO thin films, where many studies report very low electron (and hole) mobility values. Thin films are complicated by degenerate interface layers arising from poor substrate wetting and/or low-temperature buffer layer. By varying the magnetic field strength and temperature in a Hall effect measurement system, it is possible to separate the different carriers. For example, where single-field Hall effect yields a mobility of less than 50 cm@super 2@/Vs for one molecular beam epitaxy (MBE) grown ZnO/sapphire sample, the variable field technique shows a low-mobility degenerate layer in parallel with a bulk layer having a mobility of 200 cm@super 2@/Vs, approaching the best reported bulk values. Another useful probe of electronic properties is time-resolved photoluminescence (TRPL), which yields carrier lifetime as a figure of merit. For samples with an electron concentration of 10@super 19@ cm@super -3@, a parabolic temperature dependence of carrier lifetime was observed, with a decrease in lifetime as the temperature increases from 14 K up to 150 K, followed by an increase for further increases in temperature. On the other hand, concentrations of 10@super 18@ cm@super -3@ yield lifetimes that increase monotonically as the temperature increases. Taken together, these two techniques offer a more detailed picture of the characteristics of the bulk film, which cannot be adequately evaluated by a simple single-field Hall effect measurement. This work is funded in parts by The MacDiarmid Institute for Advanced Materials and Nanotechnology, University of Canterbury and Tertiary Education Comission Doctoral Scholarship (W.C.T.L).

11:20am **EM-TuM11 On the Morphology and Conductivity Control of the Expanding Thermal Plasma-Deposited ZnO Films***, **I. Volintiru**, M. Creatore,* Eindhoven University of Technology, The Netherlands*; C.I.M.A. Spee,* TNO Science and Industry, The Netherlands*; M.C.M. Van De Sanden,* Eindhoven University of Technology, The Netherlands

The bulk of the extensive research on ZnO focuses on different applications, ranging from photovoltaics to organic light emitting diodes; the plasma and film processes during growth are not well studied and, therefore, not controllable. For specific applications, good control of the ZnO film electrical and optical properties, as well as the surface morphology, is required. In this work, undoped and Al-doped ZnO layers are deposited using an Ar-fed expanding thermal plasma in which oxygen, diethylzinc, and trimethylaluminum (for Al doping) are admixed downstream. Typical downstream ion energies in this remote plasma are <2 eV, therefore energetic ion bombardment should not affect the film growth. Conductive films (5*10@super-4@ @OHM@cm) with native roughness of ~45 nm for 1 µm thickness, suitable for solar cell applications, were already obtained in our process. The film conductivity, however, shows a strong inhomogeneous depth profile, which could affect the suitability of this material for applications requiring thinner (< 200 nm) films, i.e. diodes and thin film transistors. To make our process more versatile, the ZnO film growth was investigated by studying the overall effect of the substrate temperature, working pressure, and ion bombardment (as delivered by an external RF bias). We use in-situ spectroscopic ellipsometry to monitor the refractive index, thickness and roughness development during the film growth. Atomic force microscopy, Hall and X-ray diffraction measurements are used to determine the morphological, electronic and structural properties of the films. Preliminary results demonstrate that the working pressure and substrate temperature play an important role in controlling the surface roughness of the ZnO films: smooth films, i.e. 0.02% roughness, are obtained by decreasing the pressure from 1.6 to 0.4 mbar, whereas higher texture, i.e. 10% of the film thickness, is achieved by increasing the substrate temperature from 200 to 400°C.

11:40am **EM-TuM12 X-ray Excited Optical Luminescence Studies of ZnO Nanowires and ZnO/Mg@sub x@Zn@sub (1-x)@O Core-Shell Nanowires****, **R.A. Rosenberg**, G.K. Shenoy,* Argonne National Laboratory*; L.-C. Tien, D.P. Norton, S.J. Pearton,* University of Florida*; X.H. Sun, T.K. Sham,* University of Western Ontario, Canada

As nanostructures become more complex having additional tools to unravel their optical properties will become more valuable. Due to their inherent asymmetry, the orientation of a nanowire will strongly influence its optical absorption and emission properties. In this talk we show how core-level, x-ray-excited optical luminescence (XEOL) using tunable x-rays from a synchrotron light source can be used to understand luminescence anisotropy in a disordered array of ZnO nanostructures. Optical luminescence yields from ZnO nanostructures at the Zn L and O K edges for both the band edge (~380 nm) and defect (~510 nm) peaks will be presented. At the Zn L edge the yields of both peaks are proportional to the x-ray absorption spectrum (XAS) of the wire. However, at the O K edge, marked contrasts are observed between wire XAS and the luminescence yields. There is a distinct enhancement of the yield for the band edge luminescence following 1s to 2p@sub z@ excitation relative to 1s to 2p@sub x,y@ absorption. For the defect peak excitation dramatic differences are seen between the XEOL yield and XAS of the wire. We will discuss these results in terms of the polarization of the excited electronic states and the nature of the defect states involved in the luminescence. In addition we will present recent results of a XEOL study on nanowires with a wurtzite ZnO core surrounded by a sheath composed of cubic Mg@sub x@Zn@sub (1-x)@O. The ZnO band edge luminescence (~370 nm) is blue shifted relative to the unsheathed nanowire. We also detect a deep UV peak at ~270 nm. By determining the yields of these peaks following excitation of the O K, Zn L, and Mg K core levels we are able to determine both the atomic origin and symmetry of the sites responsible for these peaks. @FootnoteText@ *This work was performed at the Advanced Photon Source and was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. W-31-109-ENG-38.

Electronic Materials and Processing
Room 2003 - Session EM-TuA

Materials for Power Electronics

Moderator: C. Eddy, Naval Research Laboratory

2:00pm **EM-TuA1 Processing of High-k Oxide Thin Films for High Energy Density Capacitors***, **G. Sethi,*** The Pennsylvania State University, US*; M.T. Lanagan, M.W. Horn,* The Pennsylvania State University

Oxide thin films with a focus on zirconia on silicon and glass substrates were prepared with the aim of optimizing the thin film processing parameters to produce 0% crystallanity (amorphous) films. Reduction in the crystallanity will improve dielectric breakdown strength, dielectric losses and the energy density. Reactive magnetron sputtering with a metallic target (76mm) is used for producing smooth, stoichiometric and dense films with high deposition rate. It is hypothesized that crystallanity (quantified from XRD) of a film can be reduced either by high bombardment to inhibit the crystallization or by low bombardment to limit ion mobility and the crystallization. High bombardment was achieved by using a pulsed-dc deposition process at low pressure (<1.3Pa) and high power (400W). The crystallanity reduces from 70% to 40% with the high bombardment, in the 'poisoned' sputtering mode. With the transition into 'elemental' sputtering mode, the deposition rate increases (20Å/s) crystallanity reduces (22%) and films become smooth. However EDS and SEM analysis revealed that the films are highly oxygen deficient (4 wt.% O@sub 2@) and defect-full with high compressive stresses. Increasing the film oxygen content during sputtering to near-stoichiometry does not reduce crystallanity and lowers the deposition rate (1.6 Å/s). Low bombardment was achieved by using RF sputtering at high pressures (13.3Pa) and low power (<200W). As imagined, the crystallanity in the film reduces with bombardment to 5%, but the deposition rate is substantially lowered (0.3 Å/s) with maximum 100nm thickness. The films are stoichiometric and near-stress free (-200MPa). The substrate temperature rise to as low as 70°C during the sputtering is responsible for this small crystallization. The temperature rise and hence crystallanity will be reduced by using liquid Nitrogen cooled substrate. Finally, the correlation between crystal structure and dielectric properties will be presented.

2:20pm **EM-TuA2 Growth of Epitaxial @gamma@-Al@sub 2@O@sub 3@ Films on 4H-SiC***, **C.M. Tanner,*** University of California, Los Angeles*; J. Lu, H.-O. Blom,* Uppsala University, Sweden*; J.P. Chang,* University of California, Los Angeles

The development of epitaxial high-k gate dielectrics has the potential to improve the performance of SiC power MOSFETs by improving the interface and enabling operation at a higher electric field. Al@sub 2@O@sub 3@ (k = 10) is a promising candidate due to its large bandgap and demonstrated stability in several crystalline phases. Al@sub 2@O@sub 3@ thin films were grown on chemically mechanically polished n-type 4H-SiC (0001) by atomic layer deposition (ALD) at 200°C using trimethylaluminum and water vapor. The films were stoichiometric with low carbon incorporation as evaluated by in-situ X-ray photoelectron spectroscopy (XPS). The as-deposited Al@sub 2@O@sub 3@ films were amorphous as determined by in-situ reflection high-energy electron diffraction (RHEED). Upon annealing in N@sub 2@ at 1100°C, the film crystallized to the @gamma@-Al@sub 2@O@sub 3@ phase as observed by RHEED, high-resolution transmission electron microscopy (HRTEM) and X-ray diffraction (XRD). Based on the Fourier transform of the HRTEM image, an epitaxial relationship of @gamma@-Al@sub 2@O@sub 3@ (111) on 4H-SiC (0001) was observed in which @gamma@-Al@sub 2@O@sub 3@ (-110) was oriented with 4H-SiC (-12-10). This orientation was further confirmed by XRD analysis in which only the @gamma@-Al@sub 2@O@sub 3@ (111) and (222) peaks were observed. An abrupt interface of both amorphous and crystalline Al@sub 2@O@sub 3@ with 4H-SiC was determined by HRTEM. Capacitance-voltage (C-V) and current-voltage (I-V) measurements of 4H-SiC MOS capacitors fabricated with 200 Å Al@sub 2@O@sub 3@ dielectric films were performed to compare the dielectric constant, fixed charge, density of interface states, and breakdown properties of epitaxial @gamma@-Al@sub 2@O@sub 3@ films with respect to those of amorphous Al@sub 2@O@sub 3@ as well as state-of-the-art thermal silicon dioxides.

2:40pm **EM-TuA3 SiC/SiO@sub2@ Interface and Near Interface Traps in SiC Based MOSFETs***, **P.M. Lenahan,*** Penn State University, US*; M.S. Dautrich,* Penn State University*; A.J. Lelis,* US Army Research Labs **INVITED**

Considerable progress has been made in the development of metal oxide semiconductor (MOS) field effect transistors (MOSFETs) based on SiC/SiO@sub2@ structures.@footnote 1@ The most promising devices utilize the 4H SiC polytype. Although, SiC/SiO@sub2@ MOS technology holds great promise in high-power and high-temperature applications, at the present time, SiC based devices exhibit mediocre performance. The device performance is limited, in large part, by trapping centers at and very near the SiC/SiO@sub2@ interface. This presentation will deal with electron spin resonance (ESR) and conventional electronic measurements of SiC MOS devices which provide some understanding of the physical and chemical nature of these performance limiting traps.@footnote 2@ Most of the ESR results have been obtained through very sensitive electrically detected magnetic resonance (EDMR) measurements on fully processed transistors via spin dependent recombination (SDR). These measurements clearly demonstrate fundamental differences between the physical nature of the defects which limit the performance of conventional Si/SiO@sub2@ based MOSFETs and current day SiC- based MOSFETs. In Si/SiO@sub2@ MOSFETs, for example, most of the observed "interface traps" are located precisely at the semiconductor/insulator boundary. In SiC-base devices this is not the case. The magnetic resonance results clearly demonstrate the presence of fairly high densities of deep level centers which are intrinsic in nature. These defects extend below the SiC/SiO@sub2@ interface into the SiC. We argue that the dominating interface/near interface defect in 4H SiC transistors involves a vacancy center. The concentration and physical distribution of this center depends strongly upon processing variables. @FootnoteText@ @footnote 1@ J.C. Zolper and M. Skowronski, MRS Bulletin 30.4 (Apr 2005) p273-275@footnote 2@ M.S. Dautrich, P.M. Lenahan, and A.J. Lelis: To Be Published, Mater. Sci. Forum 2006.

3:20pm **EM-TuA5 Diffusion Barriers for High-Temperature Reliability of SiC Junction Field Effect Transistors***, **S.E. Mohney**, C.M. Eichfeld, B.Z. Liu,* The Pennsylvania State University*; A.V. Adedeji, J.R. Williams,* Auburn University*; S.H. Wang, A. Owen,* The Pennsylvania State University*; S.-H. Ryu, S. Krishnaswami,* Cree

Tantalum-bearing diffusion barriers show considerable promise for the protection of contacts to SiC in air at high temperatures. Such barriers include Ta-Si-N, Ta-Si, Ta-Ru-N, and Ta-Ru. In this presentation, we report the high-temperature reliability of metallization stacks aged in air at 350°C for 5,000 h or longer. For many of the diffusion barrier compositions, the ohmic contacts beneath them maintain low specific contact resistances in the mid-10@super -5@ Ohm cm@super 2@ range as well as strong adhesion between the layers. We have also used Auger electron depth profiling to help us understand why some metallization stacks survive and others fail. Contrary to our original expectations, the addition of N can be detrimental to the Ta-Ru barriers because N is lost to the environment during aging, hastening oxidation. The most promising barriers have been successfully integrated into SiC JFETs, and the devices are now being aged at 350°C in TO-258 open cavity packages and periodically tested.

3:40pm **EM-TuA6 Boride-based Schottky Contacts to p-GaN***, **L.F. Voss**, L. Stafford, J.-J. Chen, S.J. Pearton, F. Ren,* University of Florida

An important aspect of the improvement of GaN-based devices for high temperature/high power electronic devices is the development of more reliable and thermally stable Ohmic and Schottky contacts on both n-type and p-type GaN. While the most common Schottky contacts to GaN are based on Ni/Au and Pt/Au, there is an increasing interest for metallization schemes with higher melting temperatures and better thermodynamic stability. In this work, we examine the potential of boride-based Schottky contacts to Mg-doped GaN layers grown by Metal Organic Chemical Vapor Deposition. This investigation is realized using current-voltage (I-V), x-ray photoelectron spectroscopy (XPS) and Auger electron spectroscopy measurements. It is found that W2B and W2B5-based Schottky diodes exhibit an excellent thermal stability upon annealing up to ~500Â°C. At higher annealing temperatures, the diodes show deterioration in rectifying behavior due to the onset of metallurgical reactions with GaN. On the other hand, the temperature dependence of the I-V characteristics indicates that tunneling through a Schottky barrier (thermionic field emission) is the dominant transport mechanism of the diodes under forward bias conditions. The characteristic energy related to the tunneling probability is however higher (E@sub0@~80 meV) than that expected from the concentration of Mg acceptors alone (E@sub0@~50 meV). This is found to correlate with the presence of acceptor-like defects in the p-GaN

surface vicinity that enhance the tunneling probability (defect-assisted tunneling). This high concentration of defects is also believed to explain the unexpectedly high barrier heights extracted from the tunneling model (~4.5 eV) which is higher than that deduced from the heterojunction band offsets obtained from XPS measurements. The possible mechanisms for reverse-bias current are also discussed.

4:00pm **EM-TuA7 Materials Issues in Power Electronics: Silicon to Silicon Carbide***, **K. Hobart**,* Naval Research Laboratory **INVITED**

The continuous advance of silicon power electronics has been made possible due to a well established materials foundation that has allowed power switching transistors to incorporate sophisticated device concepts, e.g. superjunction, junction termination extension, etc. The push to very high voltage silicon devices is primarily limited by its modest critical electric field when compared to materials such as silicon carbide and gallium nitride which have ~10x better theoretical breakdown performance. Si may still benefit from exploratory technologies to achieve higher voltage operation. However, the trade-off between switching speed, blocking voltage, and forward voltage drop cannot be fundamentally overcome for bipolar devices as it has been for unipolar devices with the superjunction, which has pushed DMOSFETs to surprisingly new performance levels. Silicon carbide, an indirect semiconductor, is an excellent candidate for wide bandgap minority carrier device technologies with high blocking voltages and low forward voltage drop. Some limitations to ultimate performance are high quality thick epitaxial layers and surface electric field termination. These two issues have been the focus of intense research recently and progress has been steady. Stable 10kV P-i-N diodes have been evaluated in our lab at temperatures above 200°C, however more work is needed to see sufficiently long working lifetimes in both forward and reverse operation. Specific challenges lie in reducing the basal plane dislocation density within the thick epitaxial layers, which lead to stacking fault generation and reduced current flow, and finding alternative surface passivation layers to handle the high surface electric fields and high temperatures typical of SiC devices. For many power electronics applications in the 10kV or less regime, SiC unipolar devices are preferred over bipolar minority carrier devices primarily due to improved switching speed. Unipolar devices have recently demonstrated extraordinary switching performance and lower voltage (1.2kV) SiC Schottky barrier diodes are now commercial products. SiC DMOSFETs with blocking voltages over 10kV have been demonstrated with a specific on-resistance ~0.2 ohm-cm@super 2@. Common material challenges exist with bipolar devices in the area of electric field termination and high temperature, high electric field surface passivation. Additionally, reliable MOSFETs demand extremely high quality gate dielectrics with very low interface state density and low fixed charge. The wide bandgap of SiC places additional burden on the gate and passivation dielectrics against charge injection from the semiconductor. Material challenges in Si and SiC power devices will be reviewed with emphasis on the most recent results that show a trend of performance to much higher voltage operation. Beyond high voltage devices, characteristics necessary for reliable large area, high current power devices will be discussed.

4:40pm **EM-TuA9 Optimized RIE Process for High Performance SiC BJTs***, **A.B. Goulakov**, F. Zhao, I. Peres-Wurfl,* Microsemi Inc.*; B. Van Zeghbroueck,* Colorado University*; J. Torvik,* Microsemi Inc.

SiC high-power RF devices are slated to replace Si devices to enhance the system performance and to reduce overall cost. Because of mechanical stability and the lack of dopant diffusion in SiC at normal temperatures, a common SiC RF BJT fabrication process includes homoepitaxial growth of differently doped layers followed by several dry etching steps. In this paper we will focus on two critical etch processes and two inch SiC wafer fabrication. The first process is a deep (> 5 micron) etch for electrical isolation between BJT fingers. The second process is a shallow (< 0.3 micron) precise etch down to the base layer. Due to thin 100 -150 nm base layer in the vertical n-p-n structure, a non uniform RIE process is a "yield killer". In this paper, we present details on a novel etching process for SiC RF BJTs fabrication process by combining optimized RIE etch, conductivity measurements, and oxidation. RIE etch parameters were optimized resulting in smooth etched surfaces and sufficient etch depth uniformity of < 8% for shallow etch, and < 2% for deep etch across two inch SiC wafers. Our etching process provides a precision (± 10nm) emitter etch to the emitter-base junction, even when the actual epitaxial layer thicknesses are different than expected. This method was also used to measure the emitter layer thickness and resistivity uniformity across different wafers and lots, and data will be presented. Furthermore, precise etching of the emitter epitaxial layer results in improved RF performance of the BJT by optimizing the base sheet resistance. Using this RIE process, we successfully fabricated several lots of 50W UHF SiC BJTs with a dc probe yield > 90%.

Electronic Materials and Processing
Room 2003 - Session EM-WeM

New Directions in Compound Semiconductors
Moderator: R. Goldman, University of Michigan

8:00am **EM-WeM1 Growth of GaP on Nanoscopically Roughened (001)Si***, I.K. Kim, X. Liu,* ***D.E. Aspnes,*** North Carolina State University

The chemical mismatch between III-V and Group IV materials makes the growth of III-V materials on Si substrates problematic. This is true even for GaP, which is nearly lattice-matched to Si. While GaP has been grown on (001)Si at low temperatures of the order of 300°C by organometallic chemical vapor deposition using easily decomposed tertiarybutylphosphine and triethylgallium precursors, higher growth temperatures offer the promise of higher-quality material. However, growth at temperatures of the order of 750°C with phosphine and trimethylgallium (TMG) precursors on standard RCA-cleaned (001)Si substrates yields widely separated protrusions of GaP separated by regions of bare Si. Here, we show that continuous films of GaP can be grown on (001)Si at these higher temperatures if the substrate is nanoscopically roughened in situ prior to deposition. Roughening not only increases the density of nucleation sites but also increases surface area and inhibits the diffusion of mobile species over the substrate surface without compromising the crystalline quality of the substrate, all of which act to promote the growth of continuous overlayers. However, we also find that the nanoroughness of the substrate can propagate through to the GaP surface, complicating the process. We take advantage of our in situ polarimetric diagnostic capabilities to explore the effect of different deposition conditions in real time, which allows us to efficiently optimize conditions with respect to both roughness and deposition. Our best films are obtained when TMG is introduced as pulses well separated in time.

8:20am **EM-WeM2 Formation and Ordering of Ga Droplets Using a Focused Ion Beam***,* ***W. Ye****, B.L. Cardozo,* University of Michigan*; X. Weng,* Penn State University*; J.F. Mansfield, R.S. Goldman,* University of Michigan

The directed self-assembly of low-dimensional semiconductor structures has been achieved using a variety of approaches to producing topographical patterns. However, an approach for achieving highly ordered arrangements of nanostructures with well-controlled shapes and size distributions has yet to be developed. Therefore, we are exploring the formation mechanisms of Ga droplets which may in turn be used for the directed seeding of semiconductor nanopillars. Using a Ga focused ion beam, we have investigated the formation and ordering of Ga droplets on a variety of semiconductor surfaces. On GaAs and GaSb surfaces, randomly distributed Ga droplets are observed above a critical dose (~4E16/cm^2). Subsequent ion beam irradiation results in growth and coalescence of the droplets. On silicon surfaces irradiated with similar doses, droplets are not observed, suggesting a droplet formation mechanism associated with preferential group V element sputtering, and subsequent local Ga agglomeration. Under further irradiation, Ga droplet motion is observed, possibly due to Marangoni motion. Interestingly, a higher droplet velocity is observed on GaSb than on GaAs surfaces, suggesting that droplet motion is dependent on the energetics of the Ga-substrate interface. To obtain ordered Ga droplets, we have milled arrays of holes with uniform sizes and shapes. By controlling the ion beam energy, current, and position, hole arrays with various sizes, depths, and periodicities may be produced. After scanning the ion beam over the patterned area, Ga atoms agglomerate within the holes, leading to the formation of ordered arrays of nearly uniformly-sized Ga droplets. We will also discuss the interaction of Ga droplets with various N-source gases, including the formation of GaN-rich nanocrystals upon exposure to ammonia vapor. @FootnoteText@ This work was supported by an Intelligence Community Postdoctoral Fellowship, the Radcliffe Institute of Advanced Study, NSF-NER, and AFOSR-MURI.

8:40am **EM-WeM3 Advances in THz Microelectronics***,* ***M.C. Wanke,*** Sandia National Laboratories **INVITED**

Unlike rf/microwave electronics and IR/visible photonics, applications of terahertz (THz) radiation have historically not enjoyed a strong technical infrastructure in semiconductor microelectronic components. This shortcoming has been particularly apparent in coherent THz sources and THz spectrometers, where existing instrumentation such as molecular gas lasers and Fourier transform or time-domain spectrometers tend to be relatively large, reliant on mechanically moving parts, and require regular maintenance. Over the last four years, some significant new developments in THz microelectronics have offered promising solutions to these problems. THz quantum cascade lasers (QCLs) have introduced a revolutionary new compact, microelectronic continuous-wave THz source that can generate the ~ 10 mW average power necessary for many applications. Also, it has been shown that THz radiation can resonantly excite two-dimensional plasmons, rather than electrons, in a quantum well formed in a semiconductor heterostructure. The ability to electrically tune the resonant plasmon frequency via a gate voltage bias makes possible a THz spectrometer-on-a-chip requiring no mechanically moving parts to generate spectral information across a large frequency range. This talk will discuss recent advances in these two areas. THz QCL performance will be reviewed with emphasis on the particular issues that face integrating THz QCLs, acting as illumination source and/or local oscillator, with microelectronic THz direct detectors and mixers. Recent work in plasmon THz detectors will also be discussed, including improvements in sensitivity, speed, and spectral coverage.

9:20am **EM-WeM5 Recent Development of THz Wave Generation, Detection and Applications****,* ***X.-C. Zhang,*** Rensselaer Polytechnic Institute **INVITED**

Terahertz (THz) radiation offers innovative sensing and imaging technologies that can provide information unavailable through conventional methods such as microwave and X-ray techniques. With the advancement of THz technologies, THz sensing and imaging will impact a broad range of interdisciplinary fields. THz radiation in the range of 0.1-10 THz induces low-frequency crystalline lattice vibrations, hydrogen-bond stretching, and other normal vibrational modes of molecules in many chemical and biological materials including ERCs, drugs and other biomolecules. The transmitted or reflected THz spectra of these materials contain THz fingerprints which provide rich information unavailable in other electromagnetic spectra. THz waves with low photon energies (4 meV for 1 THz, one million times weaker than X-ray photons) will not cause harmful photo ionization in biological tissues. As a potential sensing and imaging modality, THz radiation is considered a safe method for the operators and targets. THz radiation can penetrate through many non-polar dielectric materials including paper, cardboard, textiles, plastics, wood, leather and ceramics, with little attenuation. Therefore, THz technologies can be used for nondestructive/noninvasive sensing and imaging of targets under covers or in containers. I will report recent development of THz wave generation, detection, and applications. @FootnoteText@ * For AVS meeting, San Francisco, November, 2006.

10:40am **EM-WeM9 Influence of Nitrogen Incorporation on Electron Transport in Selectively Doped GaAsN/AlGaAs Heterostructures***,* ***Y. Jin****, M. Reason, X. Bai, H.A. McKay, C. Kurdak, R.S. Goldman,* University of Michigan

Dilute nitride (In)GaAs(N) alloys are useful for infrared laser diodes, high efficiency solar cells, and high performance heterojunction bipolar transistors. Typically, increasing N incorporation results in substantially lower electron mobilities than (In)GaAs. The precise role of N in lowering the electron mobility is not well understood. To determine the N-related electron scattering effects in GaAsN, with minimal contributions from ionized impurity scattering, we have studied modulation-doped AlGaAs/GaAs(N) heterostructures, with Si dopants in the AlGaAs barrier layer spatially separated from the undoped GaAs(N) channel layer. AlGaAs/GaAs(N) heterostructures and corresponding GaAs(N) bulk-like films with a variety of N concentrations were grown via molecular-beam epitaxy. Samples containing GaAs or GaAsN as the channel layer are referred to as "control" or "nitride" samples, respectively. The substitutional and interstitial N concentrations were determined using nuclear reaction analysis and Rutherford backscattering spectrometry studies of the bulk-like GaAsN films. Low T magnetoresistance and Hall measurements of the heterostructures reveal similar free carrier concentrations(in the dark) for the nitride and control samples, suggesting that N is not acting as a trapping center. Manipulation of the channel carrier density via front-gating and illumination with a light emitting diode reveals electron mobilities which increase with carrier density for all samples. For the control samples, µ~n^@gamma@, where @gamma@ is typically 1~1.5, suggesting the dominant scattering mechanism is long-range ionized impurity scattering. For the nitride samples, the mobility saturates for n > 1.5x10@super 11@cm@super -2@, suggesting that short-range N-induced neutral scattering is the dominant scattering source in GaAsN. The effects of varying substitutional and interstitial N concentrations on the transport properties of (In)GaAsN will also be discussed.

11:00am **EM-WeM10 Atomic Scale Morphology, Growth Behaviour and Thin Film Properties of Ga(In)NAs Quantum Wells*, T.S. Jones,*** Imperial College London, UK, United Kingdom*; W.M. McGee, R.S. Williams, T.J. Krzyzewski, M.J. Ashwin,* Imperial College London, UK*; C.P.A. Mulcahy,* Cascade Scientific Ltd, UK **INVITED**

Dilute nitride III-V-N semiconductor alloys are attracting considerable interest because of their highly unusual electronic properties and their promise as the active layer in a wide range of (opto)electronic devices. It is widely recognised that the structural and optical quality of Ga(In)NAs quantum wells (QWs) degrades significantly at relatively high N contents further development of this materials system requires a more detailed understanding of the growth behaviour and the effects of alloy composition, layer thickness and different growth conditions. In this talk I will present results from a scanning tunnelling microscopy (STM) study of the atomic-scale morphology and growth behaviour of Ga(In)NAs thin films of different composition grown on GaAs(001) by plasma-assisted molecular-beam epitaxy (MBE). High growth temperatures and N contents lead to significant phase segregation, the formation of large pits and an undulating 3D morphology.@footnote 1,2@ Measurements as a function of film thickness provide insight into the growth behaviour, in particular the onset of phase segregation and surface roughening.@footnote 2@ Spinodal decomposition is believed to facilitate lateral compositional modulation across the film, resulting in a strain-wave oscillating between compressed In-rich regions to tensile N-rich regions. Depending on the magnitude of this strain and the curvature of the resulting strain-wave a range of surface morphologies can result. Low growth temperatures are found to suppress phase segregation for N compositions up to 5% and additional characterisation by photoluminescence spectroscopy, X-ray diffraction, transmission electron microscopy and secondary ion mass spectroscopy indicate that high quality multi-QW layers can be grown with minimal clustering and with controllable emission in the range 1000-1600 nm. @FootnoteText@ @footnote 1@W.M. McGee et al., Appl.Phys.Lett. 87 (2005) 181905@footnote 2@W.M. McGee et al., Surf.Sci.Lett. (2006) submitted.

11:40am **EM-WeM12 In-Situ Investigation of Surface Stoichiometry During YMnO@sub 3@, InGaN and GaN Growth by Plasma-Assisted Molecular Beam Epitaxy Using RHEED-TRAXS*, R.P. Tompkins***, *E.D. Schires, K. Lee, Y. Chye, D. Lederman, T.H. Myers,* West Virginia University

Reflection high-energy electron diffraction total-reflection-angle x-ray spectroscopy (RHEED-TRAXS) can use high-energy electrons from the RHEED electron gun in an MBE growth system to excite x-ray fluorescence. Since the RHEED electrons just penetrate the surface, and by using a geometry that measures x-rays at the total reflection angle, RHEED-TRAXS probes the top 20 to 30 Å of material. Surface coverage of Ga and In during growth of GaN and InGaN was probed using this technique. Studies of the evolution of the surface layer of Ga on GaN during growth at substrate temperatures between 700°C and 750°C will be reported. RHEED-TRAXS measurements were performed during growth of InGaN by measuring the ratio of the In L@alpha@ to Ga K@alpha@ intensity. A significant surface coverage of In was observed at all temperatures investigated regardless of actual In incorporation. RHEED-TRAXS was also used to investigate surface segregation of Mg in GaN, indicating near monolayer coverage. This is useful for studies of the suppression of surface segregation of Mg for p-type doping of GaN, as well as determining a critical Mg surface coverage for polarity inversion. A second RHEED-TRAXS assembly was constructed for use in an oxide MBE chamber at WVU. Preliminary oxide work was performed using the initial RHEED-TRAXS setup, including measurement of monolayer thick layers and determination of the critical angle of Y L@alpha@ and Mn K@alpha@ x-rays. RHEED-TRAXS measurements performed during growth of YMnO@sub 3@ will be discussed. Because RHEED-TRAXS has near monolayer sensitivity, it is a useful tool for determination of conditions for stoichiometric layer-by-layer growth of YMnO@sub 3@. @FootnoteText@ This work was supported by AFOSR MURI Grant F49620-03-1-0330. R.P. Tompkins was supported in part by a grant from the West Virginia Graduate Student Fellowships in Science, Technology, Engineering and Math (STEM) program.

