

Electronic Materials and Devices

Room 321/322 - Session EM+SC-MoA

Defects and Interfaces in Electronic Materials and Devices

Moderator: C.G. Van de Walle, Palo Alto Research Center

2:00pm **EM+SC-MoA1 Localized Defect States, Impurities, and Doping in Al@sub x@Ga@sub 1-x@N Epilayers, S.T. Bradley**, Ohio State University
INVITED

AlGa_N and its heterojunction alloys are used in some of the most advanced micro- and optoelectronic devices today and rely on precise control of electronic properties in multilayer film structures on a nanometer scale. Deep level defects in these materials and at their interfaces can alter transport, recombination, contact formation, and doping, yet measuring such small structures is a challenge for conventional techniques. Al-rich AlGa_N layers can enable many new applications but little is known of their deep level properties. Also, doping of AlGa_N with high Al content is difficult and may be restricted by non-intentional impurities (such as oxygen) and their associated deep levels. We have used a near-surface version of cathodoluminescence spectroscopy (CLS), termed low energy electron-excited nanoluminescence (LEEN), to probe the electronic properties of thin HFET films as a function of lateral position and depth. LEEN spectroscopy can provide electronic properties of states that are localized at the surface, buried interface, and near the middle of these nanometer-scale films. For AlGa_N/Ga_N structures, correlations have been made between deep level defects and the sheet charge density, AlGa_N/Ga_N intermixing, surface roughness, and Ga/N ratio. We have also used LEEN with secondary ion mass spectrometry (SIMS) to correlate deep levels across the AlGa_N alloy series with chemical impurities and spatial location at surfaces, interfaces, and in the bulk. Al-rich AlGa_N exhibits deep level optical emissions that correlate with O and C impurities. Temperature-dependent CL of the Si-doped films reveal donor energy increases but activation energy decreases with Al content. Coupled with the appearance of an O deep level at mid-gap at highest Al concentrations, these changes can be seen to compensate the intentional Si doping. These results demonstrate how spatially-resolved CL combined with SIMS can provide new understanding of macroscopic III-nitride properties.

2:40pm **EM+SC-MoA3 Contactless Characterization of High Electron Mobility Transistor Structures using Surface Photovoltage Spectroscopy, S. Solodky**, Tel Aviv University, Israel; *A. Khrantsov*, Ben-Gurion University, Israel; *T. Baksh*, Tel Aviv University, Israel; *M. Leibovitch*, Gal-El (MMIC), Israel; *Hava*, Ben-Gurion University, Israel; *Y. Shapira*, Tel Aviv University, Israel

GaN/AlGa_N High Electron Mobility Transistor (HEMT), AlGaAs/InGaAs/GaAs pseudomorphic HEMT (PHEMT), and InAlAs/InGaAs metamorphic HEMT (MHEMT) epitaxial structures have been characterized using surface photovoltage spectroscopy (SPS). The interplay between two opposite direction signals coming from the regions with opposite direction of electric fields define the shape of the spectra. The shape of the spectra is interpreted using self-consistent numerical simulations. The effects of the transistor delta-doping levels d_{top}, d_{bot} and surface charge Q_{sur} on the spectrum features have been studied using numerical simulations. Based on the latter, an empirical model has been developed, which allows extraction and comparison of d_{top}, d_{bot} and Q_{sur} and is applicable for both double-sided and single sided delta-doped structures. Effect of Si_N passivation on GaN/AlGa_N HEMT surface is shown. Applying of the model to passivated structure shows reduced Q_{sur}. Prediction of the final device performance by the model is shown for two MHEMT structures. Applying of the model shows sensitivity of the methodology to 7.5% difference of d_{top}. Devices produced on these structures show relative difference of 8.2% in maximum drain currents, which correlate well with d_{top} values calculated using the model.