12:00pm **EM-WeM13 Surface Electron Accumulation in Indium Nitride Layers Grown by High Pressure Chemical Vapor Deposition***, R.P. Bhatta,* ***B.D. Thoms****, A. Weerasekera, A.G.U. Perera, M. Alevli, N. Dietz,* Georgia State University

High resolution electron energy loss spectroscopy (HREELS) has been used to characterize vibrational and electronic properties of indium nitride layers grown by high pressure chemical vapor deposition. HREEL spectra acquired using incident electron energy of 7 eV from atomic hydrogen cleaned InN layers showed loss peaks due to the Fuchs-Kliewer surface phonon at 560 cm@super -1@ and bending and stretching vibrations of surface N-H at 870 and 3260 cm@super -1@, respectively, indicating N-polarity of the InN layer. HREEL spectra acquired using incident electron energies from 7 to 35 eV exhibited a peak due to a conduction band plasmon excitation. The peak position shifted to lower energy as the incident electron energy was increased indicating a higher plasma frequency and a larger carrier concentration at the surface than in the bulk, which in turn implies a surface electron accumulation layer. The peak energy of the plasmon varied from 3100 to 4200 cm@super -1@ from a set of locations across the surface of the film. Room temperature infrared reflection measurements in the range of 200-8000 cm@super -1@ were acquired at comparable locations across the film and fit to using a three phase thin film reflection model. Plasma frequencies determined from the model fits are in good agreement with plasmon peak energies observed in HREELS at higher incident electron energies. Carrier concentrations determined from the infrared data vary across the film from 8.2x10@super 19@ to 1.4x10@super 20@ cm@super -3@ and carrier mobilities vary from 100 to 210 cm@super 2@/Vs.

Electronic Materials and Processing
Room 2003 - Session EM+MI-WeA

Magnetic Semiconductors

Moderator: S.A. Chambers, Pacific Northwest National Laboratory

2:00pm **EM+MI-WeA1 Spectroscopy and Magnetism of Oxide Diluted Magnetic Semiconductors*, D.R. Gamelin,* *K.R. Kittilstved, W.K. Liu,* University of Washington **INVITED**

Diluted magnetic semiconductor (DMS) nanostructures are pivotal architectural elements in many proposed spintronics devices. DMSs of ZnO are being intensely investigated for their potential use in spintronics technologies, but such applications have been hindered by their inconsistent magnetic properties. This talk will present our group's recent advances in the use of targeted chemical perturbations to manipulate high-Tc spin ordering in ZnO DMSs predictably and controllably.@footnote 1,2,3,4@ Apart from the technological advantages of reliable, controllable, and even switchable high-Tc ferromagnetic semiconductors, these experiments are motivated by the new fundamental insights they provide into the microscopic mechanisms behind magnetic ordering in this class of materials. The results from concomitant optical, magneto-optical, structural, X-ray absorption, and magnetic data collected on the same materials will be used to evaluate dopant electronic structure contributions to magnetic ordering, and the findings will be discussed in the context of current theoretical models of high-Tc ferromagnetism in oxide DMSs. @FootnoteText@ @footnote 1@Kittilstved, K. R.; Liu, W. K.; Gamelin, D. R. "Electronic Structure Origins of Polarity Dependent High-Tc Ferromagnetism in Oxide Diluted Magnetic Semiconductors." Nature Materials, 2006, 5, 291-297.@footnote 2@Kittilstved, K. R.; Norberg, N. S.; Gamelin, D. R. "Chemical Manipulation of 300K Ferromagnetism in ZnO Diluted Magnetic Semiconductors." Phys. Rev. Lett., 2005, 149049.@footnote 3@Kittilstved, K. R.; Gamelin, D. R. "Activation of High-Tc Ferromagnetism in Mn2+:ZnO using Amines." J. Am. Chem. Soc., 2005, 127, 5292-5293.@footnote 4@Schwartz, D. A.; Gamelin, D. R. "Reversible 300K Ferromagnetic Ordering in a Diluted Magnetic Semiconductor." Advanced Materials, 2004, 16, 2115-2119.

2:40pm **EM+MI-WeA3 Deposition of Doped ZnO by Pulsed Laser Deposition Utilizing Novel Ablation Targets*, T.C. Kaspar,*** *T. Droubay, S.M. Heald, V. Shutthanandan, P. Nachimuthu, C.M. Wang, S.A. Chambers,* Pacific Northwest National Laboratory*; K.R. Kittilstved, C.A. Johnson, K.M. Whitaker, D.R. Gamelin,* University of Washington

Zinc oxide (ZnO) is a promising material for optical, electro-optical, magneto-optical, and spintronic applications. The desired properties of ZnO are obtained by doping the material, in which case distribution and substitution of the dopants is of prime importance. Doped ZnO nanoparticles can achieve the necessary dopant dispersion and speciation to create high-quality material exhibiting, for example, the room temperature ferromagnetism necessary for spintronic applications. However, these nanoparticles may not be as useful in practical devices as high-quality epitaxial films. To this end, we have explored the deposition of epitaxial Co- and Mn-doped ZnO thin films by pulsed laser deposition (PLD), utilizing well-characterized doped ZnO nanoparticles as the basis for the PLD ablation target material. Ablating a target which already contains the dopant in the desired substitutional environment in ZnO should allow full substitution of the dopant into the epitaxial film and reduce or eliminate the formation of secondary phases. Initial results on Co-doped ZnO films deposited on Al@sub 2@O@sub 3@(0001) from a Co:ZnO nanoparticle target indicate that smooth, epitaxial ZnO films can be obtained. Co K-edge x-ray absorption near edge spectroscopy and extended x-ray absorption fine structure show full oxidation of Co to Co(II) for all oxygen pressures explored (5x10@super -5@ - 5x10@super -2@ Torr), with substitution of Co for Zn in the ZnO lattice. Issues associated with the nanoparticle ablation targets, such as target densification using low-temperature processing, particle and droplet ejection during ablation, and localized dopant diffusion in the ablated region, will be discussed.

3:00pm **EM+MI-WeA4 Room Temperature Ferromagneticism in Fe Im-planted ZnO Nanotips**, R.A. Bartynski,*** *D. Hill,* Rutgers University*; D.A. Arena,* National Synchrotron Light Source*; P. Wu, Y. Lu, J.F. Al-Sharab, F. Cosandey,* Rutgers University

Transition metal- (TM-) doped ZnO is a promising candidate dilute magnetic semiconductor for room-temperature spintronics applications. Controlled synthesis of nanoscale structures of these materials offers the possibility to develop low-dimensional spin-dependent electronic devices. We have grown well-aligned ZnO nanotips on SiO@sub 2@/quartz substrates using MOCVD. The tips were subsequently Fe-doped to a dose 5 x 10@super 16@ cm@super -2@ using ion implantation at 200 keV. The magnetic, structural, and chemical properties of both as-implanted and post-implantation annealed nanotips were studied using SQUID magnetometry, electron energy loss (EELS) and X-ray Energy Dispersive (EDS) spectroscopy in high resolution transmission electron microscopy (HRTEM), X-ray diffraction (XRD) and soft X-ray absorption spectroscopy (SXAS). The as-implanted tips were ferro-magnetic at room temperature with a saturation moment of ~ 0.2 µ@sub B@/Fe-ion, a remnant magnetization of ~0.03 µ@sub B@/ion, and a coercive field of ~150 Oe. The tips exhibit a core-shell structure with a high concentration (~ 8%) of Fe in the first ~ 10 nm, and about 3% in the interior, with roughly equal concentrations of Fe@super +2@ and Fe@super +3@ oxidation states. Post implantation annealing to 700C for 10 minutes improves crystallinity, produces a more uniform ~ 5% concentration of Fe, and increases the Fe@super +3@:Fe@super +2@ ratio, but significantly reduces the saturation magnetization. However, the tips remain ferromagnetic up to at least room temperature. The reduction in magnetic response, despite the increased magnetic moment/ion expected from the increased Fe@super +3@ concentration, suggests that the redistribution of Fe ions dominates the ferromagnetic coupling in the system. @FootnoteText@ * Supported by NSF Grant ECS-0224166.

3:20pm **EM+MI-WeA5 X-ray Characterization of Oxide-based Magnetic Semiconductors*, Y.U. Idzerda,*** *A. Lussier, J. Dvorak, A. McClure, M. Liberati, J. Holroyd,* Montana State University*; E. Arenholz,* ALS/LBNL*; S.R. Shinde, S.B. Ogale, T. Venkatesan,* University of Maryland, College Park **INVITED**

Although the evidence for magnetic semiconductors (not simply semiconductors which are ferromagnetic) is compelling, there is much uncertainty in the mechanism for the polarization of the carriers, suggesting that it must be quite novel. Recent experimental evidence suggests that this mechanism is similar to the polaron percolation theory proposed by Kaminski and Das Sarma,@footnote 1@ which was recently applied specifically to doped oxides by Coey et al.@footnote 2@ where the ferromagnetism is driven by the percolation of polarons generated by defects or dopants. We have used X-ray absorption spectroscopy at the L-edges and K-edges for low concentrations transition metal (TM) doped magnetic oxides (including TiO@sub 2@, La@sub 1-x@Sr@sub x@O@sub 3@, HfO@sub 2@, and In@sub 2@O@sub 3@). We have found that in most cases, the transition metal assumes a valence consistent with being at a substitutional, and not interstitial site. We have also measured the X-ray Magnetic Circular Dichroism spectra (including TM doped GaN and GaAs systems). Although these materials show strong bulk magnetization, we are unable to detect a robust dichroism feature associated with magnetic elements in the host semiconductor. In the cases where a dichroism signal was observed, it was very weak and could be ascribed to a distinct ferromagnetic phase (TM metal cluster, TM oxide particulate, etc.) separate from the host material. This fascinating absence of a dichroic signal and its significant substantiation of important features of the polaron percolation model may help to finally resolve the issue of ferromagnetism in magnetically doped oxides. @FootnoteText@ @footnote 1@ Kaminski and S. Das Sarma, Physical Review Letters 88, 247202 (2002).@footnote 2@ J. M. D. Coey, M. Venkatesan, and C. B. Fitzgerald, Nature Materials 4, 173 (2005).

4:00pm **EM+MI-WeA7 Characteristics of Ti@sub 1-x@Co@sub x@O@sub 2@ Thin Films Deposited by MOCVD*, A. McClure,*** *A. Kayani, M. Liberati, J. Dvorak, R.J. Smith, Y.U. Idzerda,* Montana State University*; E. Arenholz,* Lawrence Berkeley National Laboratory

Polycrystalline anatase thin films of Ti@sub 1-x@Co@sub x@O@sub 2@ were prepared on TiO@sub 2@ (50nm)/Si (111) substrates using liquid delivery metal organic chemical vapor deposition (MOCVD). This growth technique allows for the arbitrary variation of the Co concentration. The precursors for these growths were titanium isopropoxide and Co(TMHD)@sub 3@ dissolved in tetrahydrofuran. These films were characterized by X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD) to determine the phase of the TiO@sub 2@ host, the Co valency, and the presence of Co clusters. Film thicknesses and Co dopant concentrations were determined from Rutherford backscattering (RBS). A vibrating sample magnetometer (VSM) revealed room temperature ferromagnetism, allowing for a determination of the moment per Co atom vs. Co concentration. I will discuss these results in the context of the bound magnetic polaron model. Recent work@footnote 1@ suggests that this model may only need oxygen vacancies and

ferromagnetism may occur with nonmagnetic doping. Our experimental results on Pt:TiO@sub 2@ and its lack of ferromagnetism will also be presented. @FootnoteText@ @footnote 1@Osorio-Guillén, J., Lany, S., Barabash, S. V. and Zunger, A., Phys. Rev. Lett., 96, 107203 (2006).

4:20pm **EM+MI-WeA8 Detection of Nanometer-Sized Inclusions in Annealed Ga@sub 1-x@Mn@sub x@As from Atypical Scaling Behavior of the Anomalous Hall Coefficient*, H.K. Choi*,** *S.S.A. Seo, W.O. Lee, Y.S. Oh, K.H. Kim, T.W. Noh, Y.D. Park,* Seoul National University, Korea

We report on the anomalous Hall coefficient (R@sub s@) and longitudinal resistivity (@rho@@sub xx@) scaling relationship (R@sub s@=c@rho@@sub xx@@super n@) on three series of annealed LT-MBE Ga@sub 1-x@Mn@sub x@As epilayers (x ~ 0.55). After growth, Mn@sub Ga@ were varied by low temperature annealing from 200°-350°C. Our report of the scaling relationship can provide new methods to detect metallic secondary phases could not be observed in HRXRD and SQUID magnetometer. As-grown samples exhibit scaling parameter n of 1, which can be attributed to extrinsic skew scattering origins of the anomalous Hall Effect@footnote 1@ or to AHE attributed to phonon-assisted hopping between localized states in the impurity band.@footnote 2@ For annealing temperatures near the optimal (~ 250°C), we find n ~ 2 to be consistent with recent theories on the intrinsic origins of AHE in Ga@sub 1-x@Mn@sub x@As.@footnote 3@ For annealing temperatures above the optimum, we note n > 3, which atypical behavior cannot be explained in terms of AHE from a DMS system. This atypical behavior is similar to nanometer-sized super-paramagnetic particles in a paramagnetic matrix such as CoAg granular systems.@footnote 4@ This observation from AHE measurements agree well with optical spectroscopy measurements with observed characteristic features attributable to spherical resonance from metallic inclusions.@footnote 5@ @FootnoteText@ @footnote 1@ J. Smit, Physica (Ultrecht) 21, 877 (1955).@footnote 2@ A. A. Burkov and L. Balents, PRL 91, 057202 (2003).@footnote 3@ T. Jungwirth, Q. Niu, and A. H. MacDonald, PRL 88, 207208 (2002).@footnote 4@ Peng Xiong et al., PRL 69 (22), 3220 (1992).@footnote 5@ S.S.A. Seo et al., APL 82, 4749 (2003); S.S.A. Seo et al., JAP 95, 8172 (2004).

4:40pm **EM+MI-WeA9 Effect of Growth Conditions on the Magnetic Properties of GaGdN*, J.K. Hite*,** *R.M. Frazier, R.P. Davies, G.T. Thaler, C.R. Abernathy, S.J. Pearton,* University of Florida*; J.M. Zavada,* Army Research Office

Due to the increasing interest in spintronics, many attempts have been made at incorporating spin-based technology into the existing semiconductor technology, with a recent focus on rare earth doped GaN. GaGdN layers were grown by gas source MBE under a broad range of thicknesses and Gd cell temperatures. Magnetic measurements obtained using a SQUID magnetometer showed ferromagnetic behavior at room temperature. Magnetization of the material was dependent both on dopant cell temperature and crystalline quality. The Gd concentration was under the detection limit of secondary ion mass spectroscopy, and from the highly insulating nature of the films is estimated to be on the order of 10@super 16@ atom/cm@super 3@. In addition, the GaGdN films were also co-doped with Si at varying Si cell temperatures. In contrast to GaGdN, the co-doped material was conductive, with resistivities reaching 0.04 @ohm@-cm. Room temperature ferromagnetism was also retained, some of which exceeded that of the singly doped films. No evidence of second phases was seen in x-ray diffraction. These materials may be useful in the development of devices such as magnetic tunnel junctions and spin valves. This work is supported by the Army Research Office under W911-NF-04-10296.

Surface Science
Room 2004 - Session SS2+EM-WeA
Organic Film Growth and Characterization

Moderator: J.N. Russell, Naval Research Laboratory

2:00pm **SS2+EM-WeA1 Organic-on-Inorganic Thin Film Deposition and Vice Versa*, J.R. Engstrom,*** Cornell University **INVITED**

Thin films of organic materials differ fundamentally in many respects when compared to inorganic materials (metals, semiconductors and oxides). A key difference involves the presence of strong covalent/ionic bonding in the latter, whereas organic materials are often bound by rather weak dispersion forces. Another importance difference involves the methods and conditions used to assemble, fabricate and/or pattern these materials. For example, inorganic materials are often deposited at high temperatures, and patterned using aggressive subtractive techniques. Organics, on the other hand, can be deposited at very mild conditions, and can be patterned using additive techniques such self assembly. Interestingly, in many emerging technologies, fabricating robust interfaces between these two diverse classes of materials is absolutely essential, yet extremely challenging. In this talk we will present a summary of recent findings concerning the formation of two important interfaces: organic-on-inorganic and inorganic-on-organic. Concerning the former, we are currently conducting studies of the deposition of pentacene on clean and modified SiO@sub 2@ surfaces using supersonic molecular beam techniques. In this work we have focused initially on the effects of incident kinetic energy, angle of incidence and substrate temperature on both submonolayer and multilayer growth. Some of our more interesting observations include an effect of incident kinetic energy on the ratio of deposition rates observed for submonolayer vs. multilayer growth, and the presence of so-called rapid roughening for multilayer thin films. Concerning the latter type of interface, we are currently investigating the use of self-assembled monolayers (SAMs) to promote nucleation and growth of ultrathin inorganic films (TiN) via atomic layer deposition. In this work we have focused particularly on the initial nucleation regime, where we find that the SAMs affect nucleation significantly and in unexpected ways.

2:40pm **SS2+EM-WeA3 Organic Semiconductor Growth: Real-Time Observation of Growth Dynamics and Structural Evolution*, S.M. Kowarik,*** University of Oxford, UK, Germany*; A. Gerlach, S. Sellner, F. Schreiber,* Universitaet Tuebingen, Germany*; L. Cavalcanti, O. Konovalov,* ESRF, France

We use in-situ and real-time X-ray scattering during growth of the organic semiconductor diindenoperylene (DIP) to study the evolution of the film structure and morphology with time. Time resolved measurements in a broad q range, i.e. sampling a large number of Fourier components simultaneously, allow to directly measure (kinetically limited) growth dynamics and reveal transient structures which would be missed in post growth experiments. We identify structural and orientational transitions for the few-monolayer (ML) regime, as well as for thick (several 10's of ML) films. We show that the differences in the interaction of DIP with the substrate change the thickness as well as temperature range of the transitions, which include (transient) strain, subtle changes of the orientation, as well as complete reorientation. These effects should be considered rather general features of the growth of organics, which, with its orientational degrees of freedom, is qualitatively different from growth of inorganics. @FootnoteText@ S. Kowarik et al., Physical Review Letters, 96, 125504 (2006).

3:00pm **SS2+EM-WeA4 Resonant Soft X-Ray Emission and Resonant Inelastic X-Ray Scattering: New Probes of Electronic Structure in Organic Semiconductors***, Y. Zhang,* Boston University*; J.E. Downes,* Macquarie University, Australia*; A. DeMasi,* Boston University*; A. Matsuura,* AFOSR*; C. McGuinness,* Trinity College Dublin, Ireland*; P.A. Glans, T. Learmonth, S. Wang, L. Plucinski,* ***K.E. Smith,*** Boston University

We report the use of synchrotron radiation-excited resonant soft x-ray emission spectroscopy (XES) and resonant inelastic x-ray scattering (RIXS) to study the electronic structure of thin film organic semiconductors.@footnote 1@ XES directly measures the element-specific partial density of states (PDOS) in materials. When excited at a core level absorption threshold, RIXS features can be observed in the spectra, which are related to low energy excitations. The materials studied to date include a selection of metal phthalocyanines (Cu-Pc, FCuPc, VO-PC, TiO-Pc, Ni-Pc), as well as other organic semiconductor materials such as Alq3 and QAD. Our results are in excellent agreement with theory, but differ significantly from previously published results. The films were found to be highly susceptible to radiation damage. We demonstrate the ability to accurately measure states near E@sub F@, and show that previously published XES studies of organic semiconductors are dominated by beam damage effects. This application of resonant XES has important consequences for the determination of band gap energies in organic molecular systems, since it allows determination of the non-ionized electronic structure. Supported in part by the U.S. AFOSR under FA9550-06-1-0157, by the Petroleum Research Fund, and by NSF under DMR-0304960. The spectrometer system is funded by the U.S. ARO under DAAD19-01-1-0364 and DAAH04-95-0014. Experiments were performed at the NSLS which is supported by the U.S. DOE, Divisions of Materials and Chemical Sciences. @FootnoteText@ @footnote 1@ Y. Zhang, S. Wang, T. Learmonth, L. Plucinski, A.Y. Matsuura, S. Bernardis, C. O'Donnell, J.E. Downes, and K.E. Smith, Chem. Phys. Lett. 413, 95 (2005); J.E. Downes, C. McGuinness, P.A. Glans, T.

Learmonth, D. Fu, P. Sheridan, and K.E. Smith, Chem. Phys. Lett. 390, 203 (2004).

3:20pm **SS2+EM-WeA5 Structure in Self-Assembled Organic Thin Films**, ***S.L. Bernasek***, *F. Tao,* Princeton University; *Y. Cai,* Brookhaven National Laboratory **INVITED**

In the self-assembly of long chain hydrocarbons and substituted hydrocarbons on solid substrates, three classes of interaction energies govern the self-assembly process. They are chain-chain interactions within a lamella on the surface, interactions between ordered lamellae, and interactions between the adsorbate molecules and the underlying substrate. These interactions may be dispersive, or more directed interactions such as hydrogen bonding or acid-base interactions. We examine the interaction energies in these self-assembled organic monolayers based on structural studies using molecular resolution scanning tunneling microscopy for a variety of functionalized hydrocarbon molecules. Competitive coadsorption studies, and the effects of solvent on the stability of the structures formed are examined. Long chain carboxylic acids, di-acids, esters, anhydrides, alcohols, and di-alcohols adsorbed on highly oriented pyrolytic graphite have been examined.

4:00pm **SS2+EM-WeA7 Epitaxial Nanolayers of Organic Small Band Gap Semiconductors: Growth and Electronic Properties of Quaterrylenes on Au**, ***R. Franke***, *C. Wagner, S. Franke,* TU Dresden, Germany; *S.C.B. Mannsfeld,* Stanford University; *F. Fritz,* TU Dresden, Germany

The understanding of the physical properties of organic thin films is of importance for their application in novel devices. Thin films grown by the Organic Molecular Beam Epitaxy technique often exhibit highly ordered layer structures. Their physical structure is usually governed by a fine balance between weak molecule-molecule interactions and a small lateral variation of the molecule-substrate interaction potential. In order to investigate the energetics of such a heteroepitaxial layer system, one has to consider large molecular domains.@footnote 1,2@ Here we report on films of large molecules, namely quaterrylene (QT) and quaterrylenetetracarboxylic-dianhydride-diimide (QTCDI), on Au(111) in UHV. These materials are especially interesting due to their long-wavelength absorption in the NIR. In our combined LEED and STM study we found a point-on-line coincident growth with flat lying molecules for the first monolayer (ML) of QT, while we observe alternating upstanding and flat lying molecules in the second ML.@footnote 3@ In contrast, the arrangement of the QTCDI molecules in the first ML differs strongly, due to the presence of the substituents. We will also show that our experimental results correspond nicely to potential energy calculations on large ordered QT and QTCDI domains. The electronic properties of these ultrathin films were investigated by Scanning Tunneling Spectroscopy. In case of QTCDI we found a HOMO-LUMO gap of 2.1 eV, while we obtained 2.5 eV for the smaller QT. The comparison to absorbance measurements on mica allows us to estimate the exciton binding energies. @FootnoteText@ @footnote 1@ S.C.B. Mannsfeld and T. Fritz, PRB 93 (2004) 075416.@footnote 2@ S.C.B. Mannsfeld, K. Leo, and T. Fritz, PRL 94 (2005) 056104.@footnote 3@ R. Franke, S. Franke, S.C.B. Mannsfeld, C. Wagner, T. Dienel, and T. Fritz, APL 88, (2006) 161907.

4:20pm **SS2+EM-WeA8 One-Dimensional Supramolecular Assemblies on Stepped Surfaces: What Makes Them Extend into the Mesoscale Length Regime?**, ***J. Schnadt***, University of Aarhus, Denmark, Sweden; *E. Rauls, Wei Xu, J. Knudsen, R.T. Vang, B. Hammer, F. Besenbacher,* University of Aarhus, Denmark

On perfect single crystal surfaces small organic molecules can self-assemble to form ordered one- and two-dimensional networks based on hydrogen bonding and other non-covalent interactions (see, e.g., Ref. 1). Such networks can grow very large and extend into the meso- and macroscale length regimes. Most real surfaces of interest, however, are afflicted with defects such as monatomic steps. These defects typically hinder the formation of large-scale networks. We show here for a particular example that it is possible to overcome this obstacle by choosing the right combination of surface and organic molecule. In the present case we investigated the self-assembly of 2,6-naphthalene-dicarboxylic acid (NDCA) on a stepped Ag(110) surface and compared it to the self-assembly of the same molecule on the Ag(111) and Cu(110) surfaces. The STM and XPS results show that NDCA on Ag(110) forms macroscopic-scale one-dimensional and directional structures across the step edges with maximum lengths in the micrometer range, notwithstanding the stepped character of the surface. This stands in contrast to the other surfaces, where the step-crossing behaviour is not observed. The experimental results together with density functional theory calculations show that the primary driving force for the formation of these long one-dimensional assemblies is hydrogen bonding, and that these bonds form also at the Ag(110) step edges. The bond formation across the step edges is driven by a combination of different factors, including the strength and bond directionality of the hydrogen bonds, the assembly directionality mediated by the substrate, and a sufficient flexibility of the adsorbate molecular backbone. A subtle balance of these factors, which depends on the particular adsorbate and the particular substrate, is required to achieve the observed step-edge tolerance of the assembly. @FootnoteText@ @footnote 1@ J. V. Barth, G. Costantini, and K. Kern, Nature 437, 671 (2005).

4:40pm **SS2+EM-WeA9 Controlled Self-Organization of Nanodots at Organic p-n Heterojunctions**, *E. Barrena,* ***D.G. de Oteyza,*** Max-Planck-Institut fuer Metallforschung, Germany; *J.O. Osso,* Institut de Ciencia de Materials de Barcelona, Spain; *S. Sellner, H. Dosch,* Max-Planck-Institut fuer Metallforschung, Germany

*Many organic devices like Light-Emitting Diodes (OLEDs), solar cells or ambipolar transistors rely on p-n junctions of organic semiconductors. Although numerous studies have been devoted to the characterization and optimization of the performance of p-n organic-based devices, the present-day knowledge on the physical principles of the growth of organic heterostructures is still poor. By combining atomic force microscopy with surface-sensitive X-ray diffraction, we have been able to get a detailed in-situ insight into the microscopic processes which take place during the growth of p-conducting di-indenoperylene (DIP) molecules onto n-conducting copper-hexadecafluorophtalocyanine (F16CuPc) thin films. We demonstrate the self-organization of well-ordered DIP nanodots with high crystallinity and show that their growth is intimately related to a novel type of interface reconstruction of the underlying F16CuPc film which affects three monolayers adjacent to the organic p-n interface. This self-organized nanopatterning of an organic p-n-junction opens new possibilities for organic electronic functions.

Electronic Materials and Processing
Room 2003 - Session EM+AS-ThM

High-k Dielectric Characterization

Moderator: A. Rockett, University of Illinois, Urbana-Champaign

8:00am **EM+AS-ThM1 A Study of High Dielectric Constant Magnesium Oxide Film Interfaces with Si***, **L. Yan**, R.P. Shrestha, E.A. Irene,* University of North Carolina-Chapel Hill*; L. Zhong, I. Kim, O. Auciello,* Argonne National Lab

In a recent report we have identified MgO as a potential high dielectric constant (@Kappa@) gate dielectric because of its chemical inertness enabling sharp interfaces and wide band-gap (7.3 eV) for large band offsets with silicon (Si) to minimize leakage. Our prior investigation of reactively sputtered MgO on Si revealed impressive interfacial electronic properties as compared with the conventional SiO@sub 2@/Si, in particular comparable interface trap densities (D@sub it@). The present study is aimed at a closer exploration of MgO thin films, prepared using two different oxidizing agents: molecular and atomic oxygen on reactively sputtered Mg. In situ XPS, Mass Spectrometry of Recoiled Ions (MSRI) and spectroscopic ellipsometry (SE) were used to monitor the evolution of the interfaces with MgO. This, coupled with post-deposition, ex situ cross-sectional TEM, provided an accurate materials description of the MgO/Si interface. Electronic measurements, including capacitance versus voltage (C-V), conductance (G(@omega@)) versus gate voltage (G(@omega@)-V), and current flux versus electric field (J-E), were conducted on capacitor structures to determine @Kappa@, D@sub it@, and leakage current, respectively. Our results show that thin MgO films can provide a superior high-@Kappa@ dielectric for many electronic applications. This work is supported by the National Science Foundation (NSF) Materials Research Division.

8:20am **EM+AS-ThM2 Channel Drift Mobility in High-k Transistors from Galvanomagnetic Measurements***, **R.T. Bate**, W.P. Kirk, R. Agrawal,* University of Texas at Arlington*; R.M. Wallace, B.E. Gnade, G. Pant,* University of Texas at Dallas

Effective mobility µ@sub eff@ in high-k transistors can be degraded by enhanced scattering of carriers and by trapping. The drain current is proportional to the product of the channel carrier density n and the drift mobility µ, and the capacitance measurement used to determine channel carrier density cannot distinguish between free and trapped charge. The result is that trapping can cause µ@sub eff@ to underestimate µ. We combine Hall effect and magnetoresistance (MR) measurements to determine µ of carriers in the channel. Then effective mobility reductions due to increased scattering can be separated from loss of carriers due to trapping. In the past, Hall effect measurements have been used to measure Hall mobility in MOSFET and MISFET channels, and µ has been estimated by making assumptions about the magnitude of the Hall factor r@sub H@ which is the dimensionless ratio of the Hall mobility to the drift mobility, (i.e. r@sub H@ = µ@sub H@/µ). r@sub H@ is usually assumed to be close to unity. Theory indicates that r@sub H@ is strongly dependent on the type of carrier scattering in the channel, which is usually not known a priori. This uncertainty is currently the main drawback of the Hall effect as a means of determining channel drift mobility. We propose to use the MR to estimate r@sub H@ . Analysis based on the silicon 100 inversion layer shows that the MR is strongly correlated with r@sub H@, regardless of the scattering mechanism. This is being experimentally verified on MOSFET structures where r@sub H@ and µ can be independently determined, and the results are being carried over to high-k MISFETs. Knowing r@sub H@ permits µ to be estimated, not only from Hall measurements, but also, for routine diagnosis, from MR measurements on conventional transistors (not Hall devices), even in the presence of significant trapping. @FootnoteText@ Partial support by Texas Advanced Technology Program of THECB #003656-0029-2003.