3:00pm **EM+SC-MoA4 Atomic Bonding and Electronic Changes at InGaAs/InP Heterojunctions, P.E. Smith, S.H. Goss, S.T. Bradley, L.J. Brillson, M.K. Hudait, Y. Lin, S.A. Ringel**, The Ohio State University; *S.W. Johnson*, Sandia National Laboratories

Lattice-matched In_{0.53}Ga_{0.47}As/InP heterojunctions have attracted considerable interest for many opto- and microelectronic applications. Achieving abrupt interfaces is difficult since both group III and V elements must be switched at the interface during MBE growth. To minimize structural defects, growers often employ a sequence of source switching such that new group V elements are switched on for brief

exposure times before growth of subsequent layers. Interface-specific atomic bonding and diffusion can occur that can alter local electronic properties. We combined secondary ion mass spectrometry (SIMS) depth profiling with micro-cathodoluminescence spectroscopy (CLS) in cross section to measure atomic bonding and compositional changes and their effect on electronic properties. SIMS and CLS measurements of InGaAs-on-InP interfaces subjected to exposure times of 40, 80, 110, 140, and 170 sec reveal: (1) interface broadening (both As and P) that increases from < 5 to 15 nm with the length of time the InP surface is exposed to As prior to InGaAs growth, (2) InGaAs near band edge (NBE) emissions at ~0.79 and 0.80 eV, whose intensities shift to higher energies with proximity to the heterojunction on a submicron scale and become more evident with increasing As exposure time. These electronic changes suggest either lower In interface concentration and/or local defect formation - the latter consistent with increasing trap densities with As exposure measured via photoconductivity decay. Overall, local electronic structure at a lattice-matched III-V compound heterojunction depends sensitively on the competition of atomic species in the transition region during growth.

3:20pm **EM+SC-MoA5 Nanoscale Electronic Characterization of Semiconductor: from Operating Devices to Atomic Scale Defects, Y. Rosenwaks, R. Shikler**, Tel-Aviv University, Israel; *Th. Glatzel, S. Sadewasser*, Hahn-Meitner Institut, Germany
INVITED

Scanning probe microscopy has opened new opportunities to image semiconductors electronic properties with unprecedented spatial resolution. The recently developed Kelvin probe force microscopy (KPFM) technique has already been demonstrated as a powerful tool for measuring nanoscale electronic properties and has found many diverse applications in recent years. In this talk several novel applications of the KPFM technique recently developed and demonstrated by our group will be presented. The long-range electrostatic force between the AFM tip and the semiconductor surface deteriorates drastically the KPFM spatial resolution, and poses the problem whether surface atomic scale defects can be quantitatively measured. In addition, the physical understanding of the observed contrast in atomic resolution images is still under discussion. We show that by combining ultrahigh vacuum (UHV) KPFM measurements with rigorous modelling of the tip-semiconductor electrostatic interaction it is possible to extract the surface charge density at the atomic steps of a GaP (110) surface. The third part of the talk will be devoted to the use of KPFM for direct measurement of surface states parameters in semiconductors. The method is based on the measurement of very asymmetric cleaved p++n or n++p junctions. The absolute surface band bending, U_s, and the surface charge density, N_{ss}, can be extracted because one side of the junction is degenerate, and all the band bending is taking place in the low doped semiconductor. Methods to obtain the surface states energy distribution are also discussed.

4:00pm **EM+SC-MoA7 STM Observation of Subsurface Boron Dopants on the Si(001)-2x1 Clean Surface, M. Nishizawa, L. Bolotov, T. Kanayama**, National Institute of Advanced Industrial Science and Technology, Japan