8:40am **EM+AS-ThM3 Interface Composition and Band Alignment in Nano-electronics***, S. Rangan, E. Bersch, R.A. Bartynski, L.V. Goncharova, T. Gustafsson, **E. Garfunkel**,* Rutgers University **INVITED**

We outline some key issues relevant to characterization of interfaces in next-generation highly-scaled CMOS devices. Selected experimental results as well as conceptual approaches to addressing the structure, bonding and band alignment problems will be discussed. The semiconductor/high-K and high-K/metal interfaces will be the primary focus of the discussion. Ion scattering, photoemission, inverse photoemission, electron microscopy, and other methods have been used to examine (i) amorphous high-K gate dielectrics and their interfaces on Si, Ge and GaAs, (ii) epitaxial oxides on Si, and (iii) metal-dielectric interfaces for gate metallization. From a comparison of experimental and theoretical results we are able to develop a better understand the electronic properties of the different structures. We find that the band gap, barrier height and dielectric response of this class of materials are very phase-dependent. An understanding and control of band alignment for charge injection and carrier confinement must be realized if novel materials are to be incorporated in future nano-electronic devices.

9:20am **EM+AS-ThM5 Band Offsets Measurements of Metal/High-k/Semiconductor Structures***, **S. Rangan**, E. Bersch, R.A. Bartynski, E. Garfunkel,* Rutgers University

The study of high-k dielectrics and metal gate electrodes has been ongoing in order to thoroughly understand the properties of these materials and to contribute to their implementation in Metal/Oxide/Semiconductor Field Effect Transistors. The band offsets are an important property of Metal/Oxide/Semiconductor (MOS) stacks in that the leakage current depends directly on them. An understanding of the band offsets, particularly the role played by the interface dipole, may enable the development of tunable band offsets at the interfaces. We have used in situ photoemission and inverse photoemission as well as synchrotron photoemission to measure the band offsets between the layers of MOS stacks. UV, X-ray, and inverse photoemissions give us a direct measurement of the bandgap of the dielectric and offsets between dielectric and semiconductor bands. With sequential metallization (Al, Ru, Ti) shifts of the band edges are measured as a function of metal coverage. The band offsets we measure for the metal/oxide and oxide/semiconductor interfaces are, to first order, in good agreement with the modified Schottky Mott model which treats the interface with bare bulk (metal, oxide or semiconductor) properties. But as expected, photoemission reveals much more complicated interfaces, and in particular strong effects on the chemistry of the entire stacks upon metal deposition. We report here the energy gap and band offsets of several HfxSi1-xO2 oxides on a Si substrate, as well as the effect of Ru (high work function metal) and Al (low workfunction metal) deposition on theses dielectrics. Both Ru and Al induce an energy shift of the core levels (Hf4f, Si2p), the valence and conduction bands â?" the shift depends both on the oxide and on the metal choice. Ru stays metallic upon deposition on the oxide, whereas Al is shown to be oxidized even at room temperature. We will show that the source of oxygen can be the dielectric or the interface layer between the substrate and the oxide.

9:40am **EM+AS-ThM6 A Soft-X-Ray Photoelectron Spectroscopy Study of D-State Contributions to Valence Band States in Nanocrystalline HfO2, TiO2, and Hf1-xTixO2 Alloys***, **L.B. Fleming**, M.D. Ulrich,* NC State University*; J. Rowe,* University of North Carolina at Chapel Hill*; C.C. Fulton, G. Lucovsky,* NC State University

This paper compares d-state contributions to valence band, and valence band edge defect states determined from i) synchrotron soft x-ray photoelectron spectroscopy (SXPS) at photon energies between 40 and 80 eV, with d-state contributions determined from ii) ultra-violet photoemission spectroscopy (UPS) at 21.2 eV. Measurements have been performed on thin films of HfO@sub 2@, TiO@sub 2@ and Hf@sub 1-x@Ti@sub x@O@sub 2@ alloys prepared by reactive evaporation, and subjected to post deposition annealing at 700°C. The atomic Hf, Ti and O contributions to the valence band states in the SXPS and UPS spectra are at approximately the same energies with respect to the Fermi level, but have different spectral weighting. The only significant differences in the USP and SXPS spectra are defect state features at, and above the valence band edge. The UPS spectra, limited by the incident photon energy, yield a single feature with a spectral peak ~1 eV above the valence edge, whereas SXPS spectra, performed with higher incident photon energies can defect electronic states deeper into the forbidden band gap. The SXPS spectra confirm the band edge features, as well as identifying a second defect states at higher energy, ~3 eV above the valence band edge. The defect states in TiO@sub 2@, and the alloys are interpreted in as O-atom vacancy states in which the formal valence of Ti is 3+ rather than 4+. This assignment is based on comparisons between SXPS spectra, and epsilon 2 spectra obtained from analysis of reflection spectra of Ti@sub 2@O@sub 3@ over a spectra range from 0.01 eV to 10 eV. Defect states in HfO@sub 2@ are similar, and assigned to d-states of Hf@super 3+@ at O-atom vacancies.

10:00am **EM+AS-ThM7 Line-Width and Symmetry Changes in Jahn Teller Term-Split Sc 3d-States in LaScO3 as a Function of Deposition and Annealing Temperatures***, **H. Seo**,* NC State University*; L.F. Edge, D.G. Schlom,* Penn State University*; N.A. Stoute, G. Lucovsky,* NC State University

LaScO@sub 3@ conduction band states are derived in part from Jahn-Teller-split Sc 3d-states in distorted octahedral arrangements of O-neighbors. Conventional XRD for films deposited at ~300°C, and annealed to 700°C display no evidence for crystallinity, while films annealed to >800°C display strong crystalline features. New studies of conduction band states by i) vacuum ultra-violet spectroscopic ellipsometry (VUV SE), and ii) x-ray absorption spectra (XAS) for transitions from (a) spin-orbit split Sc 2p core states (Sc L@sub 2,3@) and (b) the O 1s core state (O K@sub 1@), are compared, providing insights into scales of order. XRD results are indicative of grain sizes >5 nm for >800°C anneals, but do not distinguish between i) amorphous films, and ii) nanocrystalline films with grain sizes

10:20am **EM+AS-ThM8 Trends in Core Level Binding Energies of Mixed Oxide Candidates for High-@kappa@ Dielectrics***, **A. Mathew**,* University of Delaware*; L. Bao,* Dupont Inc.*; K. Demirkan,* University of Delaware*; C.-G. Wang, G.D. Wilk,* ASM America Inc.*; R.L. Opila,* University of Delaware

Hafnium silicates and lanthanum aluminates are among the many proposed candidate materials for replacing the SiO@sub 2@ gate dielectric in transistors for low standby power applications. Photoelectron spectroscopy with its sensitivity to local chemical bonding is an invaluable tool for investigating these interfaces. Hafnium silicates were deposited using Atomic Layer Chemical Vapor Deposition (ALCVD@super TM@), and the lanthanum aluminates were sputter deposited. Systematic trends in core level binding energies are observed for the unannealed mixed oxide systems as a function of composition. The degree to which such shifts occur is seen to be a function of both the amount of charge transfer between the component cations as well as the local lattice potential, both initial state effects. The O 1s photoemission peak and the N 1s peak (in the case of nitrided films) reflects the local bonding environment in the film, and its variations with different concentrations of a number of cations are studied as well. The O 1s and N 1s peaks can be deconvoluted into components arising from its bonding with a higher or lower electronegativity cation, and their relative intensities vary with composition. These insights into the local bonding structure are important for improving our capability to engineer the ideal semiconductor / high-@kappa@ interface for optimal device performance.

Electronic Materials and Processing
Room 2001 - Session EM-ThM

Organic Electronic Materials and Devices

Moderator: D.J. Gundlach, NIST

8:00am **EM-ThM1 Organic Thin Film Transistors with an Organic/High-k Inorganic Bilayer Gate Dielectric Layer***, **Y.G. Seol**,* Sungkyunkwan University, Korea*; S.S. Lee, J.H. Lee,* Hanyang University, Korea*; N.-E. Lee,* Sungkyunkwan University, Korea

To develop the high performance OTFT devices, low threshold voltage (V@sub T@), low-leakage current, high current on-off ratio, and channel mobility are needed. To achieve low V@sub T@ and low-leakage current level, use of thin high-k gate dielectrics is required. For this purpose, the organic/inorganic (high-k) bilayer gate dielectric layers were investigated in this work. Flexible organic thin film transistors were fabricated using pentacene as a semiconducting layer and electroplated nickel (Ni) as a gate electrode on polyimide substrate. Electroplated gate electrode formed on the plasma-treated polyimide substrate provides a good adhesion. First, poly(4-vinyl phenol) (PVP) as an organic gate dielectric layer was deposited by spin coating after Ni gate electrode formation. Ultra-thin (10 nm) HfO@sub 2@ as a high-k dielectric deposited by ALD (atomic layer deposition) on the spin-coated PVP layer. ALD of HfO@sub 2@ layer was carried out at the substrate temperature 220 ~ 240°C. Pentacene as a semiconductor layer was thermally evaporated on the gate dielectric layer using a shadow mask in vacuum chamber at the substrate temperature of 80°C and then the thermal evaporation of gold source and drain electrodes was followed. The OTFT devices with no ALD HfO@sub 2@ layer were also fabricated for comparison. The channel length varied from 10 to 110µm, and the channel width was 800µm. The measured I-V characteristics indicated the significant reduction in the leakage current for thinner PVP layer and improvement of current on-off ratio.

8:20am **EM-ThM2 Low Voltage Organic Field-Effect Transistors with High k Nanocomposite Dielectric Gate Insulator***, **A. Rasul**, J. Zhang, D. Gamota,* Motorola Inc.*; C.G. Takoudis,* University of Illinois at Chicago

Solution processed nanocomposite dielectric material with a high dielectric constant was demonstrated as a gate insulator for organic electronics applications. A nanocomposite consisting of cross-linked Propylene Glycol Methyl Ether Acetate and Barium Titanate (BTO) nanoparticles was developed and utilized as the gate insulator. The high relative permittivity (k=35), bimodal nanocomposite utilized had two different filler particle sizes 200 nm and 1000 nm diameter particles. Bottom contact organic field-effect transistors (OFETs) were demonstrated using a combination of printing and spray coating technologies. A metal coated plastic film was used as the flexible gate substrate. An amorphous organic semiconductor was utilized as the active layer. OFETs with the solution processed nanocomposite dielectric had a high field-induced current and a low threshold voltage and thus a low operating voltage due to the high capacitance gate insulator. We review the characteristics of the nanocomposite material and discuss the processing and performance of the printed organic devices. To the knowledge of the authors, this nanocomposite has the highest reported dielectric constant of a solution processed gate insulating material for an OFET worldwide.

8:40am **EM-ThM3 New Materials and Processes for Organic Transistors, Inorganic Transistors, and Printed Electronics***, **T.J. Marks**,* Northwestern University **INVITED**

Materials chemists are exceptionally skilled at designing and constructing individual molecules with the goal of imbuing them with defined chemical and physical properties. However, the task of rationally assembling them into organized, functional supramolecular structures with precise, nanometer-level control is a daunting challenge. In this lecture, approaches to addressing this problem are described in which the ultimate goal is the fabrication of organic electronic circuit by printing techniques. Issues here concern not only the rational design of high-mobility p- and n-type organic semiconductors, but also dielectrics with ultra-high capacitance, low leakage, and high breakdown fields.

9:20am **EM-ThM5 Organic Thin-Film Transistors with Novel SAM-Modified Dielectrics***, **I.G. Hill**, M. McDowell,* Dalhousie University, Canada*; J.E. McDermott, S.L. Bernasek, J. Schwartz,* Princeton University

Pentacene organic thin-film transistors (OTFTs) exhibit charge carrier mobilities very similar to their amorphous silicon counterparts. Several impediments remain, however, which hinder their use in consumer electronic devices, including long-term stability and poor sub-threshold performance. While the implications of the former are obvious, those of the latter are subtler. The sub-threshold slope (a measure of the sharpness of the off-to-on transition) and the threshold voltage impact the total voltage swing which must be applied to the device gate to switch between the on and off states, and thus dictate power supply requirements and power dissipation. Pentacene devices utilizing bare silicon dioxide as a gate dielectric exhibit poor sub-threshold slopes (several volts/decade) and, typically, large positive threshold voltages. Both effects can be attributed to a high dielectric/semiconductor interfacial charge trap density. We have investigated the use of phosphonate-linked self-assembled monolayers (SAMs) to modify the electronic structure to the dielectric/pentacene interface. The SAM molecules were chosen to present a surface for pentacene growth which resembled an existing organic semiconductor layer, thus reducing the density of interfacial defects and charge trapping sites. Devices incorporating these SAMs have demonstrated near-zero threshold voltages and sub-threshold slopes less than 200 meV/decade of current, which is only 3x the thermodynamically allowed limit.

9:40am **EM-ThM6 Growth of Pentacene Films: Influence of Substrates***, **G. Witte**, D. Kaefer, Ch. Woell,* Ruhr-University Bochum, Germany

In recent years organic semiconductors have gained wide-spread attention due to their promising potential as active materials for organic electronic applications. Of particular interest among such materials are oligoacenes, such as pentacene, because of their ability to form crystalline phases which reveal remarkable high carrier mobilities. In view of the interrelation between intermolecular packing and electronic properties a precise control of the molecular packing and orientation in thin (poly-) crystalline films is of vital interest especially for devices such as OFETs where high charge carrier mobilities are required. Here we report the result of a comprehensive growth study of thin pentacene films deposited by OMBD under vacuum conditions onto various metal surfaces. By combining different microscopy techniques including STM, AFM, SEM with X-ray absorption spectroscopy (NEXAFS) the evolution of such organic films has been analyzed as a

function of thickness and deposition parameters (rate and temperature). We demonstrate that the resulting molecular orientation and the film morphology depend critically on the roughness and chemical termination of the substrate whereas growth rate and substrate temperature mainly affects the grain size. Dewetting phenomena which usually dominate the morphology of pentacene films on clean metal substrates can be suppressed by first coating the substrate with self-assembled monolayers (SAMs) which leads to rather smooth films. Possible driving forces for the appearance of the various film structures and strategies for a rational control of the microstructure of such organic films are discussed.

10:00am **EM-ThM7 In-Plane Anisotropy of Pentacene Crystals on Surface Alignment Layers and its Influence on Photovoltaic and Thin-Film Transistor Device Characteristics***, **A. Amassian**, A.C. Mayer, A. Kazimirov, D.-M. Smiglies, G.G. Malliaras,* Cornell University

Significant research effort has gone into understanding and controlling the growth of pentacene thin films, with the ultimate goal of enhancing charge transport by favouring 2D over 3D growth on surfaces. As pentacene behaves as a 2D powder on insulating surfaces, and electron transport is limited by charge trapping at grain boundaries, electron mobility can be further improved (in some directions) by orienting crystal growth using surface alignment layers. In this paper, we report on our recent efforts to induce in-plane anisotropy in pentacene crystals on a variety of mechanically rubbed surfaces, including conducting polymer (PEDOT:PSS) surfaces, high-k dielectrics (fluorinated ter-polymer) and various self-assembled monolayers (SAMs). In situ x-ray scattering measurements carried out at the Cornell high energy synchrotron source (CHESS) in a variety of measurement configurations show evidence of in-plane alignment in monolayer-thick pentacene films vacuum evaporated on some of these rubbed surfaces. Rubbing-induced preferential orientation of pentacene grains is shown to lead to an increase of the pentacene mobility by a factor of ~2.5 for current flow in the direction perpendicular to alignment in organic thin film transistor devices (OTFT).

10:20am **EM-ThM8 Metallic Thin Films of Molecular Metals***, I. Malfant, K. Rivasseau, D. de Caro, L. Valade,* Laboratoire de Chimie de Coordination (CNRS), France*; **J. Fraxedas**,* Institut de Ciencia de Materials de Barcelona (ICMAB-CSIC), Spain

Intrinsically metallic molecular materials become in most cases activated semiconductors when prepared as thin films due to the formation of segregated domains, the so-called grains boundaries. The transport properties of such polycrystalline films are thus determined by the morphology of the films. Needless to say that there is tremendous interest in circumventing the extrinsic effects of grain boundaries in order to exploit the intrinsic physical properties of the pristine materials when targeting technological applications. We show two examples of truly metallic organic thin films (thickness ca. 4 µm) grown by electrocrystallization on silicon wafers of TTF-based molecular metals, where TTF stands for tetrathiafulvalene. Our first example is TTF[Ni(dmit)@sub 2@]@sub 2@, dmit = dithiolethionedithiolate. The films show a reversible metal-insulator transition at 12 K.@footnote 1@ The second example concerns the single-component neutral molecular metal Ni(tmdt)@sub 2@, tmdt = trimethylenetetrathiafulvalenedithiolate. The films exhibit a room temperature conductivity of ca. 100 S/cm.@footnote 2@ We confirm that electrocrystallization is the technique of choice to obtain metallic films of single- and multi-component organic materials and we pursue the preparation of superconducting films. @FootnoteText@@footnote 1@D. de Caro, J. Fraxedas, C. Faulmann, I. Malfant, J. Milon, J.- F. Lamère, V. Collière, L. Valade, Adv. Mater. 16, 835-838 (2004) @footnote 2@I. Malfant, K. Rivasseau, J. Fraxedas, Ch. Faulmann, D. de Caro, L. Valade, L. Kaboub, Jean-Marc Fabre, F. Senocq, J. Am. Chem. Soc. 128, 5612-5613 (2006).

10:40am **EM-ThM9 Mobility Optimization Study of Organic Semiconductor Based Thin Film Transistors***, **R.P. Shrestha**, D. Yang,* University of North Carolina at Chapel Hill*; Y.X. Li,* Shandong University, China*; L. Yan, E.A. Irene,* University of North Carolina at Chapel Hill

Optical and electronic properties of two spin cast organic semiconductors N,N '- bis (3-phenoxy-3-phenoxy-phenoxy) -1,4,5,8-naphthalenetetracarboxylic diimide (NDA) and poly (o-methoxyaniline) POMA have been previously reported. In this study, the effect of various process changes (annealing, dielectric layer, device geometry) on the mobility of organic thin film transistors (OTFT) fabricated using NDA and POMA is explored. Low dielectric constant (K), non-polar dielectric materials improved charge mobility as did judicious annealing and bottom contact geometry. For example, the initial mobility of 10-3 cm2 V-1 s-1 for POMA can be improved by an order of magnitude by using polyethylene (PE) (low K) and degraded using polyvinylidene trifluoroethylene P(VDF-TrFe) (high K) dielectric layers. Similar results are reported for NDA OTFTs. Other performance parameters such has turn-on/off ratio and threshold voltages are also reported for the devices.

Surface Science
Room 2004 - Session SS2+EM-ThM
Self-Assembled Monolayers

Moderator: C. Wöll, Ruhr-Universitat Bochum, Germany

8:00am **SS2+EM-ThM1 Odd-Even Effects in Self-Assembled Monolayers of Biphenyl-Substituted Alkaneselenolates on Noble Metal Substrates***, **M. Zharnikov**, A. Shaporenko,* Universität Heidelberg, Germany*; J. Müller, A. Terfort,* Universität Hamburg, Germany

Self-assembled monolayers (SAMs) of selenolates can be considered as an alternative to thiolates for the functionalization of noble metal surfaces. In view of this option, we studied SAMs formed from biphenyl-substituted dialkanediselenides (CH@sub 3@(C@sub 6@H@sub 4@)@sub 2@(CH@sub 2@)@sub n@Se-)@sub 2@ (BPnSe, n = 1 - 6, 10, 11) on polycrystalline (111) gold and silver substrates. The SAMs were characterized by several complementary experimental techniques. Similar to the analogous systems with the thiolate headgroup, the packing density of the SAM constituents and the orientation of the biphenyl moieties in the BPnSe films exhibited a pronounced odd-even variation with the number of methylene groups in the aliphatic linker, which was opposite on silver as compared to gold. A higher packing density and a corresponding smaller inclination of the biphenyl moieties was observed for odd numbers of the methylene units in BPnSe on Au, and for even numbers of these units in BPnSe on Ag. The observed odd-even effects are explained by the strong dependence of the bending potentials in the metal-Se-C bond on the deviation of the respective angle from an optimal value of about 104° for Au and about 180° for Ag. The optimal metal-Se-C angles are presumably determined by the hybridization of the selenium in the metal-selenolate bond, which seems to have sp@super 3@ hybridization on Au and an sp hybridization on Ag, respectively.

8:20am **SS2+EM-ThM2 Structure and Stability of Acene-SAMs***, **D. Kaefer**, G. Witte, A. Bashir,* Ruhr-University Bochum, Germany*; P. Cyganik,* Institute of Physics Krakow, Poland*; J. Mueller, A. Terfort,* University Hamburg, Germany*; Ch. Woell,* Ruhr-University Bochum, Germany

In addition to tailoring mechanical and chemical surface properties self-assembled monolayers (SAMs) have also attracted significant interest in connection with studies on molecular electronics or as contact primers for organic electronic devices. The high electrical conductivity required for the latter applications has favoured the use of aromatic SAMs which generally reveal a more complex ordering mechanism as compared to aliphatic SAMs. While an improved ordering has been achieved by using additional alklyl-units within the backbone this in turn reduces the conductivity and increases the band gap of the molecular film. Recently, we have demonstrated for the case of anthracene-2-thiol that also well ordered SAMs with a completely conjugated backbone can be prepared on Au(111).@footnote 1@ In the present study we have further varied the anchoring group and prepared also an anthracene-2-selenol SAM. Here we present a comprehensive multi-technique study (based on XPS, NEXAFS, TDS, STM and LEED measurements) on the formation, molecular structure and thermal stability of both acene-based SAMs on gold. Interestingly, a remarkably improved long-range ordering and a somewhat reduced thermal stability is obtained for the anthracene-2-selenol SAM. The different films were also analyzed theoretically in the frame of DFT calculations and the microscopic interactions and energetics of both films are compared and discussed. @FootnoteText@@footnote 1@D. Kaefer et al., J. Am. Chem. Soc. 128, 1723 (2006).

8:40am **SS2+EM-ThM3 A Survey on the Structural Properties of Alkanethiols Self Assembling on Au(111)***, **E. Barrena**, C. Munuera, C. Ocal,* Instituto de Ciencia de Materiales de Madrid, Spain **INVITED**

The potential application of Self-Assembled Monolayers (SAMs) in different fields of both science and technology has motivated a large number of studies in recent years. It has become clear that the design of films with specific controlled properties requires a better understanding of the parameters governing the self-assembling process. Without doubt Alkanethiols (SH-(CH@sub 2@)@sub n-1@-CH@sub 3@ on Au(111) are the archetypal systems among SAMs. They posses important characteristics as

stability, structural simplicity and well-defined order, which make them ideal for understanding the role that the fundamental interactions play in determining the self-assembled structure. In spite of their simplicity, a rich spectrum of structures has been reported. In this talk I will present a survey on the structural properties of Alkanethiols on Au(111) mainly focused on the submonolayer regime. I will show that molecular configurations consisting of molecules presenting different tilt angles and periodicities are formed for submonolayer coverage with an extraordinary degree of order. Experimental studies carried out by combining Atomic Force Microscopy and X-ray diffraction measurements will be presented showing different aspects on their growth, structure, stability including chain length dependent investigations.

9:20am **SS2+EM-ThM5 The Electronic Structure and Polymerization of a Self-Assembled Monolayer*, D. Feng,* *D. Wisbey,* University of Nebraska-Lincoln*; Y. Tai,* Universit@um a@t Heidelberg, Germany*; Y. Losovyj,* Louisiana State University*; M. Zharnikov,* Universit@um a@t Heidelberg, Germany*; P. Dowben,* University of Nebraska-Lincoln, U.S.A

Although organic adsorbates and thin films are generally regarded as "soft" materials, the effective Debye temperature, indicative of the dynamic motion of the lattice normal to the surface, can be very high, e.g., in the multilayer film formed from [1,1'-biphenyl]-4,4'-dimethanethiol (BPDMT).@footnote 1@ The effective Debye temperature, determined from core level photoemission from the all carbon arene rings, is comparable to that of graphite, and follows the expected Debye-Waller behavior for the core level photoemission intensities with temperature, but this is not always the case. (We associate this rigidity to the stiffness of the benzene rings, and the ordering in the ultrathin multilayer molecular thin film.) We find that a monomolecular film formed from [1,1â?T;4â?T,1'-terphenyl]-4,4'-dimethanethiol deviates from Debye-Waller temperature behavior and is likely caused by temperature dependent changes in molecular orientation.@footnote 2@ Intermolecular Ï?-Ï? lateral interactions for [1,1â?T;4â?T,1'-terphenyl]-4,4'-dimethanethiol (TPDMT), were evident from the considerable dispersion of the TPDMT molecular orbitals with changing the wave vector k. The highest occupied molecular orbitals hybridize to electronic bands, with a band dispersion of about 300 to 400 meV. The wave vector dependence is consistent with a lateral spacing of about 5.1 @Ao@, found in STM. We also find evidence for the increase in dielectric character with cross-linking in spite of the decrease in the HOMO-LUMO gap upon irradiation of TPDMT. The cross-linking processes are also accompanied by changes in molecular orientation. @FootnoteText@@footnote 1@D.Q. Feng, R. Rajesh, J. Redepenning and P.A. Dowben, Applied Physics Letters 87 (2005) 181918 @footnote 2@D.-Q. Feng, D. Wisbey, Y. Tai, Ya. B. Losovyj, M. Zharnikov and P.A. Dowben, J. Phys. Chem. B 110 (2006) 1095-1098.

9:40am **SS2+EM-ThM6 Kinetics and Mechanism of Displacement in 1-Adamantanethiolate Self-Assembled Monolayers*, H.M. Saavedra,* *C.M. Barbu, T.J. Mullen, V.H. Crespi, P.S. Weiss,* The Pennsylvania State University

We have investigated the kinetics of solution-phase displacement of 1-adamantanethiolate self-assembled monolayers on Au{111} by n-dodecanethiol molecules using Fourier transform infrared-external reflectance spectroscopy (FTIR-ERS) and scanning tunneling microscopy (STM). The displacement reaction can be divided into three regions: a fast insertion and nucleation of small n-dodenathiolate islands around defects in the 1-adamantanethiolate monolayer; an island growth regime in which the rate of growth is dependent on the perimeter of the island; and a final slow ordering of the n-dodecanethiolate domains leading to denser and more crystalline n-dodenathiolate domains. A study of displacement as a function of concentration revealed that the full displacement of 1-adamantanethiolate monolayers has a [n-dodecanethiol] x time@super 2@ dependence. An analytical model has been derived to describe the displacement process, and using this model a rate constant has been determined.

10:00am **SS2+EM-ThM7 High Thermal Stability of Cross-Linked Aromatic Self-Assembled Monolayers: New Pathways for Nanopattering by Selective Desorption*, A. Turchanin,* *M. El-Desawy, A. Gölzhäuser,* University of Bielefeld, Germany

Molecular structures with high thermal stability are very desirable for applications in nanoscience and nanotechnology. We report on the thermal stability of cross-linked aromatic self-assembled monolayers (SAMs) on gold surfaces. Cross-linked monolayers were formed by low-energy electron irradiation of biphenylthiol SAMs. The pristine and the cross-linked monolayers were heated in ultra high vacuum to temperatures from 300 up to 1000K and then analyzed by X-ray photoelectron spectroscopy (XPS). We found that the pristine SAM desorbs at 400K, which is accompanied by a breaking of C-S bonds. Despite of a similar C-S bond cleavage of cross-linked SAMs in the same temperature range, their carbon matrix shows a high thermal stability and remains on the surface up to 1000K. We present a detailed analysis of the temperature transformations in pristine and cross-linked SAMs on the basis of XPS data. Using a stencil mask to locally cross-link the SAMs, it is then shown by scanning electron and atomic force microscopy that after the temperature treatment monomolecular sheets of aromatic molecules, corresponding to irradiated areas in the SAM, persist at the surface. This opens a new pathway for nanopattering by the selective desorption of non-cross-linked regions on a e-beam patterned monolayers and for technological applications of SAM coatings.

10:20am **SS2+EM-ThM8 In-situ Studies of Protein Resistance of Oligo(Ethylene Glycol) Self-Assembled Monolayers*, M. Skoda,* Oxford University, UK*; F. Schreiber,* Universit@um a@t T@um u@bingen, Germany*; J. Willis, R. Jacobs,* Oxford University, UK*; R. Dahint, M. Grunze,* University of Heidelberg, Germany*; M. Wolff,* ESRF, France

The structure of the interface between organic matter, such as self-assembled monolayers (SAMs), and water is currently subject of intensive studies due to its importance for the understanding of surface-solvent and surface-surface interactions.@footnote 1,2@ Our focus here are OEG-terminated SAMs which are used to make surfaces resistant to protein adsorption. We report our recent results from a combined Neutron Reflectivity (NR) and Polarisation Modulated (PM) Fourier Transform Infrared Spectroscopy (FTIR) study. The PM technique enables us to address the local interaction of water with OEG groups, and is ideally complementary to NR. Our data suggest a rather strong interaction of water molecules with the EG section of the SAM, potentially the penetration of water into the SAM. Also, the measurements reveal changes in the structure of water and the protein solution in the vicinity of the SAM upon changes in temperature. Our combined NR and IR investigation helps to shed light on the problem of the subtle interactions at the organic solid-liquid interface. The benefit of using IR along with NR is also that we are more sensitive to the defect structure of the organic interface, which has an impact on the interaction with water. @FootnoteText@@footnote 1@F. Schreiber, J. Phys.: Cond. Matter 16 (2004) R881 @footnote 2@D. Schwendel et al., Langmuir 19 (2003) 2284

10:40am **SS2+EM-ThM9 Thiol-Modified Diamondoid Monolayers on Gold Studied with Near-Edge X-ray Absorption Fine Structure Spectroscopy*, T.M. Willey,*** Lawrence Livermore National Laboratory*; J.D. Fabbri,* Stanford University*; J.R.I. Lee,* Lawrence Livermore National Laboratory*; P.R. Schreiner, A.A. Fokin, B.A. Tkachenko, N.A. Fokina,* Justus-Liebig University Giessen, Germany*; J.E. Dahl, R.M.K. Carlson, S.G. Liu,* MolecularDiamond Technologies*; T. van Buuren,* Lawrence Livermore National Laboratory*; N.A. Melosh,* Stanford University

Higher diamondoids, hydrocarbon cages with a diamond-like structure, have evaded laboratory synthesis and have only recently been purified from petroleum sources. Initial calculations on these unique diamond-like molecules show they may have highly desirable properties similar to hydrogen-terminated diamond surfaces. Readily available adamantane, the smallest diamondoid, can be thiolated and has shown to absorb on gold with high coverage. The availability of diamantane, triamantane, and tetramantanes opens new possibilities for surface-modification as multiple sites are available for thiol or other chemical functionalization. Surface-attached diamondoids have technological possibilities as high-efficiency field emitters in molecular electronics, as seed crystals for diamond growth, or in other nanotechnological applications, and fundamental studies of the properties of these molecules are a necessary precursor. We have investigated the effects of thiol substitution position and polymantane order on diamondoid film morphology. Using Near-Edge X-ray Absorption Fine Structure Spectroscopy (NEXAFS) we show that the orientation of the diamondoids within each type of monolayer depends highly upon both the location of the thiol and the diamondoid used. We thus demonstrate control over the assembly, and hence the surface properties, of this exciting new class of diamond-like carbon molecules.