As the feature size of integrated circuits approaches nanometer dimensions, dopant distribution in device regions plays an increasingly larger role in determining device performance. This has motivated research in recent years to identify a suitable technique to profile dopant distribution with atomic scale resolution. Among the more promising technologies is Scanning Tunneling Microscopy (STM). While a number of studies have been made to measure individual dopants on cleaved compound-semiconductor surfaces and cleaved or hydrogen-terminated Si surfaces using STM, no studies have been made on the Si(001)-2x1 clean surface. From a surface science perspective, the Si(001)-2x1 is one of the most widely studied and documented surfaces. However, it has not received attention in dopant measurement studies, as it is believed that surface states in the band gap obscure observation of dopant features. In this report, we show that Boron-dopant features can be successfully observed on the Si(001)-2x1 surface using STM. On the Boron-doped Si(001)-2x1 surface (sheet resistance is 0.01 @ohm@ cm) we have observed a number of specific features which are a few nanometers in size and appear as round-shaped protrusions superimposed on the corrugation of surface reconstruction in the filled-state image. The appearance of these features is quite similar to the dopant images observed previously on the other surfaces. These features can be recognized starting at a sample bias voltage (V@sub s@) of -1.0 V and tunneling current (I@sub t@) of 0.2 nA, can be enhanced by increasing V@sub s@ to -0.4 V and I@sub t@ to 2.0 nA. Area density of these features changes with dopant concentration of the substrate. From these results, we conclude that the specific features

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observed here are related to the Boron dopant located in a subsurface layer. This study was supported by NEDO.

4:20pm EM+SC-MoA8 Surface Defects After the Growth of Highly P and Sb Doped Si, G.G. Jernigan, P.E. Thompson, US Naval Research Laboratory

Doping in semiconductors is crucial to the formation of electronic devices, but our knowledge of the physical characteristics of electrical interfaces, as they are formed during device fabrication, is limited. We will present a unique study of Si doping with P and Sb during MBE growth on Si (100) wafers using an in vacuo STM. The process of doping affects the surface morphology, as compared to an undoped film, leading to surface defects. Under dopant flux conditions of $\sim 10^{12}$ atoms/cm²/s and Si growth rates ~ 0.10 nm/s, we will report the changes to the Si surface morphology and the production of defects at growth temperatures of 500 °C. The segregation of the n-type dopants, P and Sb, is observed to affect Si adatom attachment at step-edges resulting in an increase in island formation. For thin films of P less than 50 nm, where less than 0.1 monolayers (ML) of P has segregated, the surface roughness is not increased significantly but line defects parallel to dimer rows can be observed. At high P surface coverages observed on films greater than 50 nm, there are blockages at step-edge sites to form pothole-like defects with a density of 2×10^{10} /cm². For all Sb films grown, there is an increase in surface roughness with increasing film thickness (>2.0 nm) and Sb surface coverage (>0.01 ML). At high Sb surface coverages (0.8 ML), Si islands form into pyramid-like defects with a density of 8×10^{10} /cm², and this casts concern for the use of Sb in surfactant assisted growth. The evolution of the surface morphology and defect appearance with film growth and dopant segregation will be discussed.

4:40pm EM+SC-MoA9 The Effect of Strain on Impurity States in Si and Methods of Calculation Thereof, A. Rockett, D.D. Johnson, University of Illinois; B.R. Tuttle, University of Pennsylvania; S.V. Khare, University of Illinois

We propose a simple model for estimating the contribution of strain to the ionization energy of defect states in semiconductors. The model is illustrated for group III and V impurities in Si. The approach uses an extrapolation technique to determine the ionization energies from the results of density functional theory (DFT) calculations. The method is shown to produce reliable results for a range of dopants with no parameters and none of the usual corrections required in DFT. The results are generalized through an analysis of the resulting energies based on a screened electrostatic interaction, strain, and a bonding localization term.

5:00pm EM+SC-MoA10 New Mechanism for Coupling between Properties of Interfaces and Bulk Semiconductors, K. Dev, E.G. Seebauer, University of Illinois at Urbana Champaign

A new mechanism is described by which interface electronic properties can affect bulk semiconductor behavior. In particular, experimental measurements by photoreflectance of Si(100)-SiO₂ interfaces show how a controllable degree of band bending can be introduced near the interface by ion bombardment and annealing. The resulting electric field near the interface can affect dopant concentration profiles deep within the semiconductor bulk by drastically changing the effective interfacial boundary condition for annihilation of charged interstitial atoms formed during bombardment. Kinetic measurements of band bending evolution during annealing show that the bending persists for substantial periods even above 1000 C. Unusually low activation energies for the evolution point to a distribution of energies for healing of bombardment-generated interface defects. The transformations take place at temperatures higher than those characterizing other defects known to exist at the Si-SiO₂ interface. The findings have significant implications for pn junction formation during CMOS device processing.

Nanometer Structures

Room 308 - Session NS-TuM

Nanowires

Moderator: D.G. Cahill, University of Illinois, Urbana-Champaign

8:20am **NS-TuM1 Growth and Characterization of Single-Crystal ZnO Nanowires**, *Z. Zhu, T. Chen, Y. Gu, G. Neumark, R.M. Osgood Jr.*, Columbia University

One-dimensional ZnO nanowires have attracted increasing interest for both fundamental and applied studies of short-wavelength optoelectronic nanodevices. This talk reports a systematic study of effect of the variation of growth parameters, including growth temperature, growth time and catalyst (Au) film thickness, in determining the collective and individual structure of ZnO nanowires. Our single-crystal ZnO nanowires were grown on different-orientation silicon and sapphire substrates via vapor-phase transport. The synthesized ZnO nanowires were characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), energy dispersive x-ray spectroscopy (EDS) and photoluminescence (PL) spectroscopy. Room-temperature photoluminescence spectra of the ZnO nanowires revealed a strong, narrow excitonic emission at ~ 380 nm and a very weak green emission band at ~ 508 nm. The full width at half maximum (FWHM) of the excitonic emission at ~ 380 nm was ~ 95 meV, indicating that the ZnO nanowires are of good optical quality. SEM measurements were made of ZnO nanowires grown on silicon substrates with Au films of different-coverage. The growth studies have shown that, as the Au-thin-film coverage decreases, the width and area density of the nanowires decreases while the length of the nanowires increases. In addition, the SEM measurements of the ZnO nanowires, grown at different substrate temperatures, show that the spatial uniformity of ZnO nanowires is strongly dependent on substrate temperature. Strategies of manipulating the spatial orientation of ZnO nanowires for practical applications are being explored by using nanofabrication techniques such as electron-beam lithography to pattern the substrates and build blocks to confine the growth of the ZnO nanowires; these studies will be reported in this talk.

8:40am **NS-TuM2 Growth and Characterization of ZnO Nanowires**, *J.B. Baxter, E.S. Aydil*, University of California, Santa Barbara

ZnO is a wide band gap semiconductor with applications in UV optoelectronics, transparent conducting oxide coatings, piezoelectronics, and photovoltaics. Nanostructured ZnO can exhibit quantum confinement effects and enable applications requiring high surface area such as sensors and dye sensitized solar cells. We have grown monodisperse ZnO nanowires by chemical vapor deposition (CVD) using the organometallic precursor zinc acetylacetonate ($\text{Zn}(\text{acac})_2$) in the presence of oxygen. Nanowire diameters depend on the growth conditions and range from 16 nm to 100 nm. The growth morphology depends sensitively on the substrate and the partial pressure of $\text{Zn}(\text{acac})_2$. On a-plane sapphire, nanowires grow epitaxially and perpendicular to the substrate in dense arrays and with in-plane rotational order. X-ray diffraction pole figures confirm the epitaxial relationship $\text{ZnO}(0001) \parallel \text{Al}_2\text{O}_3(11\bar{2}0)$ and $\text{ZnO}(11\bar{2}0) \parallel \text{Al}_2\text{O}_3(10\bar{1}0)$. Conversely, nanowires grow on c-plane sapphire in one of three directions relative to the substrate owing to $\text{ZnO}(0001) \parallel \text{Al}_2\text{O}_3(10\bar{1}0)$ epitaxy and the trigonal symmetry of the substrate. Controlled sublimation and delivery of the solid precursor is challenging. However, we are improving our ability to control nanowire growth by studying the evaporation and decomposition of $\text{Zn}(\text{acac})_2$ using thermogravimetric analysis and mass spectrometry and by monitoring the presence of the $\text{Zn}(\text{acac})_2$ with in situ Fourier transform infrared (FTIR) spectroscopy. Dense ZnO nanowires with high surface area can be grown on various oxide substrates, making them suitable for replacing the mesoporous semiconductor in dye sensitized solar cells. Single crystal ZnO nanowires offer improved conduction pathways compared to sintered nanoparticles used currently, where electron transport occurs by a hopping mechanism.