Electronic Materials and Processing
Room 2001 - Session EM1-ThA

Contacts to Organic and Molecular Devices

Moderator: D.B. Janes, Purdue University

2:00pm **EM1-ThA1 Interfacial Transport Properties in Metal-Molecule-Semiconductor Diodes**, ***J.W.P. Hsu,*** Sandia National Laboratories; *W.J. Li,* Simon Fraser University; *Y. Jun,* University of Minnesota; *C. Highstrete, C.M. Matzke,* Sandia National Laboratories; *K.L. Kavanagh,* Simon Fraser University; *X.-Y. Zhu,* University of Minnesota; *A.A. Talin,* Sandia National Laboratories, 94550; *S.V. Faleev, F. Leonard,* Sandia National Laboratories; *M.D. Halls, R. Krishnan,* Indiana University **INVITED**

Integrating molecular functions with conventional semiconductors opens up new possibilities for future electronic devices. However, the formation of molecular monolayers on semiconductors is much less mature than their counter parts on metals, and the study of buried molecular junctions is hampered by the dearth of experimental tools. In this talk, I will discuss the formation of alkanethiol or alkanedithiol monolayers on (001) GaAs and electronic transport across these molecular layers by ballistic electron emission microscopy (BEEM). Using X-ray photoemission spectroscopy and ellipsometry, we found that the monolayer thicknesses of hexadecanethiols (C16MT) and of octanedithiols (C8DT) are about the same even though C16MT is almost twice as long as C8DT. Using BEEM, we examined transport properties of Au-molecule-GaAs and Au-molecule-metal-GaAs diodes where molecule = C16MT or C8DT. BEEM is one of the very few experimental techniques that are capable of measuring the local electronic transport through such buried interfaces. The barrier heights determined from BEEM are compared with Schottky barrier heights determined from temperature dependent current-voltage (I-V-T) measurements. A major difference between the two measurements is that the local barrier height determined from BEEM is without applying a bias across the molecular layer while a large field could exist across the molecules. We found that the presence of the molecule dramatically increases the BEEM threshold voltage compared to reference Au/GaAs diodes while the I-V barrier heights are about the same. Comparing the experimental results to a 1D model with two tunneling barriers, we concluded that ballistic electron transmission through the molecular layer occurs through the lowest unoccupied level. The BEEM threshold is in a reasonable agreement with the position of lowest unoccupied level from quantum chemical calculations.

2:40pm **EM1-ThA3 Oxygen-Modified Interaction of Evaporated Titanium with Organic Monolayers**, ***J.J. Blackstock,*** Hewlett Packard Labs; *W.F. Stickle,* Hewlett Packard Company; *C.L. Donley, D. Ohlberg, D.R. Stewart, R.S. Williams,* Hewlett Packard Labs

Due to ease of integration with conventional fabrication techniques, the evaporation of metal onto organic monolayers is a common method for making electrical contact to one side of a molecular electronic junction. In particular, titanium has frequently been employed as the deposited metal in molecular electronic devices, based on the assumption that the Ti atoms would interact with the top of the monolayer and form a covalent titanium-carbide bond. However, a range of recent studies have demonstrated that under some deposition conditions, titanium is more reactive than originally anticipated, and can cause significant damage to the organic monolayer. Herein we present data on the evaporation of titanium onto Langmuir-Blodgett (LB) monolayers of alkane chains. We utilize a new technique, based on the cleaving of molecular electronic device stacks at the organic interface in UHV, to investigate the interaction of the titanium with the alkane chains as a function of the underlying substrate. UHV XPS and in-situ IR data reveal that the previously observed damage to organic monolayers by evaporated titanium is strongly mitigated by the presence of available oxygen from the underlying substrate. Furthermore, angle-resolved XPS data on these systems elucidate a kinetic mechanism by which the damage to an organic monolayer proceeds beyond the top layer of the monolayer when available oxygen is not present in the substrate. In combination with previous studies, these data suggest the potential to engineer substrate-monolayer systems to produce desirable interactions between evaporated titanium contacts and organic monolayers.

3:00pm **EM1-ThA4 Silicon-on-Insulator Based Nanogap Electrode Device for DNA Conductivity Measurements**, ***S. Strobel,*** *A.G. Hansen,* Walter Schottky Institute, TU Munich, Germany; *K. Arinaga,* Fujitsu Laboratories Ltd., Japan; *M. Tornow,* Walter Schottky Institute, TU Munich, Germany

The objective to investigate DNA in hybrid bio-molecular electronic devices originates from the fundamental interest in DNA charge transfer mechanism, its potential role in future self-assembled nano-electronic networks, and from its prospective role in novel bio-sensing applications. Here, an electrical scheme allowing for the contacting of short DNA (few 10 nm) in an array-like chip format, and supporting in-situ measurements, i.e., with the DNA in aqueous buffer solution, at the same time, would be highly advantageous. We have developed a novel nanogap electrode concept based on standard Silicon microtechnology. Starting material is a Silicon-on-Insulator (SOI) substrate with a thin buried oxide layer (thickness 10-40 nm). Using standard optical lithography and reactive ion etching a large array of individual, pillar-like device structures is prepared with the buried oxide layer exposed at their edges. After selectively recess-etching this layer and evaporating a metal thin film from an angle, nanogap electrodes of predetermined spacing are formed. We successfully verified the functionality of our devices by electrically trapping gold nanoparticles onto the gap, both, on bare metal electrodes, and on those previously functionalized with monolayers of oligonucleotides. In the latter case a pronounced non-linear I-V characteristic develops at T=4.2 K which can be related to Coulomb blockade effects. Concepts for measuring DNA conductivity under aqueous conditions will be discussed.

3:20pm **EM1-ThA5 Metallization of Organic Semiconductors: Interface Chemistry and Surface Morphology**, ***K. Demirkan***, *C. Weiland, A. Mathew, J.J. Krajewski,* University of Delaware; *D. Allara,* The Pennsylvania State University; *R.L. Opila,* University of Delaware

Aluminum was thermally evaporated onto the conjugated semiconducting polymer, poly(2-methoxy-5,2'-ethyl-hexyloxy-phenylene vinylene) (MEH-PPV) and polystyrene. The interface formation and chemical interactions between the polymers and Al were investigated using X-ray Photoelectron Spectroscopy (XPS) and synchrotron based Ultraviolet Photoelectron Spectroscopy (UPS). The C-O bonds in MEH-PPV decreased with increased Al evaporation. Reaction between Al and the carbon backbone of the polymer leading to the creation of carbon-metal bonds was also observed. Scanning electron microscopy (SEM) images of Al surface deposited on MEH-PPV showed agglomeration of the Al. The poor surface wetting and agglomeration of the Al causes a non uniform and porous metallic layer with a much higher surface area and a potential for greater oxidation and presumably elevated device degradation. UPS spectra (at photon energy =120 eV) of MEH-PPV and polystyrene at considerably high Al coverage (equivalent to 6 nm of uniform Al film) showed features from the organic layers, and supports the idea of a non-uniform Al film and the existence of poorly metallized regions on the polymer surface. Atomic Force Microscopy (AFM) studies of Lithium Fluoride (LiF) evaporated on MEH-PPV surfaces also show very rough surfaces compared to the MEH-PPV surface, indicating poor wetting of LiF on MEH-PPV.

3:40pm **EM1-ThA6 Characterization of Device Grade ITO/Conductive Polymer Interfaces Using Low Intensity Photoemission Spectroscopy and Electrospray In-Vacuum Deposition**, ***Y. Yi,*** *J.E. Lyon, M.M. Beerbom, R. Schlaf,* University of South Florida

Photoemission spectroscopic (PES) characterization of indium tin oxide (ITO) surfaces, that were exposed to the ambient prior to insertion into the vacuum results in a work function reduction of more than 0.5 eV within a short period of time (seconds to minutes, depending on x-ray or ultraviolet photon flux during measurement). This artifact impairs the characterization of charge injection barriers at ITO interfaces using the typical PES measurement protocol, consisting of a multi-step deposition sequence with PES characterization in between deposition steps. Particularly, the investigation of device grade ITO interfaces is affected by this phenomenon, since in most device fabrication protocols the ITO electrode is usually exposed to the ambient before the polymer is deposited. The presented experimental results focus on the quantification of the artifact, and the determination of the maximum "photon budget" that can be used for characterization, before a significant work function reduction is observed. Based on these data, a technique for ITO interface characterization based on low intensity x-ray photoemission spectroscopy (LIXPS) was developed. The technique was demonstrated on polythiophene/ITO interfaces, yielding injection barriers similar to those determined by others using current based methods. The results also

demonstrate that exposure to UV flux immediately results in a change of the orbital line-up due to the work function lowering of the substrate.

4:00pm **EM1-ThA7 Contact-Related Effects in Organic Thin Film Transistors***, **D.J. Gundlach,*** National Institute of Standards and Technology **INVITED**

Organic thin film transistors (OTFTs) have received considerable attention in recent years and it is anticipated that OTFTs will find wide use in low-cost large-area electronic applications. OTFT performance can be limited by (1) the charge injection at the contacts or (2) the transport of charge in the field accumulated channel. In this presentation we will discuss parasitic contact related effects in OTFTs for different designs and compare experimentally observed contact-related effects with results from numerical simulations for devices employing inverted coplanar and inverted staggered designs. Organic single crystals with considerably fewer structural defects, such as grain boundaries, and having a low deep state density of electrically active traps provide ideal systems for studying charge injection and transport. The current-voltage characteristics of thin lamellar organic single crystals with gold contacts formed to opposite sides reveal that contact formation is complex and variable, even when high quality crystals and well-controlled contact formation methods are used. The current-voltage characteristics under low-level injection conditions provide a first indication of the contact quality. However, considerably more insight to the contact quality and injection process are gained from an analysis of the dependence of the activation energy on the applied voltage (extracted from the temperature dependence of the current-voltage characteristics), where a monotonic decrease in activation energy is expected when ohmic contacts are formed to crystals. Importantly, we discuss challenges in using OTFTs and organic single crystal field-effect transistors to study charge transport in organic semiconductors and possible contact-related limitations to the device reliability.

4:40pm **EM1-ThA9 Ag Islands Decorated by C@sub 60@***, **C. Tao**, T.J. Stasevich, T.L. Einstein, E.D. Williams,* University of Maryland, College Park

It is increasingly clear that a great challenge in nanoscale electronics will be understanding and controlling the interaction between the active nanoscale element and the conductive electrodes in devices. At nanoscale structural changes involving the displacement of even a single metal atom will be closely related to the electronic properties and reliability. Here I will introduce our study on a specific metal-molecule interface formed at Ag monolayer islands decorated by C@sub 60@. At room temperature, equilibrium monolayer islands on clean Ag(111) surfaces are hexagonal. At extremely low coverage of C@sub 60@, C@sub 60@ molecules are found preferentially at sections of the island edge near corners. Individual C@sub 60@ is found at different position in sequential images. When more C@sub 60@ is deposited, C@sub 60@ molecules form more stable chains along the Ag island edge near the corners of the island. The shape of the islands changes at this point with smoother corners. As coverage increases further, C@sub 60@ chains become longer and the hexagonal islands become round. By controlling C@sub 60@ coverage, we can make Ag island edges fully covered by C@sub 60@ chains, which become closed rings. The equilibrium shape of Ag islands decorated by the surrounding C@sub 60@ ring is approximately circular and shows dynamic thermal fluctuations. The mechanism for C@sub 60@ distribution and shape change of islands will be discussed in the context of the 2D equilibrium crystal shape (ECS). By rapid STM scanning, we obtain sequential images of the C@sub 60@ rings and analyze the corresponding dynamic properties. The shape fluctuation of C@sub 60@ rings are clearly displayed by movies made of sequential images. Quantitative analysis of the shape fluctuation using correlation functions will be presented, and discussed in terms of the correlated motion of the C@sub 60@ molecules and underlying Ag atoms. @FootnoteText@ --Supported by NSF, MRSEC at the University of Maryland.

Electronic Materials and Processing
Room 2003 - Session EM2-ThA

Electronic Properties of High-k Dielectrics, Ferroelectrics, and Their Interfaces

Moderator: R.M. Wallace, University of Texas at Dallas

2:00pm **EM2-ThA1 Ab Initio Study of High-k Gate Stack***, J. Ha, B. Magyari-Kope, P.C. McIntyre,* Stanford University*; **K. Cho,*** UT Dallas **INVITED**

At nanometer scale, materials behave differently from their bulk properties. Material properties become a function of their size and shape at 1-100 nm scale due to strong quantum mechanical effects and surface effects. In this talk, we will apply quantum simulations to study high-k gate stack materials. We will focus the main discussion on the modeling study of high-k gate stack system with emphasis on two interface problems: silicon/high-k oxide and high-k oxide/metal gate electrode interfaces. For the silicon/high-k oxide interface, we examine the effects of interlayer SiO2 between silicon substrate and high-k oxide (HfO2 or ZrO2). The driving force for SiO2 formation at the silicon/high-k oxide interface is identified and the correlation between the interface atomic structure and the band offsets is elucidated. Furthermore, the internal SiO2-HfO2 interface is investigated to understand the source of fixed charge problems of high-k oxides. Our modeling study has identified the source of fixed charges, and we have proposed a practical solution to passivate the fixed charge source at the interface. For the high-k oxide/metal gate interface, we have studied the work function of candidate metal gate electrodes and identified the key mechanisms which control the work function of different metals at the interface. Our study has shown that the interface work function is determine by 1-3 monolayers of metal at the interface and that the work function control requires a direct control of atomic structures at the interface rather than the overall structure of electrode materials.

2:40pm **EM2-ThA3 Material and Electrical Properties of HfRuN Gate Electrodes on HfO@sub 2@***, **M. Sawkar Mathur**, J.P. Chang,* University of California, Los Angeles

Many alternative gate dielectric candidates for future generation MOSFET devices, including Hf based dielectrics, will require the use of a metal gate, because of the instability issues, sheet resistance, gate depletion, and dopant penetration experienced with polysilicon gates. Hf based gate electrode materials are promising candidates because they are likely to reduce charge transfer and subsequent dipole formation at the interface as a result of the homo-nuclear bonds that form between the Hf in the metal gate and the Hf in the gate dielectric. This paper discusses the material and electrical properties of Hf-Ru and Hf-Ru-N gate electrodes deposited atop HfO@sub 2@. Four compositions of HfRu were synthesized with varying amounts of N (0 - 15 at.%), and their material characteristics before and after annealing, such as composition, interface bonding, and crystalline phases were determined by X-ray photoemission spectroscopy (XPS), Rutherford backscattering (RBS), and X-ray diffraction (XRD). Capacitance-voltage (C-V) and current density-voltage (J-V) characteristics of fabricated metal-oxide-semiconductor (MOS) capacitors are used to determine the effective work functions (EWFs), the barrier heights, and the leakage current density across the metal gate/HfO@sub 2@ interface. Pure Hf and pure Ru gate electrodes deposited on HfO@sub 2@ exhibited EWFs of 4.1 eV and 5.5 eV, respectively, which correspond well with what has been reported in literature.@footnote 1,2@ HfRu alloys with EWFs of 4.8eV and 5.2 eV have been achieved, and N incorporation was found to have a modest effect on the attained EWFs. Detailed analyses of EWFs as a function of alloy composition, microstructure, and interfacial bonding will be presented to determine the optimal composition for n-MOSFET devices and p-MOSFET devices. @FootnoteText@ @super 1@ P. Majhi, et. al., 2005 IEEE VLSI-TSA (2005).@super 2@ M. Tapajna, et. al., Materials Science in Semiconductor Processing 7, (2004).

3:00pm **EM2-ThA4 Spectroscopic Detection of Electronically Active Defects in Nanocrystalline Ti/Zr/Hf Elemental Oxides***, G. Lucovsky, L.B. Fleming, M.D. Ulrich, **H. Seo**, N.A. Stoute,* NC State University*; J. Luning,* Stanford Synchrotron Radiation Lab

The performance and reliability of advanced Si field effect transistors (FETs) with high-k transition metal gate dielectrics are limited by intrinsic bonding defects within the nanocrystalline oxides, and at internal device interfaces with i) Si/other semiconductor substrates, and ii) gate metals. This paper employs (a) several spectroscopic approaches: i) near-edge soft-x-ray absorption spectroscopy (NESXAS), ii) soft x-ray photoelectron spectroscopy (SXPS), iii) ultra-violet photoelectron spectroscopy (UPS), and iv) visible and vacuum ultra-violet spectroscopic ellipsometry (VUV SE), and (b) ab initio molecular orbital (MO) theory to study band edge defects. Occupied O-vacancy defect states have been identified at Ti/Zr/HfO@sub 2@ valence band edges by SXPS and UPS. These states have different crystal field splittings for Ti, and Zr and Hf oxides, as expected from the respective 6-fold, and 8-fold coordinations to O. Additionally, occupied defect states display Jahn-Teller term-splittings that remove their respective d-state degeneracies. Transitions from the J-T split ground states to empty defect states below the respective conduction band edges have been identified in O K@sub 1@ NESXAS spectra, epsilon 2 spectra obtained from analysis of VUV SE response functions, and in photoconductivity. Defect densities are ~1-3x10@super -13@ cm@super -2@, consistent with

vacancies being clustered along grain boundaries of nanocrystalline oxides. In contrast, these types of defects are not observed spectroscopically in non-crystalline Zr/Hf Si oxynitride alloys, or in ultra thin HfO@sub 2@ dielectrics that have been exposed to post deposition anneals (PDAs) in different nitrogen ambients.

3:20pm **EM2-ThA5 Combining Ferroelectric Oxides and Semiconductors for Smart Transistors***, **J. Singh**,* University of Michigan, usa **INVITED**

Semiconductors have been exploited for decades in creating intelligent devices. However, oxides and other insulators have at most provided passive roles as insulators or passivation layers. Recent work has been showing that it is possible to grow reasonable quality oxide-semiconductor interfaces. Is it possible to have oxide-semiconductor heterostrucutres where the best of semiconductors and the best of oxides (polar charge, tailorable polarization, large bandgap, tailorable dielectric response etc.) can be exploited? There are a large number of potential material systems that have polar character which are not (yet) considered to be relevant to semiconductor technology. These include ferroelectrics, pyroelectrics and piezoelectric materials where polar charges as high as 1 electron per surface atom can be present.For these structures to make an impact a number of parameters need to be evaluated. These include: (i) band lineup; (ii) polarization vs. thickness; (iii) dielectric response vs. thickness; (iv) and most importantly defect structures. In absence of all this knowledge it is still possible to examine the potential of new heterostructures that exploit polar materials. Theoretical studies can provide estimates of the level of perfection needed to make new devices possible. Polarization differences at interfaces can be used to create very large band bending which in turn can be used to induce electron (hole) gas, create tunnel junctions, cause lateral as well as vertical band engineering. Most interestingly these structures can result in smart FETs which have high transconductance and respond not only to gate bias but to pressure, temperature variations, etc. At this point in time these structures can serve as test cases to examine the potential of oxide-semiconductor structures and to see if the interfaces can reach the needed quality for functional devices.

4:00pm **EM2-ThA7 Theoretical Analysis of the Interface between Zr(Hf)O@sub 2@ and Ge(100) for Ge-based MOSFET Devices***, **T.J. Grassman**, S.R. Bishop, A.C. Kummel,* University of California, San Diego

In recent years there have been many attempts at the fabrication of high-quality Ge-based MOSFETs. One of the most successful dielectric materials used in these studies is ZrO@sub 2@, producing some of the best Ge-based MOS devices to date; HfO@sub 2@ has also found a fair amount of use in the field, with varying results. In order to better understand these MOS systems, and particularly the often-problematic SC/oxide interface, a systematic density functional theory study of the Zr(Hf)O@sub 2@/Ge(100) interfaces has been undertaken. Multiple initial first-layer bonding configurations of ZrO@sub 2@ and HfO@sub 2@ on Ge(100)-2x1/4x2 have been simulated in order to elucidate, through adsorption energy comparisons and comparison with experiments, what the interfacial configuration between the semiconductor and oxide actually is. These sites were also modeled for electronic structure in order to help explain or clarify the experimental results. It has been found that ZrO@sub 2@ bonds to the Ge(100) surface very strongly in both Zr- and O-end down configurations, with the Zr-end down geometry the strongest. It is also seen from the electronic structure calculations that the Ge-Zr bonds are covalent rather than metallic, and neither Zr- nor O-end down bonding configurations result in an increase in near-Fermi level DOS. Such results are consistent with the experimental findings that ZrO@sub 2@ is a good gate dielectric material for Ge(100). In addition, the calculations indicate that H-passivation of dangling bonds at the ZrO@sub 2@/Ge(100) interface, and potentially within the oxide itself, may be an effective method to improve MOS device properties. However, while H-passivation of dangling bonds on both Zr and O atoms produces a considerable reduction of near-Fermi level DOS, only the passivation of the O atoms is thermodynamically stable enough to be achievable in device processing conditions. All of these same calculations are currently being performed on HfO@sub 2@.

4:20pm **EM2-ThA8 Sub-1 nm Equivalent Oxide Thickness Zirconium Doped Hafnium Oxide High-k Gate Dielectrics***, **J. Yan**, C.-H. Lin, A. Birge, J. Lu, Y. Kuo,* Texas A&M University

Implementation of high-k gate dielectrics for the continuous scale-down of MOSFETs requires the equivalent oxide thickness (EOT) be less than 1 nm.@footnote 1@ In order to achieve this kind of ultra-thin film with high dielectric quality, the gate dielectric deposition and post-deposition annealing (PDA) processes need to be carefuly studied. Previously, we reported that sub-2nm EOT Zr-doped HfO2 could be prepared by the reactive co-sputtering method.@footnote 2@ In this work, we report new results on preparing the ultra-thin, e.g., EOT as low as 0.89 nm, Zr-doped HfOx dielectric films by sputtering from a composite target. Effects of PDA conditions, such as temperature and gas atmosphere, on material and electrical properties were investigated. The interface layer formation mechanism, which is critical to the low EOT, low interface states density, and low charge trapping density, was studied. The resulting films have Dit E11 to E12 cm-2eV-1, hysteresis less than 4mV, and leakage current 4 orders of magnitude lower than that of SiO2. The interface and bulk film material properties were characterized with the angle-resolved x-ray photoelectron spectroscopy and AFM. @FootnoteText@ @footnote 1@ ITRS, SIA (2005).@footnote 2@ Y. Kuo, et al., ECS Proc. High Dielectric Constant Gate Stack III, in press (2005).

4:40pm **EM2-ThA9 Evaluation of Various Ru-insulator-Ru Capacitors with CVD-Ru Thin Films for Both Top and Bottom Electrodes***, **B.S. Kim**, C.S. Hwang, H.J. Kim,* Seoul National University, Korea*; S.Y. Kang, J.Y. Kim, K.H. Lee, H.J. Lim, C.Y. Yoo, S.T. Kim,* Samsung Electronics Co., Ltd., Korea

Ruthenium has been considered as one of the most promising materials for capacitor electrodes in gigabit-scale DRAM due to its low electrical resistivity and good dry etching property in addition to the capability of conductive oxide formation. To deposit the Ru thin films into a typical concave type storage node with a high aspect ratio, the development of metalorganic chemical vapor deposition (MOCVD) process, which provides an excellent conformality, is necessarily required. However, there are few reports about the structural and electrical characterization of Ru-insulator-Ru (RIR) capacitors, of which both the top and bottom Ru films were grown by MOCVD. Therefore, in this study, we fabricated the RIR capacitors with CVD-Ru and various dielectric materials and evaluated their properties by structural and electrical analysis. The Ru thin films were deposited by hot-wall MOCVD using liquid precursor of (2,4-Demethylpentadienyl)(Ethylcyclopentadienyl)ruthenium (DER) to fabricate the top and bottom electrodes. All the dielectric thin films such as ZrO@sub 2@, TiO@sub 2@ and SrTiO@sub 3@ were formed by atomic layer deposition (ALD) method. The electrical properties of the fabricated RIR capacitors were evaluated by the capacitance-voltage measurement combined with the current-voltage measurement. The thermal stability of as-grown capacitors was also tested under several annealing ambient and temperatures. The structural analysis to elucidate the relation with electrical properties was conducted by the x-ray diffraction (XRD), atomic force microscopy (AFM), scanning electron microscopy (SEM) and transmission electron microscopy (TEM).

Electronic Materials and Processing
Room 3rd Floor Lobby - Session EM-ThP
Electronic Materials and Processing Poster Session

EM-ThP2 Effect of the Oxygen Partial Pressure on the Photoluminescence Emission from Heterostructures SiO2/Si/SIO2 Growth by RF Reactive Sputter Magnetron, ***E. Mota-Pineda***, *M. Melendez-Lira, J. Falconi-Guajardo,* Cinvestav-IPN, Mexico*; J. Jesus-Araiza,* University of Zacatecas, Mexico*; W. Calleja-Arriaga,* NAOE, Mexico

We prepared heteroestructures SiO2/Si/SiO2 by sputter reactive magnetron deposition on Si (100) and corning glass substrates at 400Â°C. We employed a polycrystalline Si target with Ar and O2 as working gases. We investigate the effect of the partial pressure of oxygen and the thickness of the Si interlayer on the electronic properties of the heterostructure. Crystallographic properties were studied by X-ray diffraction and chemical composition was determinate by EDX. The electronic properties were determined by transmission and Raman spectroscopies at room temperature. The Raman spectrum of the as-deposited samples has two broad features due to scattering by TO and LA phonons in a-Si respectively. UV-Vis transmission spectroscopy shows that the absorption edge shifts as function of the thickness of Si interlayer. The FTIR absorption spectra of as-deposited films show absorption peaks associated with vibration modes of the SiO2 and Si-Si. The thicknesses of the films were determinate by scanning electron microscopy and vary between 500 and 600nm. We observed the superficial topography of the material through AFM. Transmission electron-microscope micrography confirms the growth of the SiO2/Si/SiO2 heterostructure and the electron diffraction pattern shows the presence of nanocrystalline phases. A broad lumininescent band (around 1.7 eV) appears by effect of the Si interlayer and its intensity increases with the Si layer thickness. The results are discussed in terms of a model of quantum confinement of Si embedded in a SiO2 matrix. The effect of rapid thermal annealing under Ar and O2 atmospheres on the photoluminescent characteristics are also discussed.

EM-ThP3 Light Emission from SiO@sub x@ Films Deposited on Silicon by Laser Ablation*, *J.G. Ramirez-Mora,* U. Autonoma de Zacatecas, Mexico*;* ***M. Melendez-Lira,*** Fisica, Cinvestav-IPN, Mexico*; J.J. Araiza-Ibarra,* U. Autonoma de Zacatecas, Mexico*; C. Falcony,* Fisica, Cinvestav-IPN, Mexico

We have produced SiO@sub x@ films by laser ablation employing a silicon target under a O@sub 2@ atmosphere. Films were prepared employing the 1064 nm and 532 nm wavelength obtained from a Nd:Yag pulsed laser. Power intensity applied to the target was modulated by focusing the laser beam. Film thickness was controlled by the number of pulses applied on the silicon target. Chemical composition obtained by EDX shows that films produced present an excess of silicon. This was corroborated from results of the refraction index value obtained by ellipsometry measurements. Raman spectroscopy results show the presence of amorphous silicon regions. Room temperature photoluminescence measurements were carried out with 632.8 nm and 457.9 nm wavelengths from a HeNe and Ar@super +@ lasers. A broad emission was detected under the HeNe excitation, a stronger intensity was obtained from the thinner films. For thicker films narrow peaks are developed on the broad emission. When luminescence is excited with the Ar@super +@ laser a narrow peak around 580 nm is observed. Surface topography obtained by AFM shows the presence of square columm-like features. We will present transmission electron micrographies. Results are discuss in terms of the presence of silicon clusters embedded within a SiO@sub 2@ matrix. @FootnoteText@ *work partially funded by CONACyT-Mexico.

EM-ThP4 UV-Detecting Top-Gate ZnO-TFTs with Polymer Dielectric for Optical Inverter Application, ***K.M. Lee***, *J.-M. Choi,* Yonsei University, Korea*; J.H. Park, E. Kim,* Hongik University, Korea*; C.S. Kim,* Yonsei University, Korea*; H.K. Baik,* Yonsei University, Korea, South Korea*; S. Im,* Yonsei University, Korea

Very recently ZnO thin-film transistors (TFTs) have attracted much interest from researchers and engineers because they have potentials to realize transparent electronics. However, most of the reported devices were based on bottom-gate structures. We have successfully fabricated ZnO-based TFTs of a top-gate structure with organic polymer dielectric and also realized optical inverters by using their UV-detecting properties. ZnO channel layers were patterned by rf magnetron sputtering on glass substrate, and then Al source/drain electrodes were deposited by thermal evaporation. PVP dielectric layers were subsequently deposited by spin casting. Finally, semi-transparent conducting NiOx gate windows were patterned on the PVP layers. In spite of the relatively lower mobilities (~0.01 cm@super 2@/Vs) than those of other bottom-gate ZnO TFTs with inorganic dielectric layers, our ZnO-TFT with polymer dielectric has a good UV responsity (at wavelength ~364 nm) as a photo-detector and showed a fast response for optical gating (including detecting and inverting actions). For these demonstrations of optical inverters, we set up an appropriate array of photo TFTs and load registers. Furthermore, we attempt to enhance the mobility and to lower the operating voltage of our top gate ZnO-TFTs by adopting a hybrid gate dielectric of high-k inorganic/organic (PVP) sandwich structure. More and advanced details will be discussed in the meeting.

EM-ThP5 Etching Characteristics of ZnO Thin Films using by BCl@sub3@/Ar Inductively Coupled Plasma, ***J.C. Woo***, *C.M. Kang, J.S. Kim, G.H. Kim, K.T. Kim, C.I. Kim,* Chung-Ang University, Korea

The specific electrical, optical and acoustic properties of Zinc Oxide (ZnO) are important for semiconductor process which has many various applications. Piezoelectric Zinc Oxide (ZnO) film has been widely used for transducers, bulk and surface acoustic- wave resonators, and acousto-optic devices. Also, it has advantages relative to GaN because of its availability in bulk, single-crystal form, and its larger exciton binding energy (~60 meV, cf. ~25 meV for GaN). Research and development of ZnO have been rapidly accelerated to improve materials for the last decades. But, etch properties of ZnO have not established yet. In this study, we investigated etch characteristics of dry etching of the ZnO thin films in the inductively coupled plasma etch system with (BCl@sub 3@/Ar) gas mixture. The etching characteristics of ZnO thin films were investigated in terms of etch rates and selectivity as a function of (BCl@sub 3@/Ar) gas mixing ratio, rf power, dc bias voltage and chamber pressure. The plasmas were characterized by optical emission spectroscopy (OES) and Langmuir probe analysis. The chemical states on the etched surface were investigated with x-ray photoelectron spectroscopy (XPS). Scanning electron microscopy (SEM) was used to investigate the etching profile.