9:00am **NS-TuM3 Structure, Defect and Cathodoluminescence Studies of GaN Nanorods and Nanowires**, *L.C. Chen*, National Taiwan University, Taiwan; *C.S. Shen, S.C. Shi*, National Taiwan University; *S. Dhara, C.T. Wu, K.H. Chen*, Academia Sinica, Taiwan; *C.W. Hsu, C.C. Chen*, National Taiwan Normal University

Single-crystalline GaN and related 1D nanostructures, specifically, binary InN, AlN along with their ternary $\text{In}_x\text{Ga}_{1-x}\text{N}$ and $\text{In}_x\text{Al}_{1-x}\text{N}$ counterparts have been successfully grown by catalytic

chemical vapor deposition. Their structure and optical properties are investigated by scanning and transmission electron microscopy, Raman, photoluminescence (PL) as well as cathodoluminescence (CL) techniques. Diameter and position selective growth of these 1D nitride nanostructures has been demonstrated by pre-treatment of the substrate surface with size-controlled catalyst. Oriented growth of the nanorods was also obtained under hetero- or homo-epitaxial conditions. While PL measurements usually give spectral data from numerous nanowires and nanorods with a broad distribution of diameter, the CL measurements (from room temperature down to 4 K) can easily be performed on single nanowire or nanorod. A higher CL peak position of individual GaN nanorod than that of bulk GaN film was observed, indicating the presence of strain in the pristine nanorod, which is also confirmed by X-ray diffraction analyses. In addition, a blue shift of CL peak position with decreasing the diameter of GaN nanorod was noticed. However, the magnitude of the peak shift is much more pronounced than that estimated from quantum confinement. Finally, Ga⁺ ions implantation of these GaN 1D nanostructures has been studied using 50-keV Ga⁺ focused ion beam. Phase transformation and defect structure evolution as a function of irradiated ion-beam fluence is also investigated by electron-microscopy-based techniques.

9:20am **NS-TuM4 Onset of Nanowire Growth by Vapor-Liquid-Solid (VLS) Epitaxy**, *J.W. Dailey, J.L. Taraci, T. Michael, J.C. Thorp, S.T. Picraux*, Arizona State University

We report on CVD growth of Ge and Si nanowires on Si substrates by the Vapor Liquid Solid (VLS) technique. While many groups have formed random clusters of Si nanowires at high pressures by VLS, relatively little effort has been directed at the controlled CVD growth of epitaxial arrays of nanopillars or nanowires directly onto Si substrates. In our studies Au nanodots are formed by UHV evaporation on hydrogen terminated Si (100) and (111) substrates. Subsequent selective area growth is carried out using digermane or disilane at pressures from 1×10^{-2} to 1×10^{-5} T and temperatures from 400 to 600 C. At the lower pressures (representative of gas phase MBE) we observe the growth of Ge nanopillars that nucleate at the AuSi eutectic and grow vertically and laterally, undergoing coalescence as growth continues. RBS and ion channeling are used to establish the VLS substrate orientation and temperature dependent kinetics of the Ge nanopillar growth, and SEM elucidates the morphological evolution of the nanopillars. At pressures above 10⁻⁴ T we observe an abrupt change in the nature of the growth from a relatively slow nanopillar growth to a much more rapid nanowire growth. The nanowires are distinguished by long narrow axial growth structures with much slower lateral growth. The transition from nanopillar to nanowire growth is interpreted in terms of a nucleation-limited process. Due to the small lateral dimensions (10 to 50 nm) of these 3-D structures lateral strain relief is expected to occur and large lattice mismatches should be accommodated without defects, in contrast to large area heteroepitaxy. These CVD nanoscale structures could form the basis for new in situ synthesis of 3-D Si device structures on Si substrates.