EM-ThP6 Electroluminescence from ZnO Nanowire/Polymer Composite p-n Junction, ***C.-Y. Chang***, *F.-C. Tsao, C.-J. Pan, G.-C. Chi,* National Central University, Taiwan*; H.T. Wang, J.-J. Chen, F. Ren, D.P. Norton, S.J. Pearton,* University of Florida*; K.-H. Chen, L.-C. Chen,* National Taiwan University, Taiwan

Zinc oxide (ZnO) is an attractive candidate for UV light emission since it is an environmentally friendly material which be grown at low temperatures on cheap transparent substrates and has both a direct wide band gap of 3.3 eV and a very large exciton binding energy of 60meV,important for robust light emission. In addition, it has been suggested that semiconducting nanowires may offer additional advantages for light emission due to the increased junction area, reduced temperature sensitivity, enhanced polarization dependence of reflectivity and improved carrier confinement in 1-D nanostructures. The characteristics of a hybrid p-n junction consisting of the hole-conducting polymer poly(3,4-ethylene-dioxythiophene)-poly(styrene-sulfonate)(PEDOT/PSS) and n-ZnO nanorods grown on a n-GaN layer on sapphire are reported. To fabricate the nanowire light emitting devices, the nanowire array was first coated with polystyrene, followed by photoresist. Spin-coating of polystyrene was used to electrically isolate neighboring nanorods and a top layer of transparent conducting indium-tin-oxide (ITO) was used to contact the PEDOT/ PSS. Multiple peaks are observed in the electroluminescence spectrum from the structure under forward bias, including ZnO bandedge emission at ~383 nm as well as peaks at 430,640 and 748 nm. The threshold bias for UV light emission was <3 V, corresponding to a current density of 6.08 A.cm-2 through the PEDOT/ PSS at 3 V. These initial results show that a low-cost, low temperature process holds strong potential for ZnO-based UV light emission and reduces the requirement for achieving robust p-doping of ZnO films or substrates.

EM-ThP7 Reliability of Gate Dielectrics for ZnO Thin-Film Transistors Operating at Low Voltages, ***M.S. Oh***, *K.M. Lee, K.H. Choi, S. Im,* Yonsei University, Korea

ZnO-based thin-film transistors (TFTs) have attracted much attention from researchers and engineers because of their novel potentials: the realization of transparent TFTs, replacing amorphous Si-TFTs, and being a component of effective ultraviolet (UV) detecting devices. PECVD(Plasma Enhanced Chemical Vapor Deposition) SiN@sub x@ has been used as a gate dielectric in the fabrication of amorphous silicon (a-Si:H) TFT arrays for large area liquid crystal displays(LCDs). Since PECVD is a low-temperature process and the SiN@sub x@ layer is a transparent materials, SiN@sub x@ is one of the

powerful candidates for the dielectric layer in transparent electronics applications using ZnO-based TFTs. Additionally the dielectric constant of SiN@sub x@ is quite high (~7), so that we may drive the ZnO-TFTs at low voltage(~5V) if the dielectric is as thin as 200 nm (resultant capacitance ~31 nF/cm@super 2@). We have fabricated the ZnO-based TFTs with 200 nm-thick SiN@sub x@ dielectric layers which were deposited by PECVD. The undoped ZnO was used for a channel layer and was deposited by rf sputtering at room temperature. For the source/drain electrodes, we have used the Al and the substrate was an ITO glass. The field mobility of our ZnO-TFT was ~0.7cm@super 2@/Vs while the turn-on voltage was less than ~5V. However, our ZnO-TFT also showed inferior on/off current ratio of less than 10@super 3@ and unreliable gating with a large gate voltage hysteresis, of which the origin is not clear but probably related to deposition-induced-hydrogen in SiN@sub x@. In the present work, the reliability of SiN@sub x@ dielectric for ZnO-TFT will be discussed in detail and another results from adopting different gate dielectric such as rf sputter-deposited AlO@sub x@ will also be presented.

EM-ThP8 Metal Oxide Gas Microsensors for Sensing & Recognition of Low Concentrations of Hazardous Chemicals*, **J.K. Evju**, B. Raman,* National Institute of Standards and Technology*; Z. Boger,* OPTIMAL - Industrial Neural Systems, Israel*; D.C. Meier, K.D. Benkstein, C.B. Montgomery, S. Semancik,* National Institute of Standards and Technology

Considerable motivation exists for developing solid-state microdevices that can reliably detect chemical hazards. We describe our efforts on metal oxide-based conductometric sensor arrays, where the semiconducting oxides on the elements transduce surface chemical interactions into measurable electronic signals. The temperature dependent adsorption, desorption and reaction processes on the thin metal oxide sensing film surfaces give rise to carrier concentration changes that are readily measured on our microhotplate chemical sensor arrays. By utilizing addressable heating of individual sensor elements, together with thermally activated chemical vapor deposition (CVD), we grow different types of oxides onto our microhotplate gas sensor array elements in a self-lithographic process. The selectivity offered by these oxides, coupled with rapid temperature modulation of individual sensor elements, provides a basis of tunability that we take advantage of for gas sensing and recognition. We will illustrate how we harness information from the physical surface processes on our individually addressable sensor array elements, that are comprised of controlled temperature MEMS based microhotplate devices. Our focus will be on challenges associated with recognition of chemical warfare simulants (CWSs) and toxic industrial chemicals (TICs) at low concentrations (ppt to ppb) in air.

EM-ThP9 Micro-Optical Switch Device Based on Semiconductor-To-Metallic Phase Transition Characteristics of W-doped VO@sub 2@ Smart Coatings*, **M. Soltani**, M. Chaker,* INRS-Energie, Matériaux et Télécommunications, Canada*; E. Haddad, R.V. Kruzelecky,* MPB Communications Inc.*; J. Margot,* Université de Montréal, Canada

Thermochromic vanadium dioxide (VO2) smart coatings undergo a reversible semiconductor-to-metallic phase transition (SMT) at a transition temperature of Tt = 68°C. This phase transition is accompanied by an important modification of the electrical resistivity, optical transmittance and reflectance in the infrared region. The Tt can be controlled by doping the coating with donor-like or acceptor-like centers. In addition, the SMT of VO2 thin films can be controlled by external parameters such as temperature, pressure, photo-carrier injection into a VO2 heterostructure, and an electric field. VO2 smart coatings are thus excellent materials for technological applications such as optical fiber switching devices,@footnote 1@ smart radiator devices for spacecraft,@footnote 2@ all-optical and electro-optical switching devices.@footnote 3@ Recently, we have optimized the reactive pulsed laser deposition (RPLD) parameters to grow either an undoped or metal (W and Ti) doped VO2 smart coatings on large area substrates@footnote 4@ as well as on small area substrates such as ends of cleaved fibers and optical fibers connectors. Also, we were able to control the SMT of the VO2 layers by photo-excitation (i.e., all-optical switching), as well as by an external electric-field (i.e., electro-optical switch). In this paper, we present our recent results on the fabrication and characterization of micro-optical switch device exploiting the semiconductor (on) to metallic (off) states of W-doped VO2 active layers driven by an external voltage. The active layers were synthesized on sapphire substrate by means of RPLD. The micro-optical switch was patterned by photolithography and plasma etching. While the NiCr electrical contacts were patterned by means of the lift-off process. The transmittance switching (on/off) of the fabricated device was investigated at @lambda@ = 1.55 µm as a function of the applied voltage through the NiCr electrical contacts. An extinction ratio (on/off) as high as 20 dB was achieved with this device.@FootnoteText@@footnote 1@M. Soltani, M. Chaker, E. Haddad, R. V. Kruzelecky, and D. Nikanpour, J. Vac. Sci. Technol. A 22, 859 (2004).@footnote 2@R.V. Kruzelecky, E. Haddad, W. Jamroz, M. Soltani, M. Chaker, and G. Colangelo, Proc. SAE, Paper 2005-01-2906 (2005).@footnote 3@M. Soltani, M. Chaker, E. Haddad, and R. V. Kruzelecky, Meas. Sci. Technol.17, 1052 (2006).@footnote 4@M. Soltani, M. Chaker, E. Haddad, R. V. Kruzelecky, and J. Margot, Appl. Phys. Lett. 85, 1958 (2004).

EM-ThP10 Characteristics of Ohmic Contact Properties on N-polar Face n-type GaN with Dry and Wet Etching Method*, **T. Jang**, Y.J. Sung,* Samsung Advanced Institute of Technology, Korea, South Korea*; O.H. Nam, Y. Park,* Samsung Advanced Institute of Technology, Korea

Recently, remarkable progress on the development of blue and violet laser diode (BV-LD) has been made by several companies (Nichia, Sony and Samsung). BV-LD is a key component as a light source for high density optical storage systems and large scale display systems. Most of the commercialized high-power BV-LDs are fabricated on the free standing GaN wafers because of their high thermal conductivity, ease of cleaving and simple fabrication process. Free standing GaN wafer has a wurtzite crystal structure which has two different polarities along the c-axis direction, (0001) Ga face and (0001(_)) N face, respectively. The (0001) surface is composed of three nitrogen dangling bonds which points upward the c-plane surface, while (0001(_)) surface has a single nitrogen dangling bond that points upward. This difference in surface structure affects the device characteristics, especially ohmic contacts properties. Instead of using just Ga-face surface (0001), both Ga-polar face (0001) and N-polar face (0001(_)) surfaces would be used with free standing GaN wafers to fabricate LDs. One of the serious concerns in the fabrication of high-power BV-LDs is the difficulty of achieving reliable ohmic contact property on N-polar face n-type GaN. In this study, the effects of surface treatments such as ICP (Inductively Coupled Plasma) and wet etchings prior to the ohmic contact formation were investigated by measuring the contact resistivity of TLM (Transfer Length Method). Ohmic contact materials comprised of the layer sequence of Al/Ti and Pd/Ti/Al were deposited and contact resistivities were measured with respect to the annealing temperatures. The results of contact resistivity and AFM (Atomic Force Microscopy) confirmed that the area of contact is directly related to the improvement of ohmic contact property on N-polar face n-type GaN.

EM-ThP12 The Structural and Optical Properties of InN Layers Grown by High Pressure CVD*, **M. Alevli**, G. Durkaya,* Georgia State University*; W. Fenwick,* Georgia Institute of Technology*; A. Weerasekara, V.T. Woods,* Georgia State University*; I. Ferguson,* Georgia Institude of Technology*; U. Perera, N. Dietz,* Georgia State University

Indium nitride (InN), with its high mobility and small effective electron mass among the nitrides, is a promising material for advanced optoelectronic device applications. Indium-rich alloys, e.g. (Ga@sub 1-y-x@Al@sub y@In@subx@)N will enable the fabrication of high-efficient light emitting diodes tunable in the whole visible spectral region, as well as advanced high speed optoelectronics for optical communication. The present limitation in this area is the growth of high quality InN and indium-rich group III-nitride alloys as documented in many controversial reports on the true physical properties of InN. The difficulties arise from the low dissociation temperature of InN that requires an extraordinarily high nitrogen overpressure to stabilize the material up to optimum growth temperatures. We developed a novel high-pressure chemical vapor deposition (HPCVD) system, capable to control and analyze the vast different partial pressures of the constituents. Our results show that the chosen HPCVD pathway leads to high-quality single crystalline InN, demonstrating that HPCVD is a viable tool for the growth of indium rich group III nitride alloys. The structural analysis of InN deposited on GaN-sapphire substrate by XRD show single phase InN(0002) peaks with full width half maximum (FWHM) around 430 arcsec. Infrared reflectance spectroscopy is used to analyze the plasmon frequencies, high frequency dielectric constants, the free carrier concentrations and carrier mobilities in these layers. For nominal undoped InN layers, free carrier concentrations in the mid 10E+19cm-3 and mobilities around 600 cm+2-V-1-s-1 are observed. A further improvement is expected as the growth parameters are optimized. At present, the growth of InN is carried out at temperatures as high as 1150 K for reactor pressures around 15 bar, which is a major step towards the fabrication of indium rich heterostructures due to the closer match to the ideal processing temperatures of (Ga1-y-xAlyInx)N.

EM-ThP13 Reliability Performance and Electrical Comparison of TiB@sub 2@ ,CrB@sub 2@ and W@sub 2@B@sub 5@ Based Ohmic Contacts on n-GaN*, **R Khanna**, S.J. Pearton, F. Ren, I.I. Kravchenko,* University of Florida

Three different metal borides (TiB@sub 2@, CrB@sub 2@ and W@sub 2@B@sub 5@) were examined for use in Ti/Al/boride/Ti/Au Ohmic contacts on n-type GaN and the reliability compared to the more usual Ti/Al/Ni/Au metal scheme. The minimum specific contact resistance obtained was in the range 10@super -5@ @ohm@.cm@super 2@ with CrB@sub 2@ and W@sub 2@B@sub 5@ and approximately an order of magnitude lower with TiB@sub 2@. In all cases, the minimum contact resistance is achieved after annealing in the range 700-900°C. The main current transport mechanism in the contacts after this annealing is tunneling as determined by the absence of any significant measurement temperature dependence to the contact resistance. The TiB@sub 2@ and CrB@sub 2@ contacts retain smooth morphology even after annealing at 1000° C. Auger Electron Spectrosopy depth profiling indicated that formation of an interfacial TiN@sub X@ layer is likely responsible for the Ohmic nature of the contact after annealing. All three boride-based contacts show lower contact resistance than Ti/Al/Ni/Au after extended aging at 350°C.

EM-ThP14 Decay Mechanism of Negative Electron Affinity (Cs/O Activated)InP(100) Photocathodes*, **D.-I. Lee**,* Stanford University, U.S.*; Y. Sun, Z. Liu,* Stanford Synchrotron Radiation Laboratory*; S. Sun,* Stanford University*; P. Pianetta,* Stanford Synchrotron Radiation Laboratory

Negative Electron Affinity (NEA) III-V photocathodes prepared by Cs and oxygen co-deposition have been widely used in technological applications of image intensifiers and e-beam sources due to its beam properties such as high quantum efficiency (Q.E), high spin-polarization, and low energy spread. One of the concerns raised in the usage of these photocathodes is the relatively short lifetime since industry desires that photocathodes last for a long period of time without losing its reliable performance. This lifetime issue is induced by the fact that very thin Cs oxide layer is extremely sensitive to contamination, which destroys the NEA properties of the surface and reduces its Q.E. The lack of understanding of the very thin Cs oxide activation layer, however, prevents researchers from providing a profound way to achieve long-lifetime stability especially when the photocathode is not in a sealed tube. In this study, we have investigated the decay mechanism of Cs/O activated InP(100) photocathode by Synchrotron Radiation Photoemission (SR-PES) and Energy Distribution Curve (EDC) measurements. We found that decay of Q.E. and the increase of electron affinity are due to the transformation of Cs peroxide into Cs superoxide and subsequent oxidation of InP substrate. These changes can be explained by thermodynamics. Furthermore, a simplified lateral distribution model of Cs oxide layer on the surface is proposed based on the angular dependence of O1s and valence band spectra. The redeposition of Cs was performed in order to simulate the sealed photocathode tube, and it is found that redeposited Cs recovers Q.E. by building up partial dipoles, and prevents Cs peroxide from transforming into Cs superoxide by acting as a protective layer.

EM-ThP15 Electronic Properties of Adsorbates on GaAs(001)-c(2x8)/(2x4)*, **D.L. Winn**, M.J. Hale, A.C. Kummel,* University of California, San Diego

The key issue in fabricating a III-V MOSFET is forming an unpinned interface between the gate oxide and the semiconductor. A systematic experimental and theoretical study has been performed to determine the causes of oxide pinning and unpinning on GaAs(100). Scanning tunneling spectroscopy (STS) and density functional theory (DFT) were used to study four different adsorbates (O@sub 2@, Ga@sub 2@O, In@sub 2@O, and SiO) bonding to the GaAs(001)-c(2x8)/(2x4) surface. The STS results revealed that out of the four adsorbates only one left the Fermi level unpinned, Ga@sub 2@O. DFT calculations were used to elucidate the causes of the Fermi level pinning. Two distinct pinning mechanism were identified: direct (the adsorbate induced states in the band gap region) and/or indirectly pinning (generation of undimerized As atoms). In the cause of O@sub 2@ adsorbing onto GaAs the Fermi level pinning was found to result only from indirect case, while, In@sub 2@O was shown to pin the Fermi level directly. SiO however, was found to exhibit both indirect and direct (build-up of local charge, and formation of partially filled dangling bonds on some of the Si atoms) Fermi level pinning. The close correlation between experiment and theory suggest that DFT can be used to predict oxide pinning and unpinning on III-V semiconductors.

EM-ThP16 Bonding Geometries of In@sub 2@O on InAs(001)-(4x2)*, **J. Shen**, D.L. Winn, N.M. Santagata, A.C. Kummel,* University of California, San Diego

The key to fabricating a high mobility MOSFET is forming an electrically passive oxide-semiconductor interface on a very high molibity semiconductor. The absence of As-As dimers makes the InAs(001)-(4x2) surface ideal for gate oxide deposition, since the surface should not readily react with deposited oxides. Scanning tunneling microscopy (STM) and density functional theory (DFT) were used to definitively identify the InAs(001)-(4x2) reconstruction along with ascertaining how In@sub 2@O adsorbates bond onto the clean surface. The clean surface consists of single In-In dimers that run in the [110] direction. Between the row dimers is a trough region that contains 2 additional In-In dimers. After the InAs(001)-(4x2) reconstruction was identified, In@sub 2@O was deposited onto the clean surface using MBE. The lowest coverage In@sub 2@O adsorption site was identified as an In atom from In@sub 2@O bonding to a tricoordinated As atoms at the edge of the row. When this occurs, it causes the second In atom in In@sub 2@O to bond nonspecifically in the trough region. Evan at low coverage (20% monolayer (ML)), the In@sub 2@O adsorbates formed islands that are elongated in the [110] direction. Prior to all the first layer sites being occupied with In@sub 2@O molecules, second layer growth was observed on the islands. This was attributed to the In atom, in the In@sub 2@O molecule, that protruded into the trough region being highly reactive. Most importantly, the In@sub 2@O adsorbates never causes the abstraction of any surface atoms on the InAs(001)-(4x2) surface. This is consistent with the formation of a smooth interface between the oxide and the semiconductor. STS measurements are being performed to determine the electronic properties of the interface.

EM-ThP17 High Thermal Stability Ag-based Ohmic Contacts for InAlAs/InGaAs/InP High Electron Mobility Transistors*, L. Wang, W.F. Zhao, **I. Adesida**,* University of Illinois at Urbana-Champaign

InAlAs/InGaAs/InP HEMTs are promising for microwave applications due to their high-frequency and low-noise characteristics. Low-resistive and high thermal stable ohmic contacts are desirable to fully exploit their potential. The Au-Ge-Ni contacts used for GaAs are also applied in InP-based devices with further optimization. However, the optimum annealing temperatures of these contacts are low (~250 °C). Due to the high diffusivity of Au and low eutectic point of AuGe alloy, these contacts are intrinsically unstable when subjected to thermal processes of fabrication or electrical stresses during operation. We showed that the optimum contact resistance of Au-Ge-Ni is achievable only within a narrow window of ~50 °C which makes the reliable control of device performance problematic. Ge/Ag/Ni ohmic contacts with excellent contact resistance of 0.07 Î©-mm were obtained after annealing at 425 °C. These contacts have a large processing window of >130 °C. A SiNx layer deposited prior to annealing could suppress the degradation of the devices. Storage tests at 215 and 250 °C indicate that this metallization is far superior to the Au-based contacts in term of thermal stability. TEM studies confirm that metal spikes successfully link the 2DEG layer with the metal layer to produce excellent ohmic characteristics. The spikes are mainly Ag and Au, respectively, as identified by EDS. For the optimum annealed samples, the Ag and Au spikes have similar area density and penetration depth. This is a logical result since the injection properties/efficiencies of the metal spikes, which are dictated by the density, size, and shape of the spikes, determine the ohmic performance. The formation of liquid Au-Ge eutectic phase in Au-Ge-Ni at 300 °C and the fast diffusion of Au are believed to be the reason of overannealing. The eutectic temperature of Ag-Ge is 300 °C higher rendering Ag-contacts a higher annealing temperature and a wider processing window.

EM-ThP18 Ion-channeling Damage Profiles in Ferromagnetic Mn-implanted Si*, **C. Awo-Affouda**, M.B. Huang, V.P. LaBella,* University at Albany-SUNY

Semiconductor devices which exploit the spin of the electron have potential to produce devices with increased functionalities. Making conventional semiconductors such as GaAs and Si ferromagnetic via doping with Mn will aid in fabricating these future spintronic devices. It has been suggested that the residual implant damage after post implant annealing plays a role in the magnetic behavior of Mn-implanted Si. To further investigate this, lattice disorder depth profiles were obtained from RBS-channeling experiments on Mn implanted p-type Si samples. These profiles reveal a strong influence of the Mn fluence and the post implant annealing temperatures upon the defects generated from implantation. Specifically, above 800C, the back scattering yield from Si lattice defects decreases

which is coincident with a decrease in the magnetization. Modeling is also performed to help understand the type of defects and their distributions.

**EM-ThP19 Ferroelectric Properties of Na@sub 0.5@ K@sub 0.5@ NbO@sub 3@ Thin Films for Nonvolatile Ferroelectric Random Access Memory*, K.T. Kim,* *C.I. Kim,* Chung-Ang University, Korea

The ferroelectric sodium-potassium niobate Na@sub 0.5@ K@sub 0.5@ NbO@sub 3@ (hereafter NKN, a solid solution of KNbO@sub 3@ and NaNbO@sub 3@) thin films have received the intent attention for their excellent ferroelectric, crystalline properties and lead-free materials. It was shown that NKN thin films are able to overcome the drawbacks of other materials, such as SBT and PZT, for nonvolatile memory applications. The NKN thin films were prepared by using metal organic decomposition method. The structure and morphology of the films were analyzed by x-ray diffraction (XRD), atomic force microscope (AFM), and Scanning electron micrograph (SEM). SEM and AFM showed uniform surface of the films. From the XRD analysis, the NKN thin films were grown using a Pt bottom electrode showed a polycrystalline phase. The remanent polarization Pr and coercive field is 13.5 µmC/cm@super 2@ and 89 kV/cm. The BLT thin films on Pt bottom electrode exhibited no significant degradation of switching charge at least up to 5 x 10@super 9@ switching cycles at a frequency of 50 kHz below cycling fields of 5 V.

**EM-ThP20 Fatigue Characteristics of PZT Thin Film Capacitors with Controls of CMP Process Parameters and Slurry Contaminations*, Y.-K. Jun,* *N.H. Kim, W.-S. Lee,* Chosun University, Korea

Pb(Zr,Ti)O@sub 3@ (PZT) is very attractive ferroelectric materials for ferroelectric random access memory (FeRAM) applications because of its high polarization ability and low process temperature. In this study, PZT thin film capacitors were fabricated by damascene process instead of plasma etching process. Damascene process of PZT thin film was first applied for the densification of devices and the protection of plasma damages including ion charging. However, chemical mechanical polishing (CMP) pressure and velocity must be carefully adjusted because FeRAM shrinks to high density devices. The probability of CMP damage such as microscratch surely existed although the removal rate of PZT thin films increases and the yield improves through the each increase of CMP pressure and velocity. The contaminations such as slurry residues due to the absence of the exclusive cleaning chemicals are enough to influence on the degradation of PZT thin film capacitors. The fatigue characteristics of the degradations of PZT thin film capacitors were investigated by the change of process parameters and the cleaning process. Both the low CMP pressure and the cleaning process must be employed, even if the removal rate and the yield were decreased, to reduce the fatigue of PZT thin film capacitors fabricated by damascene process. Like this, fatigue characteristics were partially controlled by the regulation of the CMP process parameters in PZT damascene process. And the exclusive cleaning chemicals for PZT thin films were developed in this work. Acknowledgement: This work was supported by Korea Research Foundation Grant (KRF-2004-005-D00007).

EM-ThP21 Molecular Beam Epitaxy of YMnO@sub 3@ on c-plane GaN*, C.B. Keenan*, *T. Liu, K. Lee, R.P. Tompkins, E.D. Schires, Y. Chye, D. Lederman, T.H. Myers,* West Virginia University

Ferroelectric oxide thin films on semiconductors have attracted attention for their potential applications in nonvolatile memory, piezoelectric, and microwave devices. Interest is now emerging in the potential of new devices based on active interfaces between ferroelectric oxides and polar semiconductors such as GaN or ZnO. YMnO@sub 3@ is an obvious candidate of oxide films on GaN because they both have a hexagonal lattice structure and the lattice constant of YMnO@sub 3@ is approximately twice that of GaN. Here we report on the epitaxial growth of YMO thin films directly on GaN using MBE. YMnO@sub 3@ films are grown on GaN (0001)-on-sapphire templates using MBE. The structure of the films as characterized by in-situ RHEED, x-ray diffraction, and atomic force microscopy will be discussed. Atomic force microscopy revealed that the YMnO@sub 3@ films grown at different temperatures have significantly different morphologies. Samples grown at the optimal growth temperature are ferroelectric at room temperature, and magnetic at low temperatures. The YMnO@sub 3@ samples exhibit a remnant polarization of approximately 3.2 @micro@C/cm@super 2@ and saturation polarization of about 12 @micro@C/cm@super 2@. The difference between magnetic field-cooled and zero-field-cooled behavior at low temperatures suggests the presence of either antiferromagnetic frustration or ferromagnetic behavior. The effects of different growth temperatures and post-growth annealing will also be discussed. This research was supported by US Office of Naval Research (Grant N00014-02-1-0974), the US Air Force Office of Scientific Research (MURI Grant F49620-03-1-0330), and by the US National Science Foundation through the West Virginia EPSCoR program.

**EM-ThP22 Integration of Barium Ferrite on the Wide Bandgap Semiconductor 6H-SiC Through Molecular Beam Epitaxy*, Z. Cai,* *Z Chen, T.L. Goodrich, V.G. Harris, K.S. Ziemer,* Northeastern University

Integration of nonreciprocal ferrite microwave devices with semiconductor platforms would allow for reduced volume and weight in phased array radar electronics, in addition to enhanced bandwidth and power management. Barium hexaferrite (BaM, BaFe@sub 12@O@sub 19@) is ideal for microwave device applications because of its large (17kOe) uniaxial magnetocrystalline anisotropy, high resistivity and permeability at high frequencies (>40GHz). The performance of current ferrite devices would be enhanced and novel devices would be possible if BaM were integrated with wide bandgap semiconductors (e.g. SiC), which can function in high-temperature, high-power, and high-frequency environments. However, oriented, single-crystalline BaM films with the desired magnetic properties (high saturation magnetization and low FMR linewidth) have not yet been successfully grown on any semiconductor substrate. In order to produce BaM thin films with desired stoichiometry, structure, and magnetic properties needed for microwave device applications, the nucleation and growth mechanisms of BaM on 6H-SiC were investigated using a remote oxygen plasma source producing a chamber oxygen pressure of 5x10@super -6@ Torr, and solid source Ba and Fe effusion cells. In-situ x-ray photoelectron spectroscopy (XPS) and reflection high-energy electron diffraction show oxygen rich (@>=@69%) and iron deficient (@<=@20%) polycrystalline films, which suggest complex surface reactions among the metals and the oxygen. Preliminary XPS studies of BaM films deposited by pulsed laser deposition (PLD) show different compositions and O bonding states with respect to the thickness of the films. Films grown on SiC by PLD are porous with either FMR linewidth of >500 Oe or no FMR at all. Using a MgO interlayer structure between the BaM and SiC has been shown to prevent silicon diffusion into BaM films and reduce bond mixing at the interface, which results in FMR linewidths

**EM-ThP23 Ferroelectric and Dielectric Properties of BLT Capacitors Fabricated by Damascene Process using Chemical Mechanical Polishing*, S.H. Shin,* *P.J. Ko, N.H. Kim, W.-S. Lee,* Chosun University, Korea

Nonvolatile memory devices using ferroelectric thin films such as PZT, SBT and BLT have attracted attention because of their non-volatility and high-speed operations. However, commercial use of PZT ferroelectric memory devices has been hindered largely by fatigue, defined as the decrease of switchable polarization with electric field cycling in ferroelectrics. Whereas, as a fatigue-free material, SBT is limited in the practical application due to its small polarization and high processing temperature. More recently, BLT is of particular interest, as it is not only crystallized at relatively low processing temperature, but also shows highly fatigue resistance and large remanent polarization. Meanwhile, these submicron ferroelectric capacitors were fabricated by a damascene process using Chemical mechanical polishing (CMP). The fabricated capacitors consisted of BLT thin film with top and bottom electrodes. The P-E characteristics of BLT capacitors fabricated by CMP were examined at various voltages and room temperature. Remanent polarization was identified by the measuring of electric hysteresis loops for the capacitors. Dielectric property and loss factor (dissipation factor) were investigated as a function of frequency with LCR meter. Ferroelectric BLT capacitors were practicable by a damascene process using CMP, which realized a vertical sidewall.

**EM-ThP24 P Incorporation during Si(001):P Gas-Source Molecular Beam Epitaxy: Effects on Growth Kinetics and Surface Morphology*, B. Cho,* *J. Bareno,* University of Illinois at Urbana-Champaign*; Y.L. Foo,* Institute of Materials Research and Engineering, Singapore*; S. Hong,* Seoul National University, Korea*; T. Spila, I. Petrov, J.E. Greene,* University of Illinois at Urbana-Champaign

The effects of P doping on growth kinetics and surface morphological evolution during Si(001):P GS-MBE from Si@sub2@H@sub6@ and PH@sub3@ at temperatures T@subs@ = 500-900 °C have been investigated. With increasing PH@sub3@/Si@sub2@H@sub6@ flux ratio J@subP/Si@ at constant T@subs@, we observe a decrease in the film growth rate R, accompanied by increased surface roughening and pit formation. At constant J@subP/Si@, R increases with increasing T@subs@, while the incorporated P concentration C@subP@ initially increases, reaches a maximum at T@subs@ = 700 °C, and then decreases at higher growth temperatures. We use in-situ D@sub2@ temperature programmed

desorption (TPD) to follow changes in film surface composition and dangling bond density @theta@@subdb@ as a function of J@subP/Si@ and T@subs@. Measurements on both as-deposited Si(001):P layers and P-adsorbed Si(001) reveal @beta@@sub1@ and @beta@@sub2@ peaks due to D@sub2@ desorption from Si monohydride and dihydride species, respectively, as well as the formation of a third peak @beta@@sub3@ corresponding to D@sub2@ desorption from mixed Si-P dimers. Dissociative PH@sub3@ adsorption on Si(001) results in a decrease in @theta@@subdb@ and an initial increase in P surface coverage @theta@@subP@ with increasing T@subs@. @theta@@subP@ reaches a maximum value of 0.95 ML at T@subs@ = 550 °C, and decreases with T@subs@ > 600 °C due to the onset of P@sub2@ desorption. Comparison of @theta@@subP@(T@subs@) with C@subP@(T@subs@) results obtained during film growth reveals the presence of strong P surface segregation. From measurements of @theta@@subP@ vs. C@subP@ in Si(001):P layers, we obtain a P segregation enthalpy @DELTA@H@subs@= -0.86 eV. Using the combined set of results, we develop a predictive model for C@subP@ vs. T@subs@ and J@subP/Si@, incorporating the dependence of the PH@sub3@ sticking probability S@subPH3@ on @theta@@subP@, which provides an excellent fit to the experimental data.

EM-ThP25 Solid Source Phosphorous Doping in Si*, **G.G. Jernigan,*** *P.E. Thompson,* U.S. Naval Research Laboratory

Phosphorus doping in Si is being pursed as a possible single spin qubit for quantum computing and as a delta layer for use in a resonant interband tunnel diode. We are using a unique doping source, based on the decomposition of GaP, to produce P in a solid source molecular beam epitaxy machine. This has advantages over the use of phosphine gas decomposition due to the use of lower sample temperatures (< 500 °C) and higher surface coverages (due the absence of hydrogen). We will present a study of the adsorption and desorption of P in the temperature range of 25-800 °C on a Si (100) surface using in vacuo XPS and STM. P is found to adsorb up to one complete monolayer (ML) between 25 and 500 °C and does not form a multilayer. The surface consists of long rows of P dimers separated by vacancy lines. Beginning with 1 ML, P desorbs from Si between 500 and 800 °C. A simple Redhead analysis indicates a second order desorption with an activation energy of ~29 Kcal/mol. Desorption disrupts the P dimer morphology resulting in individual P atoms moving on the surface. STM IV analysis indicates that layer conductivity changes when the dimers break and when P begins to desorb. Compared to a Si surface without P, we find that annealing a surface with a submonolayer of P produces a surface whose step edges are very highly kinked. The relevance of P surface coverage and surface morphology, along with the co-deposition of P and Si, to device applications will be discussed.

EM-ThP28 Local Structure Around Germanium Atoms in SiGe Thin Films*, **Y. Uehara**, K. Kawase,* Mitsubishi Electric Co., Japan*; J. Tsuchimoto,* Renesas Co., Japan

SiGe thin films are widely studied in order to apply them as the channel layer for LSI of the next generation, because they show superior electronic properties than the current silicon channel. More germaniums in film enhance the electron mobility, while the lattice mismatch of the film with the substrate becomes large, so it is important to control the concentration of germanium in the film. Also, it should be important to control how the germanium atoms are involved in the film, however, there are few information on them. In this study, we have applied XAFS technique to investigate the local structure around germanium atoms in SiGe thin films. SiGe films were prepared by CVD method on Si(100) wafers. Si/Ge ratio of the films was controlled by the flow rate of the origin gases. The germanium concentration and the thickness of the films were confirmed by X-ray locking curve method and X-ray reflectivity method, respectively. XAFS measurements at Ge-K absorption edge were performed at BL16B2 of SPring-8. The Si(311) double crystal monochromator and the Rh-coated cylindrical mirror were used, and electrons emitted from the sample surface were collected using a conversion electron yield detection system. We could not find any changes in the Ge-K XANES region among the samples with different germanium concentration. The standard EXAFS analysis was performed to elucidate the local structure around the germanium atoms in the films. The curve fitting analysis revealed that the germanium atoms in as-deposited SiGe thin films make complete solid solution with silicon, do not conform micro-clusters of germanium, at least when the germanium concentration is less than 20%.

EM-ThP29 Inspection and Analysis of Voiding Defects in Copper Interconnects on a Test Wafer*, **S. Suzuki**, Y. Nakano, K. Umemura, T. Sato,* Hitachi High-Technologies Corporation, Japan

For improvement of yield of LSI, it is necessary to use the analysis system that consists of inspection of defects of a wafer, analysis of defects and countermeasures. Voiding of Cu interconnects affect yield and reliability of ULSI, therefore it is so useful to detect efficiently voids of Cu layer in the manufacturing process. In this study, we have investigated the efficient analysis technique of voids by using the system. Void and etching stopped defects were intentionally on a 200mm wafer with 160nm diameter Cu via pattern made by typical single damascene process. Inspection of the wafer was done by electron beam (EB) inspection and optical inspection equipments, for cross section analysis samples from the wafer were made by focused ion beam (FIB) equipment, and defects were observed by scanning transmission electron microscope (STEM) with energy dispersive X-ray spectroscopy (EDS).The 2 types of defects (called one gray defect, the other dark defect), which contrast were different, were detected by EB inspection. The STEM results confirmed that gray defect was a void defect; dark one was an etching stopped defect. By cross section observation of 10 defects, there is a coincidence that all gray defects were voids and all dark were etching stopped. In the gray defect Cu was partially missing and only Ta/TaN layer remained, and it was estimated that voiding was finally occurred at annealing step of process because Cu seed layer also was missing. We are able to explain that difference of contrast is caused difference of electrical current through via, which depends on resistivity, for example a single via with 180nm height void is 10 times resistivity of that without void by rough calculation. In addition, we tried to quantify SEM image of the 2 types of defects, and actually measure resistivity of via by means of electrical probing equipment with SEM. Finally we find that EB inspection and quantification of SEM image is an efficient method to detect and classify defects.

EM-ThP30 Oxidation of Thin Y-Si Film on Silicon*, **S.Y. Chiam**,* Imperial College, United Kingdom*; W.K. Chim,* National University of Singapore*; A.C. Huan,* Nanyang Technological University, Singapore*; J. Zhang,* Imperial College, UK*; J.S. Pan,* Institute of Materials Research & Engineering, Singapore

Oxidation studies are investigated on sputtered films in the formation of yttrium silicate by a two step process. Firstly, an in-situ low temperature annealing of yttrium (Y) metal on silicon (Si) is performed to obtain a Y-Si film. The Y-Si film is then oxidized ex-situ in a horizontal furnace of either nitrogen (N2) or oxygen (O2) ambient. Deposited films are investigated by depth profiling X-ray photoelectron spectroscopy (XPS). We report on self-limiting formation of yttrium silicate at room temperature which is insensitive to annealing ambient. We also found that oxygen pressure plays an important role in the extent of Si oxidation at mid-annealing temperature. Finally, we report that a relatively high temperature is needed for the complete oxidation of Y-Si films in the formation of yttrium silicate films. This is attributed to a high diffusion barrier for oxygen caused by initial yttrium silicate films formed on the top of the film which is the limiting mechanism for the oxidation of Y-Si film.

EM-ThP31 Effects of NO Addition on Chemical Dry Etching of Silicon Oxide Layers in F2/Ar and F2/Ar/N2 Remote Plasma Processing*, **Y.B. Yun**, D. Kim,* Sungkyunkwan University, Korea*; Y.-C. Jang, G. Bae,* Atto Inc in Korea

Chemical dry etching and cleaning process of silicon oxide layers in Si device manufacturing fabs have been carried out using PFCs. Etching process utilizing F@sub 2@gas is of a great interest. We carried out etching experiments using F@sub 2@/Ar, F@sub 2@/Ar/N@sub 2@ remote plasma generated from a toroidal-type remote plasma source in a commercial PECVD system. And the effect of directly-injected NO gas on the SiO@sub 2@ etching in F@sub 2@/Ar/N@sub 2@ remote plasmas was investigated. Etching experiments were carried out by varying the gas flow ratio, flow rate, RF power, and temperature. The effects of NO addition to F@sub 2@/Ar, F@sub 2@/Ar/N@sub 2@ etching were characterized by measuring the etch rates and by analyzing the emitted species during etching. The results showed that the addition of NO gas increased the etch rates significantly. The mechanism for etch rate enhancement will be discussed in detail in conjunction with the gas emission analysis using FT-IR and RGA and chemical composition of the etched oxide surface using XPS.

EM-ThP32 Yield improvement of 0.13 µm Cu/Low-k Dual Damascene Interconnection by Organic Cleaning Process*, **H.K. Lee,*** Chung-Ang University, Korea*; N.H. Kim,* Chosun University, Korea*; S.Y. Kim,* DongbuAnam Semiconductor Inc., Korea*; C.I. Kim, E.G. Chang,* Chung-Ang University, Korea

Cu/low-k dielectrics are required to reduce RC delay and parasitic capacitance of the back-end-of-line (BEOL) interconnection. Integration of Cu/low-k dielectrics for BEOL interconnection in the 0.13 µm technology has gained wide acceptance in the microelectronics industry in recent years. In this paper, we discuss the process integration issues of the 0.13 µm Cu/low-k (Black Diamond) dual damascene integration for SRAM device yield. The same scheme of 0.13 µm Cu/ fluorinated silicate glass (FSG) based device was used for full process in making low-k based device. Black diamond was used as a low-k material with a dielectric constant of 2.95. To reduce the damage of low-k and improve the yield of low-k based device, H@sub 2@O ashing, organic cleaning, and low down pressure in chemical mechanical planarization (CMP) were selected for the study. Specially, the organic cleaning process after ashing process is very effective on the removal of organic residues in via and trench, and surface contaminant. There is an increase of 40% SRAM device yield, compared to low-k based device which is uncleaned after ashing process. As a result, we successfully integrated 0.13 µm Cu/low-k (Black Diamond) dual damascene interconnection with excellent yield performance after process improvement of organic cleaning.

EM-ThP33 Etch Induced Sidewall Damage Evaluation in Porous Low-k MSQ Films*, **B. Kong**,* Sungkyunkwan University, Korea*; T. Choi, S. Sirard,* Lam Research Corporation*; D. Kim,* Sungkyunkwan University, Korea

As device feature sizes shrink down to 45nm and below, films with lower dielectric constants (k) are needed to reduce the RC delay in copper backend applications. The plasma etch-induced damage (carbon depletion, moisture uptake, silanol formation) of porous low-k methyl silsesquioxane (MSQ, k=2.2) films was investigated. Etch-induced damage was characterized on both blanket and trench patterned MSQ materials. The MSQ materials were etched with CF4 and C4F8-based chemistries under various process conditions. Simple CF4/O2 chemistry minimized the damage of porous MSQ during plasma etching. The addition of Ar or H2 increased the damage. The highest damage levels were observed with simultaneous Ar, H2 and N2 addition. Also, the use of higher powers and/or lower pressures resulted in more etch-induced damage.

EM-ThP34 Arsenic Ultra Shallow Junction Deactivation Investigated by Multi-Technique Analytical Approach*, **M. Bersani**, G. Pepponi, D. Giubertoni, S. Gennaro, M. Anderle,* ITC-irst, Italy*; R. Doherty, M.A. Foad,* Applied Materials

New processes are needed to satisfy the requirements of modern ULSI C-MOS fabrication. In particular for source and drain extension laser sub-melt annealing has arisen as an emerging tool able to produce high level of dopant activation together with ultra shallow distribution. Nevertheless arsenic (the most used n-type dopant) is known to easily deactivate when further thermal annealings are carried out after laser treatment. A detailed study is required in order to understand its behavior in high concentration regime and in close proximity of the surface as in the case of ultra shallow distribution. In this work ultra shallow arsenic implants (2 keV implant energy, dose ranging from 3E13 to 3E15 at/cm2) laser sub-melt annealed have been submitted to further thermal processes in conventional furnace. The samples so produced have been characterized by a multi-technique analytical approach: Secondary Ion Mass Spectrometry (SIMS), Hall Effect measurements, Extended X-ray Absorption Fine Structure (EXAFS). This approach has been chosen to enable the correlation among dopant electrical activation, spatial distribution and the local order structure around arsenic atoms. Results show how Arsenic diffusion and electrical behavior after post laser treatment depend on laser annealing conditions.

EM-ThP37 Effects of Additive C@sub 4@F@sub 8@ on Dry Etching of TaN/HfO@sub 2@ Gate Stack Structure using Inductively Coupled BCl@sub 3@/Ar Plasma*, **J.H. Ko**, M.S. Park, D.-Y. Kim,* Sungkyunkwan University, Korea*; S.S. Lee, J. Ahn,* Hanyang University, Korea*; N.-E. Lee,* Sungkyunkwan University, Korea

As the advanced nano-scale CMOS (complementary-metal-oxide-semiconductor) device dimensions continue to be scaled down below 50 nm, development of advanced high-k gate dielectrics with metal gate electrodes and their integration has obtained considerable interests. Among many integration issues, selective etching processes of metal gate electrodes over the high-k gate dielectrics and the high-k gate dielectrics over the Si substrate are expected to be the critical steps in the process integration of the front-end of the line (FEOL). In this work, we compared the etching characteristics of the TaN/HfO@sub 2@ gate stack structure and etch rate selectivity of the TaN over the HfO@sub 2@ layer in the BCl@sub 3@/Ar and BCl@sub 3@/C@sub 4@F@sub 8@/Ar plasmas by varying the process parameters such as the top electrode power, the DC self-bias voltage (V@sub dc@), and BCl@sub 3@/C@sub 4@F@sub 8@ gas flow ratio. To understand the role of etch gas chemistry in ICP etching, the relative change in the densities of ions and radicals in the plasma and chemical binding states of etched TaN and HfO@sub 2@ surfaces were measured by optical spectroscopy (OES) and X-ray photoelectron spectroscopy (XPS), respectively. The results of the etch rates and etch selectivity measured as a function of the various process parameters will be discussed in detail in conjunction with the OES and XPS analysis data. Keywords: HfO@sub 2@, TaN, plasma etching, ICP (inductively coupled plasma), metal gate stack.

EM-ThP38 Characteristics of the Laminated HfO@sub2@/Al@sub2@O@sub3@ High-k Gate Oxides for Thin Film Transistors*, **S.W. Jeong**, K.-S. Kim, J.-Y. Son,* Sungkyunkwan University, Korea*; Y. Roh,* Sungkyunkwan University, Korea, Republic of Korea

Recently, high-k materials are under consideration as replacements for SiO@SUB2@. Among some metal oxides, HfO@sub2@ is an attractive candidate due to their high dielectric constant and thermal stability in contact with silicon. And Al@SUB2@O@SUB3@ is an another attractive candidate because Al@SUB2@O@SUB3@ can remain amorphous at temperature higher than 900@degree@C. The aim of this study is to investigate the thermal stability of the HfO@sub2@ based films with Al@sub2@O@sub3@. Hf metal films were deposited on the (100) p-type Si/Al@sub2@O@sub3@ substrates (100) p-type Si wafers in sequence by non-reactive magnetron sputtering at room temperature. The Hf metal films deposited on the Si/Al@sub2@O@sub3@ substrate were then subjected to oxidation in O@sub2@ ambient at 500 @degree@C for 60 minutes in furnace. We proposed a new technique to grow Al@sub2@O@sub3@/HfO@sub2@ films on the Si substrate at 500 @degree@C. Oxidation followed by annealing of sputtered Hf metal films on the Si substrate both at 500 @degree@C results in multi-layered Al@sub2@O@sub3@-HfO@sub2@ gate insulator. HfO@sub2@/Al@sub2@O@sub3@ laminate structure ware maintained, and Al@sub2@O@sub3@ layer was not useful for blocking oxygen diffusion due to interfacial layer growth. Crystallization temperature of the HfO@sub2@/Al@sub2@O@sub3@ thin films which has Al@sub2@O@sub3@ was delayed up to 900 @degree@C, and as concentration of the Al@sub2@O@sub3@ in HfO@sub2@/Al@sub2@O@sub3@ thin films increases, thermal stability improved. As an annealing temperature increases, HR-TEM analyses of the all the HfO@sub2@/Al@sub2@O@sub3@ flims show the increased interfacial layer thickness. Therefore, our results show the addition of Al@sub2@O@sub3@ is not useful for blocking oxygen diffusion through the HfO@sub2@/Al@sub2@O@sub3@ thin film. From the C-V and I-V measurements, calculated leakage current of the HfO@sub2@/Al@sub2@O@sub3@ thin films was ~16, and as an annealing temperature increases, the leakage current of the films was improved.

EM-ThP39 High-k Dielectric Lanthanum Oxide Thin Films Deposited by Spray Pyrolysis*, S. Carmona, G. Alarcon,* CICATA-IPN, Mexico*; J. Guzman-Mendoza, M. Garcia-Hipolito,* IIM-UNAM, Mexico*; M. Aguilar,* CICATA-IPN, Mexico*; **C. Falcony**,* CINVESTAV-IPN, Mexico

Lanthanum oxide thin films were deposited on silicon substrates using the spray pyrolysis technique. Several chemical solution concentrations of lanthanum acetylacetonate dissolved in acetylacetone were prepared to obtain the films at substrate temperatures in the range of 450-550 ÂºC. The total thickness of the deposited layers was of the order of 50 Ã.. At low temperatures the films resulted amorphous. In addition, the films were characterized by Ellipsometry (single wavelength and spectroscopic), Infrared Spectroscopy, Atomic Force Microscopy, and Electron Microscopy. The chemical composition was studied by Energy Dispersive Spectroscopy, and by means of nuclear reactions. The electrical behavior of the films (I-V and C-V), is discussed when they are incorporated in Metal-Oxide-Semiconductor structures. The growth of an interfacial layer of silicon oxide in the films was controlled by means of the addition of a water/ammonium hydroxide mist applied during the deposition process.

EM-ThP40 Suppression of Chemical Phase Separation in Hf and Ti Si Oxynitride Alloys with High Silicon Nitride Content*, **S. Lee**, G. Lucovsky,* NC State University*; J. Luning,* Stanford Synchrotron Radiation Lab

There are two significant materials issues that limit implementation of high and medium k dielectrics into MOS devices. These are grain-boundary defects in high-k transition metal(TM)/rare earth elemental/complex oxides, and chemical phase separation (CPS) at temperatures too low for thermal budget requirements, 35%, and approximately equal concentrations of ZrO@sub 2@ and SiO@sub 2@, ~ 30-32%, are stable for annealing in inert ambients at temperatures to 1100°C. The results of this paper demonstrate essentially the same behaviors with respect to low and high Si@sub 3@N@sub 4@ content for Hf Si oxynitrides, Ti Si oxyntirdes, and equally importantly, for Hf-Ti alloy Si oxynitrides. Three different spectroscopies have been used to detect CPS, or the absence of CPS: Fourier transform infrared spectroscopy, derivative x-ray photoelectron spectroscopy for the O 1s core level, and derivative near edge x-ray absorption spectroscopy (NEXAS) for the O K@sub 1@ and N K@sub 1@ edges. The NEXAS spectra also provide direct confirmation of a chemical bonding self-organization that prevents nucleation and growth of a nanocrystalline TiO@sub 2@ or HfO@sub 2@ phase that is a necessary precursor to a CPS process.

EM-ThP41 Room-Temperature Magnetron-Sputtered High-k Titanium Silicate Thin Films for MIM and MOS Device Applications*, **D. Brassard**,* INRS-Énergie, Matériaux et Télécommunications, Canada*; L. Ouellet,* DALSA Semiconductor, Canada*; M.A. El Khakani,* INRS-Énergie, Matériaux et Télécommunications, Canada

There is a tremendous ongoing effort for the development of a high dielectric constant (high-k) material that will replace the traditional SiO@sub x@N@sub y@ insulator in both metal-oxide-semiconductor (MOS) transistors and metal-insulator-metal (MIM) capacitors. In this context, we report on the development of a room-temperature magnetron co-sputtering process for the growth of high-k titanium silicate (Ti@sub x@Si@sub 1-x@O@sub 2@) thin films. Ti@sub x@Si@sub 1-x@O@sub 2@ mixed oxide films constitute a highly promising high-k material candidate because they offer the prospect of achieving the best trade-off between the high-k value of the TiO@sub 2@ phase and the unpaired insulating behavior of SiO@sub 2@. The sputter-deposited Ti@sub x@Si@sub 1-x@O@sub 2@ films were integrated into both MIM and MOS capacitors and their structural and electrical properties systematically investigated as a function of the relevant growth conditions (particularly the substrate bias) and the film composition (i.e., the Ti/Si ratio). It is shown that the application of an optimal bias voltage value (of ~ -15 V), during the film growth, leads to a significant densification of the films which in turn is found to improve drastically their electrical properties. Under the optimal growth conditions, the Ti@sub 0.5@Si@sub 0.5@O@sub 2@ films are shown to exhibit an excellent combination of electrical properties, namely: a k of ~17, a leakage current as low as ~10 nA/cm@super 2@ (at 1 MV/cm), and a breakdown field > 4 MV/cm. Moreover, titanium silicate based MIM capacitors showing both high capacitance density of 10 fF/µm@super 2@ and good capacitance linearity (@alpha@ < 1000 ppm/V@super 2@) were achieved. Finally, despite the inherent presence of a ~2 nm-thick SiO@sub 2@ interfacial layer, Ti@sub x@Si@sub 1-x@O@sub 2@ based MOS capacitors with a relatively low density of defects (D@sub it@ ~2x10@super 11@ eV@super -1@cm@super -2@) were achieved after annealing under forming gas.

EM-ThP42 A Study of High-k Removal by Plasma Etching and its Effect on Gate Dielectric Characterization*, **B.S. Ju**, S.C. Song, J. Barnett,* SEMATECH*; B.H. Lee,* IBM

A process to remove high-k gate dielectric films (HfO@sub 2@ and Hf silicate) from the source and drain (S/D) areas after gate electrode etching was investigated to improve the performance and increase the packing density of CMOS transistors. A vertical gate stack profile can be achieved by replacing the conventional method to remove high-k dielectric films that combined physical bombardment and wet etching. This method has been effective to remove crystallized high-k film, but causes notching in Hf silicate or footing in HfO@sub 2@. We propose a new advanced high-k dry etch process using high temperature (250°C) and high density chlorine plasmas (BCl@sub 3@/Cl@sub 2@). The plasma etch process was optimized to enhance etch selectivity to Si, thus enabling the complete removal of high-k films without any substrate recess in the S/D active regions. Optical emission spectroscopy was used to identify the plasma etching by-products, which were mainly chlorinated hafnium, during plasma etching. After plasma etching, no remaining high-k film on the S/D area was detected with Auger electron spectroscopy (AES) measurement and no residual high-k films or structural weaknesses were found with high-resolution transmission electron microscopy (HRTEM). The new process to remove high-k on a CMOSFET device was electrically compared with the conventional wet chemical removal process. A significant amount of plasma damage on high-k films at the gate edge was found to be induced during dry etching, which generated leakage sources in the gate for both HfO@sub 2@ and Hf silicate devices. In situ surface oxidation after plasma removal of the high-k films cured the damage, which dramatically improved leakage current and simultaneously reduced off current, particularly in the short channel, for both PMOS and NMOS devices.

EM-ThP43 Scanning Probe Microscopy Study of Atomic Layer Deposited Hafnium Based High-k Dielectric Films*, **X.-D. Wang**, D.H. Triyoso, R.I. Hegde, D. Roan, R. Gregory,* Freescale Semiconductor, Inc.

Here we report on surface topography and tunneling current characteristics of atomic layer deposited hafnium based dielectric (HfO@sub 2@, Hf@sub x@Zr@sub 1-x@O@sub 2@ and Hf@sub x@Ti@sub y@O@sub z@) films with different processing conditions. The process conditions explored here are: dielectric deposition temperature, post deposition anneal, with and without capping layers for the dielectric during annealing. Atomic force microscopy (AFM) was used to characterize the surface morphology. Conducting AFM (C-AFM) provided the unique capability to characterize the film uniformity by measuring the spatial distribution of the tunneling current through the film. X-ray diffraction (XRD), transmission electron microscopy (TEM) and electrical measurements were also used for the understanding of the film properties. With optimized Ti or Zr ratios, the roughness of the dielectric films is significantly improved and resulted in smaller and more uniform grain size distribution. The addition of Ti or Zr resulted in improved uniformity of tunneling current distribution. However, without a cap layer, significant re-crystallization and roughing were still observed upon 1000°C annealing. This resulted in significant leakage at grain boundaries as revealed by C-AFM images. Adding a metal capping layer prior to annealing greatly improved the stability of the films with only minor increase in surface roughness compared to as-deposited films. Films capped with metal during annealing showed dramatically improved leakage characteristics by eliminating most of the apparent grain boundaries and by improvement of overall film roughness. With the optimized Ti or Zr ratio and metal cap during annealing, better electrical characteristics were achieved based on C-V measurements.

EM-ThP44 Dependence of the Nitrogen Depth Profile on Annealing In HfSiON/SiON/Si(001) Ultrathin Films*, **A. Herrera-Gomez**,* University of Texas at Dallas and CINVESTAV-Queretaro, Mexico*; F.S. Aguirre-Tostado, G. Pant,* University of Texas at Dallas*; M.A. Quevedo-Lopez, P.D. Kirsch,* SEMATECH*; B.E. Gnade, R.M. Wallace,* University of Texas at Dallas

The chemical depth profile of nitrided hafnium silicate dielectric films has been the subject of many studies. Properties such as channel peak mobility and crystallinity depend on the distribution of the nitrogen content. The stoichiometry of hafnium silicate films deposited on a thin layer of silicon oxide was studied with angle resolved x-ray photoelectron spectroscopy (ARXPS). Through a self consistent analysis it was possible to determine the influence of rapid thermal annealing on the compositional depth profile of the film. Upon nitridation, the nitrogen was distributed throughout the films. However, after rapid thermal annealing the N left the hafnium oxide layer and diffused into the underlying silicon oxide layer. Also discussed are important issues regarding the extraction of quantitative information from ARXPS data, such as a proper characterization of the beam shape and analyzer focus area.

EM-ThP45 Electrical and Chemical Analyses of SrTiO@sub 3@/Y@sub 2@O@sub 3@ MIM Capacitors*, **C. Vallee**, M. Kahn, E. Defay, C. Dubourdieu, M. Bonvalot, O. Joubert,* LTM/CNRS, France

The voltage linearity of MIM capacitors is usually described by the following equation: @DELTA@C/C = (C(V)-C0)/C0 = ?V2 + ?V , where C0 is the capacitance value at zero applied voltage, and ? and ? are the quadratic and linear coefficients of the capacitance. According to ITRS specifications, ? must be less than 100 ppm/V2 for RF bypass devices and ? should be as small as possible. As of this date, none of the dielectric materials put on trial for MIM applications shows acceptable voltage linearity with high capacitance density value, their C(V) curve having either a positive or a negative bending. An experimental strategy consists in elaborating bi-layer of dielectric materials exhibiting opposite voltage linearity behaviour. By tuning the thickness of these two dielectrics with respect to each other, we expect to adjust their relative contribution to the overall ? value. Thus, perfectly stable capacitance density values should be observed with varying

applied voltage. In this study, SrTiO3 (STO)-Y2O3 bilayer MIM capacitors are developed. Indeed, STO and Y2O3 show respectively negative and positive ?. STO layers with several thicknesses have been prepared by dual ion beam scattering (DIBS) on Pt/TiO2/SiO2/Si stacks. A post deposition annealing treatment is carried out in order to induce crystallisation. Y2O3 layers are deposited by pulsed injection PE-MOCVD. Metal-dielectric and dielectric-dielectric interfaces are analyzed by XPS, XRR and SE in the FUV range. These dielectrics are then electrically characterized by C(V) measurements with gold electrodes in order to extract ? values and to estimate the overall dielectric constant.

EM-ThP46 Nitrogen Incorporation in Hf-based High-k Dielectrics Upon Thermal and Plasma Treatments, ***F.S. Aguirre-Tostado,*** University of Texas at Dallas; *A. Herrera-Gomez,* University of Texas at Dallas and Cinvestav-Qro, Mexico; *M.J. Kim, B.E. Gnade, R.M. Wallace,* University of Texas at Dallas; *M.A. Quevedo-Lopez,* Texas Instruments assignee at SEMATECH; *P.D. Kirsch,* IBM assignee at SEMATECH

Nitridation of SiO@sub 2@ has been demonstrated to increase the dielectric constant allowing for further scaling in conventional CMOS fabrication. The same applies for Hf-based high-k dielectrics such as HfSiO and HfO@sub 2@. For HfO@sub 2@, nitrogen incorporation helps to suppress crystallization after high temperature activation anneals. In this work we systematically study the incorporation of nitrogen in HfSiO and HfO@sub 2@ using plasma assisted nitridation and thermal treatments in ammonia. The nitrogen concentration and chemical interactions are studied using x-ray photoelectron spectroscopy, x-ray diffraction, and high-resolution transmission electron microscopy. The role of nitrogen on the electrical properties is also discussed.

EM-ThP47 Cyclic Chemical Vapor Deposition of TiAlO Ultra-Thin Films, ***X. Song***, *C.G. Takoudis,* University of Illinois at Chicago

Cyclic-chemical vapor deposited TiAlO films, a few nanometers-thick, were prepared on H-passivated Si substrates using trimethyl Aluminum (TMA), tetrakis(diethylamino)titanium (TDEAT) and O@sub 2@. The depositions were carried out in a low pressure chemical vapor deposition chamber. The reaction pressure was on the order of 1 Torr and the reaction temperature was 300°C. The film thickness was probed using spectroellipsometry. The surface roughness of both as-deposited and annealed films were measured with atomic force microscopy (AFM). Rutherford backscattering spectroscopy (RBS) was utilized for the composition analysis. The atomic compositions and interfacial reactions were probed using x-ray photoelectron spectroscopy (XPS). The morphology of the films was analyzed using x-ray diffraction (XRD). Our studies show that the properties of TiO@sub 2@ are improved even with the addition of a few percent of Al@sub 2@O@sub 3@. XRD analyses indicate that as-deposited TiAlO films have amorphous structure. Upon annealing the as-deposited film in Ar at 500°C for 5 min, the film still maintains amorphous character, while TiO@sub 2@ crystallizes at these conditions. The surface of TiAlO films is found to be smoother than that of TiO@sub 2@. Sample annealing increases the roughness of the TiAlO films but the film roughness is still much lower than that of as-deposited TiO@sub 2@ films. There is no detectable formation of interfacial silicon oxide in as-deposited TiAlO films, based on XPS analyses. The thermal stability of TiAlO is also studied at different Ti contents. The carbon absence in the RBS analyses indicates that carbon (detected by XPS) is contamination on the sample surface most likely from the ambient. Electrical characterization of the TiAlO films will also be discussed.

EM-ThP48 Preparation of Yttrium and Aluminum Oxide Thin Films through Supercritical Carbon Dioxide Assisted Deposition, ***Z. Chen***, *T. Gougousi,* UMBC

Aluminum and yttrium oxide thin films were deposited on silicon at low temperatures (<150°C) through a chemical route, where the metal-organic precursors and oxidizing agents were delivered in liquid and supercritical carbon dioxide. Aluminum acetylacetonate (99%) (Al(acac)@sub3@), aluminum hexafluoroacetyl-acetonate (min. 98%) (Al(hfac)@sub3@), and tris(2,2,6,6-tetramethyl-3,5-heptanedionato) yttrium(III), (98+%, 99.9%-Y) (Y(tmhd)@sub3@) were used as precursors and a 30% aqueous solution of hydrogen peroxide, tert-butyl peroxide, and di-tert-amyl peroxide as oxidants. Depositions were carried out in a hot wall reactor at pressures ranging from 2100 to 3500 psi at 70-140°C. The deposited thin films were investigated by using X-ray photoelectron spectroscopy (XPS) and transmission Fourier transform infrared spectroscopy (FTIR). XPS and FTIR results indicated the formation of metal oxides thin films with some bonded carbon present in the film. Substitution of the aqueous hydrogen peroxide solution by the organic peroxides resulted in substantially lower OH and carbonate content in the films. For Al@sub2@O@sub3@ deposition from Al(acac)@sub3@ and tert butyl peroxide a very narrow temperature window (110 -120°C) existed for film formation. However, for Y@sub2@O@sub3@ deposition from Y(tmhd)@sub3@ and the same oxidant we find a much broader deposition window ranging from 80 to 130°C. The results demonstrate the feasibility of the technique for the deposition of metal oxide films.