9:40am **NS-TuM5 Functional Semiconductor Nanowires and Their Optical Properties**, *P. Yang*, University of California, Berkeley **INVITED**

Nanowires are of both fundamental and technological interest. They represent the critical components in the potential nanoscale electronic and photonic device applications. In this talk, I will introduce the vapor-liquid-solid crystal growth mechanism for the general synthesis of nanowires of different compositions, sizes, orientation and doping profile. Particularly, synthesis and organization of different types of heterostructured nanowires will be discussed. Wide band gap semiconductor nanostructures with near-cylindrical geometry and large dielectric constants exhibit two-dimensional ultraviolet and visible photonic confinement (i.e. waveguiding). Combined with optical gain, the waveguiding behavior facilitates highly directional lasing at room temperature in controlled-growth nanowires with suitable resonant feedback. The nanowire optical emission has been studied in detail using high-resolution optical microscopy. The waveguiding behavior of individual zinc oxide (ZnO, GaN) nanowires depends on the wavelength of the emitted light and the directional coupling of the photoluminescence (PL) to the emission dipoles of the nanowire. Pumping at high pulse intensity leads to the transition from spontaneous to stimulated emission, and analysis of the polarization, linewidth, and spacing of the spectral features facilitates identification of the transverse and longitudinal cavity modes and their gain properties. The observation of lasing action in arrayed and isolated ZnO/GaN nanowires without requiring fabrication of mirrors suggests the single-crystalline, well-faceted nanowires can indeed function as effective resonance

Tuesday Morning, November 4, 2003

cavities. This concept of using well-cleaved nanowires as natural optical cavities may be extendable to many other different semiconductor systems. @FootnoteText@ @footnote 1@ Y. Wu, R. Fan, P. Yang, Nanolett, 2, 83, 2002. @footnote 2@ M. Huang, S. Mao, H. Feick, H. Yan, Y. Wu, H. Kind, E. Weber, R. Russo, P. Yang, Science, 292, 1897, 2001. @footnote 3@ J. Johnson, H. J. Choi, K. P. Knutsen, R. D. Schaller, R. J. Saykally, P. Yang, Nature Materials, 1, 101, 2002. @footnote 4@ J. Johnson, H. Yan, R. Schaller, L. Haber, R. Saykally, P. Yang, J. Phys. Chem. B, 105, 11387, 2001.

10:20am **NS-TuM7 Mo@sub 3@Se@sub 3@ Nanowires - Mechanical and Electrical Properties at the Nanoscale, A. Heidelberg**, Trinity College Dublin, Ireland; *J.W. Schultze*, Heinrich-Heine-Universität Düsseldorf, Germany; *G. Staikov*, Forschungszentrum Jülich, Germany; *J.J. Boland*, Trinity College Dublin, Ireland

Low dimensional organic and inorganic materials like nanowires and nanotubes have attracted much interest as potential building blocks for nanotechnology. This interest can be traced to the novel structural and electronic properties of these materials. Here we describe a study that measures the electronic and mechanical properties of the inorganic polymer (LiMo@sub 3@Se@sub 3@)@sub n@ together with nanowire-networks that have been synthesized by exchanging the Li-counterion with different alkylammonium- and pyridinium-ligands. (LiMo@sub 3@Se@sub 3@)@sub n@ forms quasi-1D crystals and is structurally related to the Chevrel phases. It can be viewed as a condensation polymer of Mo@sub 3@Se@sub 3@ units. The crystals can be dissolved in polar solvents with @epsilon@ > 45. In these solvents the crystals disassemble into single nanowires with a diameter of 0.6 nm (from crystal data and TEM) and bundles of nanowires, depending on the solutions concentration. From solution, single nanowires, bundles of nanowires or films of nanowires can be cast on various substrates. Both, the wires themselves as well as the nanowire films are highly conductive but susceptible to electrical degradation (oxidation) in air. The ion exchanged wires form self assembled networks with an inter-wire spacing determined by the length of the side chain of the alkylammonium- and pyridinium-ligands. Conductivity measurements on these nanowire networks at different temperatures and oxidation times show that conduction is activated and occurs via a percolation mechanism. The mechanical properties of single nanowires or bundles were studied using a SPM-nanomaniplator. This instrument allows us to controllably apply forces (μN -nN range) to supported Mo@sub 3@Se@sub 3@-nanowires to effect nanoscale manipulations. Using the lateral force data of the manipulations, the mechanical properties like Youngs modulus and tensile strength of the wires can be measured.