EM-ThP49 Influence of the Bottom Electrode Material in Y@sub 2@O@sub 3@ MIM Capacitors, ***M. Bonvalot***, *M. Kahn, C. Vallee, J. Ducote, O. Joubert,* LTM/CNRS, France

High quality MIM capacitors are seeing increased use in CMOS, BICMOS and bipolar chips. The economic demand for smaller devices directly leads to the request for higher MIM charge storage densities. Therefore new high @kappa@ dielectric materials, such as Al@sub 2@O@sub 3@, Ta@sub 2@O@sub 5@ and HfO@sub 2@, are being evaluated as MIM dielectrics and will be used in future applications. Nevertheless, most of these materials show very large variations of their capacitance with applied bias voltage (so-called voltage linearity, characterized by a quadratic coefficient - alpha); thus, they cannot be used for analog MIM applications. TiN/Y@sub 2@O@sub 3@/Au capacitors have already been investigated. They exhibit good electrical properties with large breakdown electrical field values (7-8 MV/cm), low leakage currents, and a capacitance density of 5 fF/µm@super 2@. The Y@sub 2@O@sub 3@ is grown by pulsed liquid injection MOCVD. The aim of the present work is to study the impact of the bottom electrode materials on the interfacial layer between the metal and the yttrium oxide and hence, on the MIM electrical properties (C(V) and I(V) characterizations). Several electrode materials will be put on trial, such as WSi@sub x@(x=1, 2, 3), Ni and Pt. Their influence on the interface will be chemically characterized by means of XPS, SE in the FUV-visible range (up to 8 eV), and SIMS. The electrical behavior C(V) will be analyzed based on the work function of the metal electrode and on the nature of the interface with Y@sub 2@O@sub 3@.

EM-ThP50 Synthesis and Dielectric Characteristics of Poly Paraxylene-C Thin Films, *P. Tewari, M.T. Lanagan,* Pennsylvania State University; ***G. Sethi***, Pennsylvania State University, US

Poly paraxylene-C thin films are particularly useful in both biomedical and electronic applications. In the current work the synthesis and electrical properties of Poly paraxylene-C (parylene-C) thin films were investigated. Parylene-C has high breakdown strength and dielectric constant of 2.8. Parylene-C thin film were deposited by pyrolitic vapor decomposition of substituted paraxylene, followed by its polymerization on metallic substrates. During the deposition, base pressure was maintained at 21mtorr while evaporator and pyrolysis furnaces were maintained at 160°C and 690°C respectively. Crystallinity of Paralyne-C thin films was analyzed with the variation of pressure in deposition chamber. Reduction in chamber pressure has shown to improve film morphology. Dielectric constant and dissipation factor variation with temperature and frequency were analyzed with LCR meter and impedance gain phase analyzer. 1µm thick parylene thin film were shown to have a dielectric constant of 3.1 at frequency of 1MHz and room temperature. A dielectric relaxation following Maxwell- Wagner behavior was noticed around 20KHz frequency. Current-voltage characteristic was analyzed to distinguish between regions of Ohmic and non-Ohmic conduction. Deposited Parylene-C thin film will be used to analyze interfacial effects in multilayer Parylene-C - Silica laminar structures.

EM-ThP51 Chemical Structure of the Bilayer Ag/Li@sub 2@O Cathode Interface in Organic Light-Emitting Diodes, ***M.H. Joo,*** LG Electronics Institute of Technology, South Korea, Korea (South); *M.K. Baik, J.K. Choi,* LG Electronics Institute of Technology, South Korea

The chemical structure of the interface between Ag with Li2O and tri (8-hydroxyquinoline) aluminum (Alq) was investigated by using in-situ characterization of x-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS). Li2O on Ag had lower barrier height than LiF on Ag. XPS and UPS results show the interaction between Li2O and Alq leads to gap state formation in HOMO of Alq.

EM-ThP52 Thickness Dependence of High Capacitance-Gate Dielectric Layer on Electrical, Structural Characteristics and OTFT Device Performance, ***C.S. Kim***, *H.K. Baik,* Yonsei University, South Korea

In this study, pentacene TFTs operating at low voltage (-2V) were successfully fabricated using the CeO2-SiO2 dielectric layer with optimum thickness. The field effect mobility and on/off current ratio, at operating voltage of -2V, were 0.97cm2/Vs and 10^4, respectively. Threshold voltage

and subthreshold slope were -0.4V and 0.58V/dec, respectively. We have also shown the correlation of surface morphology and leakage current density. In the thick films, the leakage current is not bulk limited but rather it depends on the surface roughness, which increases with film thickness. The realization of low voltage and low leakage devices make the OTFTs excellent candidates for future flexible display and electronics applications.

EM-ThP53 Luminescence Properties of Organic Light Emitting Diodes using Chemical Mechanical Polishing Process*, G.-W. Choi, W.-S. Lee,* Chosun University, Korea*; Y.J. Seo,* Daebul University, Korea, South Korea*; P.-G. Jung,* Chosun University, Korea

Indium tin oxide thin film has attracted intensive interest because of their unique characteristics of good conductivity, high optical transmittance over the visible wavelength region, excellent adhesion to the substrate, stable chemical properties and easy patterning ability. ITO thin films have found many applications in solar battery, illuminators, optical switches, liquid crystal displays, plasma display panels, and organic light emitting displays. However, some problems such as peaks, bumps, large particles, and pin-holes on the surface of ITO thin film were reported, which caused the destruction of color quality, the reduction of device life time, and short-circuit. The interface between the electrode and organic layer in OLEDs has been reported as an important factor to influence the electrical and luminescent properties. Chemical mechanical polishing (CMP) process is one of the suitable solutions, which could solve the above-mentioned problems. In this work, we report the effect of polished ITO surface on the luminescent performance of the OLEDs. This work was supported by a Korea Research Foundation grant (KRF-2004-005-D00007).

EM-ThP54 Electrical Properties of Organic Light Emitting Diodes by Indium Tin Oxide-Chemical Mechanical Polishing Process*, G.-W. Choi,* ***W.-S. Lee,*** Chosun University, Korea*; Y.J. Seo,* Daebul University, Korea, South Korea*; Y.-K. Jun,* Chosun University, Korea

Indium tin oxide (ITO) thin film is a transparent electrode, which is widely applied to solar battery, illuminators, optical switches, liquid crystal displays (LCDs), plasma display panels (PDPs), and organic light emitting displays (OLEDs) due to its easy formation on glass substrates, good optical transmittance, and good conductivity. However, some problems such as peaks, bumps, large particles, and pin-holes on the surface of ITO thin film were reported, which caused the destruction of color quality, the reduction of device life time, and short-circuit. Chemical mechanical polishing (CMP) process is one of the suitable solutions, which could solve the problems. CMP performances can be optimized by several CMP components such as equipment and consumables. In this study, the optimum process parameters and the influences of process parameters were investigated for ITO-CMP with the sufficient removal rate and the good planarity. In this work, we studied the electrical characteristics of OLED with the structure of glass/ITO/MEH-PPV/Al using polished ITO surface as a bottom electrode (anode). And then, the optical property such as transmittance and absorption efficiency were discussed in order to evaluate the possibility of CMP application for ITO film.

EM-ThP55 Strongly Enhanced Thermal Stability of Crystalline Organic Thin Films Induced by Aluminum Oxide Capping Layers*, S. Sellner, A. Gerlach, F. Schreiber,* Universit@um a@t T@um u@bingen, Germany*; M. Kelsch, N. Kasper, H. Dosch,* Max-Planck-Institut f@um u@r Metallforschung, Germany*; S. Meyer, J. Pflaum, M. Fischer, B. Gompf,* Universit@um a@t Stuttgart, Germany

We present a detailed study of the strongly enhanced thermal stability of organic thin films of diindenoperylene encapsulated by sputtered aluminum oxide layers. We study the influence of capping layer thickness, stoichiometry, and heating rate on the thermal stability of capped films and their eventual breakdown. Under optimized encapsulation conditions (thick and stoichiometric capping layer), the organic films desorb only at temperatures 200 Â°C above the desorption of the uncapped film. Moreover, the capped organic films retain their crystalline order at these elevated temperatures, whereas they would normally (i.e., uncapped) be in the gas phase. This study therefore also shows a way of studying organic materials under temperature conditions normally inaccessible. Considering results from complementary techniques, we discuss possible scenarios for the eventual breakdown. The results have implications for the performance and long-term stability of organic devices for which stability against elevated temperatures as well as against exposure to ambient gases is crucial. @FootnoteText@ S. Sellner et al., J. Mater. Res. 21 (2006) 455. S. Sellner et al., Adv. Mater. 16 (2004) 1750.

EM-ThP57 Sol-Gel Derived SiO2-TiO2 Dielectric Layer for Organic Thin Film Transistor*,* ***S.W. Lee,*** *H.K. Baik,* Yonsei University, South Korea

Solution processible gate dielectric using SiO2-TiO2 composite oxide were prepared by sol-gel method for OTFT application. The composition, crystal structure, bonding configuration and electrical properties of SiO2-TiO2 composite oxide were analyzed using X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), Fourier transform infrared spectroscopy (FTIR) and current-voltage (I-V) measurement. Si/Ti ratio was 1:1 and annealing temperature was 300^C. Dielectric constant around 8 was obtained by capacitance-voltage measurement. The modification of microstructure and chemical bonding configuration in the SiO2-TiO2 film by the annealing temperature and its influence on electrical properties are discussed. We have fabricated OTFT device using SiO2-TiO2 composite oxide as a dielectric layer. Electrical properties of OTFT show that solution processible dielectric layer produce almost same results as vacuum process. We expect this process can replace conventional vacuum process due to its simplicity and low price consumption.

EM-ThP58 Plasma Treatment Effects on the Device Performance of Organic Thin Film Transistors*,* ***S.J. Jo,*** *C.S. Kim, S.W. Lee, H.K. Baik,* Yonsei University, Korea

We investigated electronic effects of plasma treatment on device properties of pentacene based thin film transistors (TFTs) with ITO (indium-tin-oxide) source and drain electrodes. The treated ITO electrodes were investigated by both contact angle measurements and X-ray photoelectron spectroscopy (XPS). The TFTs with plasma treated ITO electrodes show significantly improved performance over the devices without plasma treated ITO. The plasma treatment of the ITO surface improved the TFT performance by enhancing the hole injections from the electrode. The change in performance was attributed to the removal of contaminants and to the change in work function of ITO.

EM-ThP59 Synthesis, Characterization, and Properties of Flexible Side-Chain-Containing Polyimides*,* ***C.-L. Cheng,*** Chung-Yuan University, Taiwan*; L. Wang,* National Taiwan University

Aromatic polyimides have found a wide range of applications in advanced aerospace, automobile, microelectronic and printed circuit industries because of their distinguished thermal stability, high chemical resistance, good mechanical strength and excellent dielectric properties. However, conventional polyimides are often categorized as an insoluble, intractable, and infusible material owing to their rigid backbone structure. These disadvantages make them extremely difficult to process and greatly limit their commercial uses. Various attempts have been developed to overcome these deficiencies, including the use of noncoplanar or alicyclic monomers and the introduction of flexible segments into the polymer backbone. The strategies of these methods are the reduction of chain crystallinity, inter-molecular charge-transfer and electronic polarization interactions. An alternate successful approach involves the incorporation of pendant groups onto the rigid polyimide backbone. These works have shown that the presence of bulky groups could effectively prevent the coplanarity of aromatic rings and reduce the packing efficiency of molecular chains without sacrificing thermal properties. In this study, we synthesized two series of polyimides containing alkyl side groups in different sizes and investigated the effect of the molecular structure of pendant groups on the thermal and dielectric properties of polyimides.

EM-ThP61 Jet-printed Organic Electronics: Display Backplanes without Vacuum Processing*,* ***J.H. Daniel,*** *A.C. Arias, B. Krusor, R.A. Street,* Palo Alto Research Center

Most electronic circuit fabrication relies on vacuum tools for the deposition or removal of materials. In large-area electronics, particularly for active-matrix display backplanes, these vacuum tools represent a considerably increased engineering challenge due the growing substrate size and the requirements on uniformity. Moreover, the capital cost is substantial. With the development of new materials, solution-based processes are being studied which will potentially enable extremely low-cost large-area electronics on flexible substrates. We are investigating low-temperature (<150degC) all-additive processes for the fabrication of flexible active matrix thin-film transistor (TFT) backplanes. The metal conductors for gate/data lines and pixel pads are defined by jet-printing of silver nano-particle solutions. The active regions of the TFTs consist of jet-printed polymeric semiconductor (PQT-12). Various polymeric gate dielectrics were investigated, including the epoxy SU-8. SU-8 strongly cross-links at temperatures below 150 degC making it chemically inert to subsequent processing steps and the surface energy of SU-8 is compatible with the printing solution to form narrow continuous lines. We were able to coat

SU-8 layers with a thickness around 200-300nm with low pin-hole density. Pixel circuits were printed on rigid and flexible substrates. The transistor performance was measured and the pixel response was determined using a picoprobe. When combined with our reflective electrophoretic display media these all-printed backplanes are promising for electronic paper or signage applications.

EM-ThP62 An Improved Method for the Derivation of Depth Profile Information from Angle Resolved XPS Data*, **P. Mack**, R.G. White,* Thermo Electron Corporation, UK*; T. Conard,* IMEC, Belgium

The construction of depth profiles from angle resolved XPS (ARXPS) data is currently receiving much attention. This is mainly due to the increasing technological importance of layers whose thickness is of the order of a few nanometres. Transistor gate dielectric layers and self-assembled monolayers are good examples of such layers. The construction of profiles from ARXPS data can be accomplished using methods involving maximum entropy but there are limits to the accuracy and repeatability of these methods if used in isolation. In this paper, we will show that the quality of the profiles can be improved by making use of additional, readily available, information. For example, the composition of the substrate is usually known as is the oxidation state of the elements in the thin film because these are available from the XPS spectrum. This information can be used to refine the profiles derived using maximum entropy thus improving the reliability of the result. The method will be described in detail and illustrated by reference to layers of nitrided hafnium oxide on silicon. The nitrogen profiles obtained using this method will be compared with those derived from other experimental techniques.

EM-ThP63 An Investigation of Thermal Management in Laser Diode Structures*, **D. Roberts**, G. Triplett,* University of Missouri-Columbia

As electronic device feature sizes decrease to several nanometers, the ability to effectively remove heat through the packaging remains a technical challenge. Thermal management issues in electronic systems have been a limiting factor for high-power as well as optoelectronic device applications. In optoelectronic applications, thermal issues dramatically affect device operation, particularly in laser diodes. The active region in laser diodes (which can be several microns thick) are particularly sensitive to heat as it pertains to the lasing threshold because of large injection current density. Whereas larger bandgap materials are less temperature dependent, they are inappropriate for optical-fiber applications. This large injection current density also results in shorter device lifetimes. Current heat removal techniques involve fluidic cooling, epi-down packaging, and thermoelectric coolers. These techniques have several advantages; however, certain limitations exist with these solutions. The ability to effectively remove heat at a rate that supports higher-power (~1kW/cm@super2@) operation remains a technical barrier. Our approach is to focus on the substrate for heat removal. In their current form, substrates lack the thermal conductivity required to deal with these operating conditions. In this paper we will discuss thermal management issues in laser diodes and discuss an additional approach to device cooling via substrate manipulation. This approach will involve neutron transmutation doping (NTD) to reconfigure the substrate properties.

Electronic Materials and Processing
Room 2003 - Session EM+TF-FrM

High-k Dielectric & Multi-Functional Oxide Growth & Processing

Moderator: R.L. Opila, University of Delaware

8:00am **EM+TF-FrM1 Chemical Analyses and Electrical Studies of HfO@sub 2@/Y@sub 2@O@sub 3@, Y@sub 2@O@sub 3@/HFO@sub 2@ Bilayered and Y@sub x@Hf@sub y@O@sub z@ Intermixed Dielectric Materials for MIM Capacitors***, M. Kahn,* *C. Vallee, C. Dubourdieu, M. Bonvalot, J.R. Plaussu, J. Ducote, T. Baron, O. Joubert,* LTM/CNRS, France

Improving the capacitance density of MIM devices constitutes a real challenge to satisfy scaling rules for next IC generations and to reduce the cost as well. Silicon dioxide and nitride have been commonly used up to date as dielectrics in conventional MIM capacitors. However, they cannot provide capacitance values larger than 2fF/µm@super 2@. With further scaling going on at an active pace, high-@kappa@ dielectric materials offer a viable alternative to provide both high capacitance density and low leakage currents. This dielectric material of a MIM device has to meet several requirements such as a high capacitance density, low leakage currents and minimum variation of capacitance values with voltage bias. In a previous work, we studied TiN/Y@sub 2@O@sub 3@/Au capacitors and showed that Y@sub 2@O@sub 3@ exhibits appropriate electrical properties with low leakage currents and a capacitance density of 5 fF/µm@super 2@ @foonote 1@. However, we observed that the capacitance density cannot be further increased without a substantial increase in the leakage current, which in turn exceeds ITRS requirements. The aim of the present work is to overpass this capacitance limitation thanks to the introduction of a bilaminate dielectric material. Studies of MIM capacitors based on HfO@sub 2@/Y@sub 2@O@sub 3@, Y@sub 2@O@sub 3@/HFO@sub 2@ bilaminate and intermixed Y@sub x@Hf@sub y@O@sub z@ dielectric materials will be presented. These high @kappa@ dielectric layers are prepared by pulsed injection MOCVD on WSi@sub x@ bottom electrodes and the gold top electrode is realized by evaporation. The electrical behavior C(V) and I(V) of the obtained structures will be presented and discussed in terms of capacitance density, capacitance linearity and leakage currents. They will be correlated to chemical analysis results (XPS and SIMS), with special attention devoted to metal/oxide and oxide/oxide interface investigations. In particular, the observation of a non symmetrical C(V) curve will be highlighted with respect to the bilaminate stack HfO@sub 2@/Y@sub 2@O@sub 3@ and Y@sub 2@O@sub 3@/HFO@sub 2@ of dielectric materials. @FootnoteText@ @footnote1@ C. Durand, C. Vallee, C. Dubourdieu, M. Kahn, M. Derivaz, S. Blonkowski, D. Jalabert, P. Holliger, Q. Fang, I.W. Boyd ; J. Vac. Sci. Technol to be published (May/June 2006).

8:20am **EM+TF-FrM2 Process-Dependent Interface States at Mo/Hafnium Oxide/Si Interfaces***, S. Walsh, L. Fang,* The Ohio State University*; J.K. Schaeffer, E. Weisbrod,* Freescale Semiconductor, Inc.*; L.J. Brillson,* The Ohio State University

A major challenge for Hafnium Oxide (HFO) and other high-K dielectric materials is the control of their interface state and trapped charge densities. Among the chief electronic and chemical requirements for their development is the identification of post-growth processes to optimize oxide bonding within the thin dielectric films and at their interfaces. This requires characterization techniques that are nondestructive, that can measure electrically-active defects that correlate with electrical device features, and that can spatially isolate these defects within ultra-thin films to help identify their physical origins. We have used low energy electron-excited nanoscale-depth-resolved (DRCLS) spectroscopy to probe the bulk and interface defect states of ultra-thin Mo/HFO/Si with 8 different process sequences. After atomic layer deposition (ALD) of 4 nm HfO@sub 2@ on Si and an O@sub 2@ post treatment, we deposited 10 nm Mo using either plasma vapor or electron beam deposition, with or without a subsequent 1000@super O@C N@sub 2@ anneal, and with or without a forming gas anneal. DRCLS revealed pronounced gap state emissions within the ultrathin films and their interfaces with Mo and Si. There are multiple deep level emissions below the 5.5 eV band gap, including 3 peak emissions at 3.4, 3.5 eV, and 3.9-4.3 eV that can be associated with HFO oxygen vacancies in different charge states predicted theoretically.[1] In addition, states at 2 -2.6 eV that resemble known SiO@sub 2@-related nonbonding oxygen hole centers (NBOHC) and E' (positively charged O vacancy) native defects increase with depth within the 4 nm HFO film suggesting the formation of a Hf silicate at the HFO/Si interface. Furthermore, different process steps produce large changes in these states and for at least one sequence, a dramatic decrease in both types of defects. The differences between process sequences can be understood in terms of known reactions at HFO-Si interfaces.

8:40am **EM+TF-FrM3 Materials Challenges for High Permittivity Gate Dielectrics and Metal Gate Electrodes***, J.K. Schaeffer, D. Gilmer, S. Samavedam, M. Raymond, D.H. Triyoso, R.I. Hegde, M. Stoker, S. Kalpat, C. Capasso, B. Taylor, P.J. Tobin, B.E. White,* Freescale Semiconductor, Inc.*; S. Walsh, L. Fang, L.J. Brillson,* The Ohio State University **INVITED**

This talk will review recent advances and remaining challenges associated with high-k gate dielectrics and metal gate electrodes with a specific focus on the fundamental materials properties responsible for critical device characteristics. Recent reports have shown that alloying ZrO@sub 2@ into HfO@sub 2@ improves device reliability and effective oxide thickness (EOT) scaling. This talk will review the structural and electrical properties of Hf@sub x@Zr@sub 1-x@O@sub 2@ films that impact EOT and device reliability. Next, to better understand the nature of the metal/HfO@sub 2@ interface, the previously established empirical relationship between the mean electronegativity and effective work function developed for Schottky contacts has been applied to multi-element electrode materials on hafnium dioxide gate dielectrics. Our data show good agreement with the pre-existing framework established for metal/insulator contacts, and illustrates the important role that sub-lattice elements such as N and C can have on effective work-function. This understanding helped lead to the development of tantalum carbide as a thermally stable NMOS gate electrode candidate. Finally, many device properties result from the electrical and chemical interactions between the various gate stack layers which can lead to differences in EOT growth, increased dielectric leakage, fixed charge, and changes in effective work function. The selection of the gate metal can have a pronounced impact on these properties. Such interactions are likely responsible for the difficulty in manufacturing devices with low PMOS device threshold voltages and scaled EOT on silicon substrates. Recent experiments are now providing new insights into the origins of this problem.

9:20am **EM+TF-FrM5 Molecular Beam Epitaxy of Multifunctional Materials Using a Chloride Refractory Metal Chemistry***, W.A. Doolittle, A.G. Carver, W. Henderson, W. Laws Calley, S.-S. Kim,* Georgia Institute of Technology **INVITED**

Multifunctional materials, materials that interact with their environment via differing force mechanisms, including but not limited to electrostatic, magnetic, acoustic, photonic, and chemical, are of great interest for future sensor and actuator applications. Lithium metal oxide multifunctional materials, including LiNbO@sub 2@, LiNbO@sub 3@, LiTaO@sub 2@ and LiTaO@sub 3@ are presented as a promising but challenging materials for multifunctional devices. Example proposed applications will be presented. A chloride based chemistry that bypasses many of the traditional pitfalls of Lithium Niobate (LN) epitaxy including the need for electron beam evaporation of refractory metals, and use of complex metal organic precursors prone to pre-reaction is described. Methods of dealing with the normally corrosive chloride based chemistry in a Molecular Beam Epitaxy (MBE) chamber are detailed. The present state of homoepitaxy and heteroepitaxy of LN on semiconductors is presented. It is shown that LiNbO@sub 2@ is preferentially grown over LiNbO@sub 3@ in the oxygen deficient MBE vacuum environment. However, LiNbO@sub 2@ is shown to be converted to LiNbO@sub 3@ by an ex-situ oxygen anneal. Dramatic changes in optical properties and crystalline lattice structure result and will be detailed. A limited stoichiometry control is demonstrated via use of ion filters on an oxygen plasma source including the ability to partially select between various valences of niobium oxides, NbO, NbO@sub 2@ and Nb@sub 2@O@sub 5@. While the demonstrated metal chloride based epitaxy is shown as a viable candidate for MBE of multifunctional refractory metal oxides, particularly for electronic applications, the possibility for thicker films, and thus impact on optical devices, is currently limited by the available Li source. Efforts to circumvent this difficulty, including a large volume valved Li source, will be described.

10:00am **EM+TF-FrM7 Magnesium Oxide Thin Film 'Bridge' on Hexagonal Silicon Carbide for Integration of Functional Oxides***, T.L. Goodrich, Z. Cai,* ***K.S. Ziemer,*** Northeastern University

Single crystalline MgO (111) films, 15 to 100 Å thick, have been grown on hexagonal silicon carbide (6H-SiC) in order to integrate complex oxides, such as lead zirconate titanate [PZT], with SiC high-power, high-

temperature, high-frequency devices with multiple functionalities. 6H-SiC substrates (0001)@sub Si@ and (000I)@sub C@ were cleaned to create atomic steps hundreds of nanometers wide and 1.5 nm high, and reduce oxygen contamination from 12% to 8% for the (0001)@sub Si@ surface and from 8% to 3% for the (000I)@sub C@ surface, as measured by x-ray photoelectron spectroscopy (XPS) and Auger electron spectroscopy. The residual oxygen concentration was determined by reflection high energy electron diffraction (RHEED) to be incorporated into a @sr@3x@sr@3 R30° silicate adlayer reconstruction. MgO films were grown using a remote oxygen plasma source to produce a constant chamber oxygen pressure (5x10@super -6@ Torr) and a solid source Mg effusion cell at various Mg fluxes but constant Mg fluence. The (000I)@sub C@ surface and the (0001)@sub Si@ surface of the SiC produce differently structured films, as measured by RHEED and atomic force microscopy (AFM), under the same molecular beam epitaxy growth conditions. All films are roughly stoichiometric as measured by XPS, with some suggestions of Mg metallic bonding near the substrate. MgO thin films grown on (0001)@sub Si@ oriented SiC substrates were three-dimensional and crystalline at low Mg flux but became more conformal and improved single crystalline as the Mg flux was increased. The opposite was observed for (000I)@sub C@ oriented SiC. At Mg fluxes than 1x10@super 14@ atoms/cm@super 2@s, the films were conformal but highly polycrystalline. As the Mg flux was increased, the crystalline MgO thin films became less polycrystalline but exhibited more 3-D morphology. Current studies will compare the deposition of BaTiO and PZT on the MgO thin films to those deposited directly on the cleaned SiC substrates.

10:20am **EM+TF-FrM8 Zirconium Dioxide Formation on Silicon Surfaces by Metal-Organic Chemical Vapor Deposition in UHV**, ***A. Sandell**, P.G. Karlsson, J.H. Richter,* Uppsala University, Sweden*; J. Blomquist, P. Uvdal,* Lund University, Sweden*; T.M. Grehk,* Hogskolan Dalarna, Sweden

Previous work has shown that deposition of zirconium tetra-tert-butoxide at elevated temperatures leads to the formation of a ZrO2 film. The previous studies also reveal the presence of an interfacial region between the Si substrate and the ZrO2 film. However, up to date, the evolution of the interface has not been comprehensively addressed using surface science techniques. In this contribution, a detailed study of the growth and interface formation on Si(100) and Si(111) in UHV is presented. Core level photoelectron spectra provide information on the growth rate, atomic oxidation state and the chemical composition of the interface, including the fate of the butoxy ligands. X-ray absorption spectra give valuable complementary information on the local geometric structure of the Zr-O units and the Zr-O electronic interaction. In addition, STM images of the first stages of nucleation are shown. These suggest that it is possible to distinguish between precursors induced defects on the Si(100) surface related to oxidation and reaction with carbonaceous fragments, respectively.

10:40am **EM+TF-FrM9 Controlling Interfacial Reactions between HfO@sub 2@and Si using Ultra-Thin Diffusion Barriers**, ***R.R. Katamreddy,*** University of Illinois at Chicago*; R. Inman, G. Jursich, A. Soulet,* American Air Liquide*; C.G. Takoudis,* University of Illinois at Chicago

Hafnium oxide has gained considerable interest in recent years as a potential high-k dielectric material for future fabrication of complementary metal oxide semiconductor devices. One of the problems with HfO@sub 2@ is its interfacial reactivity with Si at the high temperature necessary for post deposition annealing. Our previous studies have shown that HfO@sub 2@ films on Si form silicates and silicides at the interface as low as 600 °C and this is not suitable for CMOS process integration. In this study we examine the effectiveness of ultra-thin Al@sub 2@O@sub 3@ as a HfO@sub 2@-Si diffusion barrier up to 1000 °C. Al@sub 2@O@sub 3@ has superior interface stability with Si but it also has a lower dielectric constant than HfO@sub 2@. So, to minimize reduction in overall dielectric constant of the film with this barrier layer, there is a need to understand how thin the Al@sub 2@O@sub 3@ layer can be in this system and yet still maintain its effectiveness as a barrier. Our studies have shown 0.5 nm of alumina was sufficient to prevent formation of silicates and silicides of hafnium at temperatures below 1000 °C, while thicker alumina films were required to prevent the same at 1000 °C. The ultra-thin dual layer films are prepared by sequential atomic layer deposition of Al@sub 2@O@sub 3@ and HfO@sub 2@ using tetrakis(diethylamino)hafnium and tris(diethylamino)alane as the metal oxide precursors and water vapor as the oxidizer. Nitrides and oxynitrides of silicon are some other promising diffusion barriers. Silicon nitride and oxynitride are also investigated as potential barrier layers for HfO@sub 2@-Si. After deposition, the films are subjected to high temperature annealing up to 1000 °C and the extent of interfacial reactivity is examined using Fourier transformed infrared spectroscopy, x-ray photoelectron spectroscopy, and scanning transmission electron microscopy/electron energy loss spectroscopy. An explanation of the observed behavior is also proposed for these systems.

11:00am **EM+TF-FrM10 Comparison of the Calculated Electronic Structure of Oxygen and Nitrogen Adsorption onto Ge(100)**, ***S.R. Bishop**, T.J. Grassman, A.C. Kummel,* University of California, San Diego

For high-k dielectrics on Ge(100), a germanium oxynitride (GeON) interface leads to superior C-V characteristics compared to GeO@sub 2@ passivation layers. Experimental studies show GeON is both a better diffusion barrier and surface passivant than GeO@sub 2@. To understand why GeON is an effective passivating layer, it is necessary to first determine the oxygen and nitrogen binding sites independently. STM studies have shown that the initial stage of O and N adsorption is insertion into the backbonds and into the 2x1 surface dimers, while the final stage is Ge displacement by O and N. The clean Ge(100) surface, oxygen adsorption sites, and nitrogen adsorption sites were modeled using density functional theory (DFT). The DFT calculations show that all oxygen insertion and displacement sites leave the near-Fermi level density of states essentially unchanged compared to the clean surface. This is consistent with O atom insertion and displacement creating no new unfilled dangling bonds. In contrast, the insertion and adsorption sites for nitrogen all create new electronic states in the near-Fermi level region, consistent with nitrogen atoms making two bonds to the surface, but retaining a half-filled dangling bond. However, the Ge-N bonds were found to be stronger than the Ge-O bonds, consistent with GeON being more effective than GeO@sub 2@ as a diffusion barrier. Since the efficiency of GeON as an electronically passivating layer is not intrinsic to its chemisorption states on Ge(100), it may be related to the nitrogens' ability to be electronically passivated by hydrogen. The DFT calculations show that even though N atom displacement of Ge creates states near the Fermi level, hydrogen passivation greatly reduces or eliminates the density of those states.

11:20am **EM+TF-FrM11 Thermal Stability of High-k Dielectrics on Ge(001)**, *F.S. Aguirre-Tostado, M.J. Kim, **R.M. Wallace**,* University of Texas at Dallas*; R. Sreenivasan, K.-I. Seo, C.O. Chui, K.C. Saraswat, P.C. McIntyre,* Stanford University*; F.A. Stevie, R. Garcia, Z. Zhu, D.P. Griffis,* North Carolina State University

The use of high-mobility channel materials, such as SiGe and Ge has attracted substantial interest as a means to maintain integrated circuit scaling and performance. A necessary requirement for a MOSFET application is a stable gate dielectric which can be integrated into an appropriate CMOS process flow. High-k dielectrics, such as ZrO@sub 2@ and HfO@sub 2@ have been previously reported for this application with promising electrical results.@footnote 1,2,3@ This paper will describe thermal stability studies of these high-k dielectrics on Ge(001) using in-situ ARXPS and SPM analysis in conjunction with backside SIMS@footnote 4@ and HRTEM analysis. The extent of Zr, Hf and Ge interdiffusion is examined with oxide or oxynitride interfacial layers. Corresponding electrical characterization of the associated devices will also be described in view of the thermal budget where the maximum process temperature is ~500°C. @FootnoteText@@footnote 1@K.I. Seo, P.C. McIntyre, S. Sun, D.I. Lee, P. Pianetta, K.C. Saraswat, Appl. Phys. Lett. 87 (2005) 042902. @footnote 2@D. Chi, C.O. Chui, K.C. Saraswat, B.B. Triplett, P.C. McIntyre, J. Appl. Phys. 96 (2004) 813. @footnote 3@C.O. Chui, H. Kim, P.C. McIntyre, K.C. Saraswat , IEEE Elec. Dev. Lett. 25 (2004) 274. @footnote 4@C. Gu, et. al., J. Vac. Sci. Technol. B22, 350 (2004).

11:40am **EM+TF-FrM12 Oxidation Properties of Al-nanostructures on Si Surfaces**, ***P. Morgen,*** University of Southern Denmark, Denmark*; C. Janfelt,* University of Copenhagen, Denmark*; K. Pedersen,* University of Aalborg, Denmark*; Z.S. Li,* University of Aarhus, Denmark

We have explored the oxidation properties of different nanostructures of Al formed by deposition of Al on Si surfaces with surface sensitive techniques to reveal the differences in reactivity between differently organized nanostructures of Al on these surfaces. In a parallel effort some of these reactions have been modeled with surface electronic structure calculations simulating STM and photoemission spectra, based on the DFT method. Recently several theorists have looked at the initial phases of oxide formed during exposure of Al to oxygen, and found these to differ from bulk Al-oxide. Here we discuss the results for the oxidation of Al on Si (111) and Si (100) in quantities of less than a monolayer as deposited and after annealing of these systems. For the un-annealed systems we discover a route to control the formation of Al-oxide on top of Si with a sharp unmixed interface, while the reactions of the annealed systems show

mixing and enhanced reactivity of the Si surface to oxygen. Ultrathin films of Al on top of Si oxidize at room temperature and at elevated temperatures as a self limiting process, like Si itself. The structure of this oxide includes Al with a coordination number of four.

Electronic Materials and Processing
Room 2001 - Session EM-FrM
Molecular Electronics

Moderator: I.G. Hill, Dalhousie University, Canada

8:00am **EM-FrM1 Scanning Tunneling Microscopy Study of Azobenzene and Azobenzene-Derivatives***, **Y.S. Cho**, B.Y. Choi, H.J. Yang,* Seoul National University, Korea*; Y. Kuk,* Seoul National University, Korea, South Korea

Conjugated molecular chains exhibit good conductivity with @pi@ bonding for the carrier transport. If two disconnected parts of a conducting molecular chain are connected by a bond with two coupled potential energy surfaces with 2 degrees of freedom, the resulting chain will reveal non-linear characteristics. It has been shown experimentally in a scanning tunneling microscopy (STM) that these kinds of molecules switch between two potential energy minima and function as nano-molecular switches.@footnote 1@ Chemical isomers are the most appropriate target molecules, because they have the same molecular formula and connectivity but different geometric structures and conductivities. We studied geometric and electonic structures of isolated azobenzene and azobenzene derivative molecules adsorbed on Au (111) surface with scanning tunneling microscopy and spectroscopy(STM) at 5K. These molecules have two stereoisomers which can be transformed to each other by UV irradiation or thermal energy. We could induce this transformation by tunneling electrons using STM tip. In the case of azobenzne, the trans-to-cis transition is induced at ~-1.5V and the cis-azobenzene returned back ~+2.5 V. We studied three different kinds of azobenzene-derivatives; EtO-Az-C10, EtO-Az-C6, CF@sub 3@-Az-C10. Each derivative has a long alkyl-chain which enable us to control the length of switching molecules. We will show the coverage dependance of the HOMO-LUMO state and the conformational change by STM tip in azobenzene-derivatives. This results could be an possible implication to mechanism of organic-based conformational switch. @FootnoteText@ @footnote 1@ Byoung-Young Choi et al., PRL 96, 156106 (2006).

8:20am **EM-FrM2 Structural Dependence of Charge Transport in Organic Molecular Films***, **Y. Qi**, B.L.M. Hendriksen, D. Esteban, I. Ratera, M. Salmeron, J.Y. Park, F. Ogletree,* UC Berkeley and Lawrence Berkeley National Laboratory

The charge transport properties and mechanical properties of alkanethiol and trans-stilbene based self-assembled molecules on Au(111) have been investigated by using a conducting probe atomic force microscope (CP-AFM) in ultrahigh vacuum. We found that there exists a clear correlation between them. The step-wise change previously found in alkanethiol molecular film thickness and friction upon pressing the molecules with atomic force microscope tip was observed in the tip-sample current. Increasing of tip-sample current is mainly due to tilt of molecules under the high pressure. We measured the decay constant ß=0.58/Å for hexadecanethiol, significantly smaller than decay constant (~ 1/Å) that is caused by shortening the alkanethiol molecule length. Our calculation based on the two-pathway model is in good agreement with the current measurement upon molecular tilt. We will discuss the new scheme of Field Effect Transistor (FET) configuration that allows us to measure the electron transport parallel to the self-assembled monolayer.

8:40am **EM-FrM3 Temperature Dependent Conduction and Charge Tunneling in Nanoparticle-Molecule-Nanoparticle Bridging Structures***, **J.-S. Na**, J. Ayres, K. Chandra, C.B. Gorman, G.N. Parsons,* North Carolina State University

Although electronic transport across organic molecules has been widely investigated, the conduction mechanisms across a single molecule is still not well defined because of instability of metal-molecule contacts, uncertainty of number of molecules in the junction, and unavailability of temperature variable current-voltage measurements. Here we report the dielectrophoretic trapping, contact stability, and conduction characteristics of a nanoparticle/molecule/nanoparticle bridge assembly, where two ~40nm nanoparticles are linked by a phenylacetylene oligomer. The molecule/nanoparticle structures are assembled across a nanoscale (~70nm) electrode gap fabricated by angled e-beam evaporation. The nanoparticle/molecule structures are trapped by applying a dielectrophoretic force across the nanoscale electrode gap. At the optimum trapping conditions (2VAC, 1MHz, and 60s), a success rate of ~78% is achieved. Current versus voltage through the nanoparticle/molecule structure is consistent with a single molecule present between the nanoparticles, and IV results are obtained as a function of temperature (80K to 293K) and time in ambient. Analyses of ln(I/V@super 2@) versus 1/V indicates a transition from direct tunneling to Fowler-Nordheim tunneling, independent of temperature. A nonlinear fit of the IV data to the Simmons tunneling model results in barrier height of about 0.12eV, suggesting charge transport proceeds through hole tunneling. The stability of the nanoparticle electrode structure and molecular conduction over several weeks will also be presented and discussed.

9:00am **EM-FrM4 Switching and Conductance Peaks in Metal-Molecule-Silicon Devices with Nitro-Containing Molecular Layers***, **A.D. Scott**, D.B. Janes,* Purdue University

Recently there has been a large amount of interest in developing molecular electronics for miniaturization and enhancing functionality of electronic devices. Interesting transport features have been observed in metal-molecule-metal devices containing nitro-substituted species.@footnote 1@ Silicon contacts to molecular devices offer advantages over metal contacts due to the covalent nature of the molecular attachment, the technological relevance of silicon, and the ability to tune the electrical properties of the contact through doping. In this study, we present interesting transport features observed in metal-molecule-silicon devices with nitro-containing molecular layers. These devices exhibit interesting transport behavior that varies with molecular species used and substrate doping. Devices with nitrobenzene layers on p+ Si substrates exhibit bistable switching in 63% of devices. This behavior has been characterized using current-voltage measurements and current vs. time measurements of switching transients. The voltage threshold at which switching takes place is 0.9±0.15 V and the ratio of on-current to off-current is approximately 10. Devices with 2-methyl 4-nitrobenzene layers on n Si exhibit non-ideal current-voltage behavior and show peaks in the conductance-voltage curves for all devices measured. The conductance peak occurs at 0.9V forward bias. It has been observed both by numerically differentiating DC current-voltage curves and by AC conductance measurements utilizing lock-in detection. Similar devices with molecular layers that do not contain nitro headgroups and those with different substrate dopings do not exhibit these features. @FootnoteText@ @footnote 1@ Chen J, Reed MA, Rawlett AM, Tour JM (1999) Large On-Off Ratios and Negative Differential Resistance in a Molecular Electronic Device. Science 286: 1550-1552.

9:20am **EM-FrM5 Towards Molecular Electronics: Controlling and Understanding Metallic Contact Formation on Patterned Self-Assembled Monolayers***, **A.V. Walker**,* Washington University in St. Louis **INVITED**

We have developed a robust method by which to construct complex two- and three- dimensional structures based on controlling interfacial chemistry. This work has important applications in molecular/organic electronics, sensing, and other technologies. Our method is extensible to many different materials, easily parallelized, affords precise nanoscale placement and is fully compatible with photolithography. Our work to date has provided a simple method for the construction of complex 2D molecular electronic circuitry using UV-photopatterning and the reaction of deposited metals with self-assembled monolayers (SAMs). To demonstrate the method we have selectively vapor-deposited Mg on a patterned -CH@sub 3@/-COOH terminated alkanethiolate surface. The deposited metal penetrates through the -CH@sub 3@ SAM to the Au/S interface while reacting with and accumulating on top of the -COOH SAM. Applying these ideas to the rational design of metal/organic structures requires a fundamental understanding of the underlying metal-molecule interactions; we therefore shall also discuss experiments that elucidate these.

10:00am **EM-FrM7 Energy-Level Alignment at Thiol/Metal Interfaces: A Model "Molecular Wire" Chemisorbed on Ag, Cu, Au, and Pt.***, **C.D. Zangmeister**, R.D. van Zee,* National Institute of Standards and Technology*; C.A. Ventrice,* University of New Orleans

Photoemission spectra have been used to determine the energy-level alignment for self-assembled monolayers of the "molecular wire" 4,4'-bis-(phenylethynyl)benzenethiol self-assembled on Ag, Cu, Au, and Pt. We measured a shift in the hole-transport barrier with metal work function due to changes in the interfacial electrostatics. The hole-transport barrier as a function of metal work function is near the common vacuum limit (S@subB@ = 0.8). The shift of the hole-transport barrier is analyzed as an interfacial dipole and decomposed with a three term model. The current

through a model metal/molecule/metal junction is calculated using the measured values of the hole-transport barrier, and trends are found to be consistent with previously published results.

10:20am **EM-FrM8 Fabrication of Semiconductor-Molecule-Semiconductor (SMS) Devices*, A. Mahapatro*,** *M. Martinez, P. Carpenter, A.D. Scott,* Purdue University*; A. Yulius,* Yale University*; J. Woodall, D.B. Janes,* Purdue University

Molecular electronic devices have typically been fabricated using metal-molecule-metal (MMM) configurations. Recently, several studies involving semiconductor-molecule-metal (SMM) junctions have been reported, motivated by the prospects of realizing covalent bonds to one contact and exploiting the semiconductor states in device properties. The MMM and SMM junctions are the commonly used device structures for studying the electrical behavior of single/few molecules. While the SMM structures address some of the problems with reliability of MMM structures, there is still the possibility of metal penetration through the molecular layer during deposition or device operation. This study illustrates a technique to fabricate large area molecular devices in a semiconductor-molecule-semiconductor (SMS) configuration by depositing a pre-formed semiconductor island (InAs) onto a molecular self-assembled monolayer (SAM) which has been formed on another semiconductor substrate (GaAs). Micron-scale InAs islands with Au top contact layers are formed on a sacrificial substrate and transferred onto the SAM-coated GaAs substrate. Identical topography of the grains on the surface of the settled islands and freshly prepared Au surfaces, confirm that the InAs side of the island is in contact with the SAM-coated GaAs surface. In order to verify that thiol-based bonds are possible on InAs (for the top contact), we have also developed SAMS of short thiol molecules on InAs surfaces. The resulting SAMs were characterized through X-ray photoemission spectroscopy. Electrical conduction has been measured for p@super +@GaAs/xylyl-dithiol/InAs structures of 100-400 µm@super 2@ contact areas. This study demonstrates that molecular devices can be realized using exclusively semiconductor contacts.

10:40am **EM-FrM9 Molecular Tunnel Junctions Incorporating Nickel-Octanedithiol Multilayer Thin Film*, L.H. Yu*,** *J.G. Kushmerick,* National Institute of Standards and Technology

We present measurement of tunneling junctions made using self-assembled nickel-octanedithiol multilayer thin film. Multilayer structures on evaporated gold and nickel surfaces were studied by ellipsometry, Fourier Transform Infrared (FTIR) spectroscopy, and X-ray photoelectron spectroscopy (XPS). Superconducting quantum interference device (SQUID) measurements were performed on the nickel-dithiol multilayer thin films and bulk materials to characterize their magnetic properties. We will discuss the effect of applied magnetic field on the electronic transport of these ferromagnetic atoms containing tunneling junctions.

11:00am **EM-FrM10 Electrical Transport Measurements on Conjugated Molecules using Nanogap Electrodes on Cleaved AlGaAs Planes*, M. Tornow*,** *S.M. Luber, S. Lingitz, A.G. Hansen, F. Zhang,* Walter Schottky Institute, TU Munich, Germany*; F. Scheliga, E. Thorn-Csányi,* University of Hamburg, Germany*; M. Bichler,* Walter Schottky Institute, TU Munich, Germany

One of the major challenges in the realization of molecular electronic hybrid systems that comprise molecules as functional units is the reproducible fabrication of the inorganic contact electrodes. We have developed a novel technique to prepare such nanogap electrodes in a very precise manner, based on cleaved GaAs/AlGaAs semiconductor heterostructures grown by Molecular Beam Epitaxy (MBE).@footnote 1@ These electrodes of predetermined distance are macroscopically flat, coplanar and exceedingly clean. We report on electronic transport measurements on @pi@-conjugated, dithiolated Oligo-(phenylenvinylene) (OPV) derivatives of length 8.5 nm bridging a ~7 nm nanogap device. Starting from a high impedance behaviour before molecule deposition the OPV functionalized hybrid system develops a pronounced non-linear I-V characteristic measured at T=4.2 K. We compare our observations to model calculations on a simplified structure involving extended Hueckel theory and non-equilibrium Greens Function methods, and find qualitatively good agreement. @FootnoteText@ @footnote 1@ S.M. Luber et al., Nanotechnology 16, 1182 (2005).

11:20am **EM-FrM11 Dynamics of Molecular Quantum-Dot Cellular Automata Devices and Circuits*, Y. Lu*,** *M. Liu, C. Lent,* University of Notre Dame

Quantum-dot cellular automata (QCA) provides a non-transistor alternative for the design of molecular electronics. Binary information is encoded in the charge configuration of molecular cells. Information is transported from cell to cell through the Coulomb interaction. Clocked control of molecular QCA can be accomplished by employing an applied clocking field which varies regularly in both space and time. This enables binary information to be transported across molecular arrays without electrons moving between molecules. Power gain restores signal energy lost to unavoidable dissipative processes. Here we study dynamic properties of molecular QCA devices including energy dissipation, operating frequency, and defect tolerance. We use detailed quantum chemistry results for molecules to construct simpler effective Hamiltonians for each QCA molecular cell. We then solve the equation of motion of the whole molecular device using a coherence vector formalism which includes both quantum effects and dissipative coupling to the environment. This enables us to characterize non-equilibrium and finite-temperature effects on switching behavior. We explore the structure-function relation in molecular QCA at two levels: that of the individual molecules and that of the circuit layout. The specific character of the inter-dot intra-molecular linker plays a crucial role in the dynamics of molecular switching, particularly near the maximum possible switching speeds. At the level of the circuit as a whole, a key challenge for all molecular electronics is handling defects due to the fundamental thermodynamic inability to control exactly the position and orientation of each single-molecule device. The QCA approach has the advantage of being inherently robust against disorder and can be made even more so by simply using wider wires to build in redundancy.

Thin Film
Room 2022 - Session TF+EM-FrM
In-Situ/Ex-Situ & Real-Time Monitoring and Characterization

Moderator: C. Stoessel, Southwall Technologies

8:00am **TF+EM-FrM1 Parameter Uncertainties and Higher-Order Effects in the Analytic First-Order Solution for the Complex Refractive Index and Thickness of a Thin Film on a Substrate*, I.K. Kim*,** *D.E. Aspnes,* North Carolina State University

We recently reported a solution in the thin-film limit of the general problem of determining the complex refractive index ñ = n+i@kappa@ and thickness d of an isotropic film on an isotropic substrate from the changes induced in polarimetric data by deposition or removal. Here, we consider uncertainties in n, @kappa@, and d in terms of uncertainties in the measured Fourier coefficients of the intensity. Taking advantage of the fact that the uncertainty @delta@(@DELTA@R/R) in the reflectance is much higher than the uncertainty @delta@(@DELTA@@rho@/@rho@) in the relative complex reflectance ratio, we obtain an analytic expression that gives the uncertainties of n, @kappa@, and d in both relative and absolute terms. The expression can be used to establish conditions where one or the other is determined with maximum accuracy. In contrast to expectations from ellipsometry, the relative uncertainties @delta@n/n and @delta@d/d can be significantly different. By adding noise to simulated data, we investigate the range of linearity and higher-order nonlinearities. Symmetric fluctuations of the Fourier coefficients about their average values can yield highly asymmetric fluctuations about the parameter values corresponding to the coefficient averages, particularly d. We describe a procedure for correcting the results for these asymmetries. Finally, we confirm all results with polarimetric data obtained by cyclically physisorbing and desorbing a monolayer of H@sub 2@O on oxidized GaAs.

8:20am **TF+EM-FrM2 Optical and Morphological Studies on SiO@sub 2@-like Films Deposited by Means of Ion Bombardment- Assisted Expanding Thermal Plasma CVD*, A. Milella*,** *M. Creatore, M.A. Blauw, M.C.M. Van De Sanden,* Eindhoven University of Technology, The Netherlands

The role of ion bombardment in the growth of plasma-deposited thin films has been often investigated in literature as a route towards film matrix densification at low temperature, this latter being a requirement when thermally sensitive substrates, such as polymers, are studied. In the present paper we report our latest results on the densification of SiO@sub 2@-like films by applying an external rf bias to the substrate holder during film deposition by means of an Ar-fed expanding thermal plasma, in which

hexamethyldisiloxane and oxygen are injected downstream. A comprehensive study of the optical properties of the deposited films, as determined by Spectroscopic Ellipsometry, with increasing dc bias voltage will be presented. In particular, it will be shown that ion bombardment can effectively improve film density when parameters such as the energy of the ions impinging the surface of the growing film and the ion-to-depositing radical flux ratio, are carefully controlled. Densification of film network by ion bombardment can be furthermore assessed by Fourier Transform IR spectroscopy, following changes in SiOSi asymmetric stretching absorption band with dc bias voltage. Film porosity increases with increasing deposition rate which results in a different absorption band shape. Surface morphology evolution of SiO@sub 2@-like films deposited under increasing dc bias voltage conditions as determined by Atomic Force Microscopy will be presented. In absence of ion bombardment, films display growth of spherical nodules distributed uniformly across the surface, with heights and lateral dimensions depending on the process parameters selected. Quantitative analysis shows that both RMS roughness and mean peak-to-valley distance decrease almost exponentially with increasing dc bias voltage. These results correlate with refractive index trends as determined from spectroscopic ellipsometry.

8:40am **TF+EM-FrM3 Real-Time X-ray Studies of Surface and Thin-Film Processes***, **K. Ludwig**, Y. Wang, A. Özcan, G. Ozaydin, C. Sanborn, A. Bhattacharyya, R. Chandrasekaran, T.D. Moustakas,* Boston University*; R. Headrick, H. Zhou,* University of Vermont **INVITED**

A new facility for the time-resolved x-ray study of surface and thin film processes is now in use at the National Synchrotron Light Source (NSLS) of Brookhaven National Laboratory. To promote flexibility, the base spectrometer is designed so that modest-sized processing/vacuum chambers can be rolled onto it. This design allows multiple specialized chambers to be constructed, optimized for experimentation, and then moved onto the diffractometer for real-time x-ray studies. Here results from studies of wide-bandgap group III-nitride growth on sapphire by plasma assisted molecular beam epitaxy (PA-MBE) will be discussed. These experiments have examined migration-enhanced epitaxy, the early stage kinetics of sapphire surface nitridation, and Ga droplet formation with subsequent nitridation to form GaN nanodots. Studies examining the spontaneous nanopatterning and smoothening of surfaces by ion bombardment will also be presented. This research is partially supported by DOE DE-FG02-03ER46037 and by NSF DMR-0507351.

9:20am **TF+EM-FrM5 Novel Annealing Treatments Applied to Binary Alloy Thin Films***, **J.R. Skuza**, R.A. Lukaszew,* The University of Toledo*; E.M. Dufresne,* Argonne National Lab*; C. Cionca, R. Clarke,* University of Michigan, Ann Arbor*; A. Cebollada,* Instituto de Microelectronica de Madrid, Spain

Rapid thermal annealing (RTA) is widely used for electronic materials processing, from the activation of dopants to the healing of lattice defects caused by ion implantation. Here, we describe an innovative application of x-ray undulator radiation to simultaneously anneal and probe the structural evolution that occurs during annealing in real-time. X-ray Rapid Thermal Annealing (XRTA) is similar to laser annealing, but there is a unique advantage in that the x-ray energy can be tuned to the absorption edge of a particular element, thereby permitting efficient annealing of buried layers and nanostructures. In our studies at the MHATT/XOR (Sector 7) beam line at the Advanced Photon Source, we have used XRTA to enhance the degree of chemical order in epitaxial and equiatomic FePt thin films. We have chosen this particular binary alloy system because it exhibits an interesting fcc-fct phase transformation. This phase transformation allows for the real-time tracking of the degree of chemical ordering achieved due to the appearance of a forbidden reflection in fcc structures [(001) peak] and the doubling of the fundamental reflection [(002) peak]. These results will be compared to the ones obtained with traditional resistive annealing. We will demonstrate that undulator radiation offers unique possibilities for materials processing AND real-time structural probing. @FootnoteText@ This work was partially supported by the National Science Foundation (DMR Grant #0355171), the American Chemical Society (PRF Grant #41319-AC), and the Research Corporation Cottrell Scholar Award. Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Basic Energy Sciences, Office of Science, under Contract No. W-31-109-Eng-38.

9:40am **TF+EM-FrM6 In-Situ Studies of Stress Evolution during the Heteroepitaxial Growth of Group III-Nitrides***, **J.M. Redwing**, S. Raghavan, X. Weng, J.D. Acord, E.C. Dickey,* Penn State University **INVITED**

The group III-nitrides (GaN, AlN, InN and related alloys) are an important class of III-V semiconductors that form the basis for commercial high brightness blue/green light emitting diodes, laser diodes and high power microwave electronics for military and communication applications. Due to difficulties associated with the bulk crystal growth of GaN, group-III nitride thin films are grown heteroepitaxially on substrates such as sapphire, silicon carbide and silicon. These substrates have significantly different lattice constants and coefficients of thermal expansion than GaN, which can result in thin film stress, dislocation formation and film cracking. In addition to the epitaxial and thermal mismatch stresses, which are well known, growth-related stresses due to developing film morphology also play an important role, but are not as well understood for the GaN materials system. In this study, we have utilized in-situ wafer curvature measurements to study the magnitude and evolution of growth stress during the metalorganic chemical vapor deposition of group III-nitride thin films. Specific examples will be presented including the case of GaN growth on silicon and AlGaN growth on silicon carbide. By combining the in-situ measurements with post-growth atomic force microscopy and cross-sectional transmission electron microscopy, we correlate the growth stress to microstructural changes in the film arising from island coalescence and dislocation bending and demonstrate that dislocation density reduction in AlGaN films primarily occurs when the film is growing under a compressive stress. Methods to mitigate stress and reduce film cracking including the use of compositionally graded buffer layers will also be discussed.

10:20am **TF+EM-FrM8 In Situ ATR - FTIR Spectroscopy of Hf (IV) Tert Butoxide and Tetrakis Ethyl Methyl Amino Hf Adsorption on Si (100), Si (111) and Ge***, **K. Li**, S. Dubey, T.M. Klein,* The University of Alabama

Hafnium oxide ultra thin films on Si are being developed to replace thermally grown SiO2 gates in CMOS devices. In this work, a specially designed attenuated total reflectance - fourier transform infra-red spectroscopy (ATR-FTIR) reaction cell has been developed to observe chemisorption of hafnium (IV) t-butoxide (HtB) and tetrakis ethyl methyl amino hafnium (TEMAH), onto a Si (100), Si (111) and Ge ATR crystals heated up to 250Â°C and under 1 torr of vacuum allowing the observation of initial reaction pathways in real time. Chemisorption spectra were compared to spectra of the liquid precursor and to spectra generated by density functional theory (DFT) calculations of liquid, monodentate and bidentate adsorbed precursors. Asymmetric stretching modes located at 1017 cm-1 and 1250cm-1 present in the chemisorbed spectra but not in the liquid spectra of HtB indicate that the adsorbed hafnium containing group is prevalent as a bidentate ligand on Si (111). Surface concentration of the chemisorbed species was dependant on the substrate temperature and precursor partial pressure allowing for determination of heats of adsorption of the t-butyl groups, which is 26.5 kJ/mol for HtB on Si (111).

10:40am **TF+EM-FrM9 In Situ Defect Spectroscopy: Probing Dangling Bonds during a-Si:H Film Growth by Subgap Absorption***, I.M.P. Aarts, A.C.R. Pipino,* ***M.C.M. Van De Sanden***, Eindhoven University of Technology, The Netherlands*; W.M.M. Kessels,* Eindhoven University of Technology, The Netherlands, Netherlands

Detecting ultralow defect concentrations in a-Si:H thin films is of great importance for improving the efficiency of a-Si:H-based solar cells. Likewise, from a more fundamental point of view, it is essential to obtain understanding of the role of surface defect states during the growth process. Yet, a paucity of experimental techniques capable of detecting these surface and or bulk defect states is readily available. Using the technique of evanescent-wave cavity ringdown spectroscopy, we have realized a unique and absolute absorption technique capable of detecting defect states such as dangling bonds with an unprecedented sensitivity that can be applied in situ and during film growth as we will demonstrate for hotwire chemical vapor deposited a-Si:H. We deposited a thin a-Si:H film (from 0 up to 800 nm thickness), onto a total-internal reflection surface of a ultralow-loss monolithic folded optical resonator. Subgap absorption spectra between wavelengths of 1170 and 1245 nm are obtained and show the typical broad absorption feature due to dangling bonds defect states present in the bulk and at the interfaces. The minimal detectable absorption of the technique is 3 10@super -8@ optical loss, which is equivalent to 3 10@super 8@ dangling bonds/cm@super 2@. Furthermore, from the real time experiments the defect distribution in the film could be established and showed that the highest defect concentration was present at the interface of the a-Si:H with the substrate while the surface defect density was approximately ten times smaller. Moreover,

changes in surface dangling bond concentration (formation- and decay-curves) could be monitored in real-time under various growth conditions.

11:00am **TF+EM-FrM10 In Situ Monitoring of Hafnium Oxide Atomic Layer Deposition***, **J.E. Maslar**, W.S. Hurst, D.R. Burgess, W.A. Kimes, N.V. Nguyen,* NIST

In situ monitoring of atomic layer deposition processes has the potential to yield insights that will enable efficiencies in film growth, in the development of deposition recipes, and in the design and qualification of reactors. However, demonstrations of in situ monitoring of actual atomic layer deposition processes are limited. In this work, the species present in the gas phase during atomic layer deposition of hafnium oxide were investigated in an attempt to gain insight into the chemistry of this system and evaluate potential in situ gas phase optical monitors. Hafnium oxide was deposited on a silicon substrate using tetrakis(ethylmethylamino) hafnium and water as the hafnium and oxygen sources, respectively. In situ Raman and infrared absorption spectroscopy measurements were performed in a research-grade, horizontal-flow reactor under a range of deposition conditions. Density functional theory quantum calculations of vibrational frequencies of expected species were used to facilitate identification of observed spectral features. Gas phase measurements performed at the wafer surface were compared to measurements performed at the chamber exhaust to investigate the utility of exhaust-based optical measurements for deposition monitoring. Results of in situ gas-phase measurements were compared with results of ex situ hafnium oxide film characterization, vacuum ultraviolet spectroscopic ellipsometry and infrared absorption spectroscopy, in an effort to correlate observed gas phase species with deposited film properties.

11:20am **TF+EM-FrM11 In-situ and Real-Time Spectroscopic Ellipsometry on Organic Semiconductors during Growth***, U. Heinemeyer,* Universit@um a@t T@um u@bingen, Germany*; S.M. Kowarik,* Oxford University, UK, Germany*; A. Gerlach, **F. Schreiber**,* Universit@um a@t T@um u@bingen, Germany*; G. Humphreys, R. Jacobs,* Oxford University, UK

We demonstrate the use of in-situ and real-time spectroscopic ellipsometry as a non-invasive technique for following the growth of organic semiconductor thin films of diindenoperylene and pentacene. It is possible to take spectra in the spectral range between 1.25eV and 5 eV sufficiently fast (~ 1 sec) to follow organic molecular beam deposition in detail. We show how this technique can be used to detect spectral changes occurring during growth of these complex materials. From the vibrational progression of the HOMO-LUMO transition we analyze the time/thickness evolution of the exciton-phonon (Huang-Rhys) parameter S. We discuss our results and their implications for organic device fabrication in the context of a recent real-time structural study which found structural and orientational transitions during growth.@footnote 1@ @FootnoteText@ @footnote 1@S. Kowarik et al., Phys. Rev. Lett. 96, 125504 (2006).

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