10:40am **NS-TuM8 Defect Mediated Electronic Transport in Nano and Molecular Wires, D.A. Bonnell, S. Kalinin, M. Freitag, A.T. Johnson**, University of Pennsylvania

Any rational approach to nanostructure design necessitates a fundamental understanding of the properties of the constituents, as well as collective behavior of ensembles. We have developed 2 new approaches to measuring local electromagnetic properties based on scanning probes that can be applied to nano and molecular wires, Scanning Impedance Microscopy and Nano Impedance Spectroscopy. These approaches access the frequency dependence of electronic transport over 3-6 orders of magnitude, depending on experimental conditions. The frequency dependence can be used to determine mechanisms of electronic transport, particularly the processes that occur at defects. We demonstrate this approach by determining the local electronic structures of individual defects in single walled carbon nanotubes. We then generalize to nanowires and molecular wires.

11:00am **NS-TuM9 Electronic Structure and Excited States of One-dimensional Polydiacetylene Nanowire, M. Akai-Kasaya, K. Shimizu, A. Saito, M. Aono, Y. Kuwahara**, Osaka University and SORST JST, Japan

The polydiacetylene (PDA) nanowire can be fabricated at designated positions by using a STM probe tip on a self-assembled monomolecular (SAM) layer. @footnote 1@ The fabricated PDA wire grows out in a straight line and extends to a sub-micrometer length on the surface. The fully extended conjugated backbone of the PDA is not only expected to function as an electrically conducting nanowire but is also interesting in terms of exploring physics in one-dimensional (1D) systems. In this work, the density of states of individual polymers and constituent monomers were studied by STS. The STS spectrum delineating the density of states of PDA wire clearly reveals the theoretically predicted @pi@-band and band edge singularities of the 1D conjugated polymer. We have also observed a fascinating spectrum with a narrow gap, which is suggested to be due to the existence

of the charge-carrying polaron states on a polymer backbone. Furthermore, we demonstrated that an excited state took place in an isolated polymer nanowire following the polymerization. The voltage pulse initiates additive polymerization, which proceeds instantaneously to both sides of the monomer array on the SAM layer. Before and after polymerization within the disabled feedback loop, the tunneling current shows the accountable difference due to the steady-state current on the monomer and derived polymer, respectively. However, the anomalous current, which often continues for few hundred micro-seconds, has been observed simultaneously with inception of the polymerization. We have estimated statistically the time of onset and duration of the current and correlation with the length of the derived polymer wire. And then, it can be concluded that the detected anomalous current results from the vibrational excitation states of a derived molecular nanowire. These results are remarkable and interesting in terms of one molecular science. @FootnoteText@ @footnote 1@ Y. Okawa and M. Aono, Nature 409, 683 (2001).

11:20am **NS-TuM10 STM and DFT Study of Gadolinium Silicide on Si(100), B.C. Harrison**, University of North Carolina at Chapel Hill, Ireland; *J.J. Boland*, Trinity College Dublin, Ireland

The fabrication and characterization of low-dimensional nanoscale structures is motivated by the desire to produce materials and devices with novel optical, structural, and electronic properties. Due to the difficulties in nanoscale fabrication by a top-down approach, self-assembly of nanoscale materials represent an attractive alternative. Rare earth silicide on the Si(100) surface is one such system that has attracted significant interest over the past several years. Nanostructures of various silicides @footnote 1,2,3@ have been formed with high aspect ratios, micrometer length scales, large mechanical strengths, and metallic character; all of which make them potential candidates for nanoscale interconnects or device components. However, these nanowires cannot be successfully used in electronic circuits until the morphology and placement of wires are controlled. This study focuses on Gadolinium Silicide (GdSi@sub 2@) on Si(100) since this silicide forms nanowires and has the smallest lattice constant mismatch in the wire growth direction of any of the available rare earth silicides at growth temperatures. Scanning Tunneling Microscopy data and DFT calculations results are coupled to determine the morphology of the various phases of GdSi@sub 2@ on the Si(100) surface. Furthermore, STM images are acquired from room temperature to wire-growth temperatures in order to study the atomic structure and growth processes of the initial wetting layer and nanowires themselves. At least three forms of the wetting layer and two forms of wires will be discussed in connection with an overall surface phase diagram for GdSi@sub 2@ on Si(100). @FootnoteText@ @footnote 1@ Chen, Y.; Ohlberg, D. A. A.; Williams, S. J. Appl. Phys. 2002, 91, 3213. @footnote 2@ Chen, Y.; Ohlberg, D. A. A.; Medeiros-Riberio, G.; Chang, Y. A.; Williams, S. Appl. Phys. Lett. 2000, 76, 4004. @footnote 3@ Nogami, J.; Liu, B. Z.; Katkov, M. V.; Ohbuchi, C.; Birge, N. O. Phys. Rev. B 2001, 63, 233305-1.

11:40am **NS-TuM11 Theoretical Calculation of the Thermal Conductivity of Semiconducting Nanowires, N. Mingo, L. Yang**, NASA-Ames Research Center

An atomistic Green function theoretical formalism to compute phonon transport in nanostructures will be presented, and its application to several different problems will be discussed. In particular, we present calculations of the thermal conductivity of Si and Ge nanowires, and compare these with some experimental results [D. Li et al., submitted]. One important problem that has not yet been extensively studied in an atomistic framework, is that of ballistic vs. diffusive phonon transport. Using our atomistic Green function approach, we study the transition from ballistic to diffusive phonon transport, occurring as the system's length increases. The way in which this transition takes place is largely determined by properties of its boundary. We will discuss the ballistic-diffusive transition in terms of atomic properties of the wire and its coating. Differences between (111) and (110) orientated nanowires are shown to be of more importance in the ballistic regime than in the diffusive one. Finally, a two parameter model, with the parameters depending only on bulk material properties, is also derived. Using this method we obtained good predictive calculations of the thermal conductivity of Si nanowires. The method employs the full phonon dispersion relations of bulk Si. The relative importance of specific nanowire modes not present in bulk, as the system's size becomes smaller, will be discussed. The results and methods presented offer an exciting new range of possibilities in the study and development of thermal transport through nanosized devices.

Organic Films and Devices

Room 318/319 - Session OF+EM-TuM

Molecular and Organic Films and Devices-Electronics

Moderator: A.R. Duggal, GE Global Research

8:20am **OF+EM-TuM1 Charge Transport and Charge Injection in Polymer Field Effect Transistors**, *H. Sirringhaus*, University of Cambridge, UK
INVITED

Conjugated polymer semiconductors have been intensely researched over the last 15 years as active layers in solution-processed semiconducting devices, such as field-effect transistors. Here we will discuss recent progress in understanding the charge transport physics of conjugated polymer semiconductors. Particular emphasis will be on polaronic relaxation effects, distinction between interchain and intrachain charge transport, and the physics of charge injection from a metal electrode into a polymer semiconductor. Polymer field effect transistors offer new opportunities for the controlled manufacturing of active electronic circuits by a combination of solution processing and direct printing. Control over the morphology of the polymer semiconductor is obtained by making use of self-organization mechanisms, such as liquid-crystalline phase behaviour. Techniques such as surface energy-assisted inkjet printing or embossing can be used to manufacture integrated polymer transistor circuits.

9:00am **OF+EM-TuM3 High Mobility Organic Field Effect Transistors**, *S.E. Sysoev, V.V. Podzorov, E.M. Loginova, M.E. Gershenson*, Rutgers University
Both organic thin film transistors (OTFTs) and organic single crystal field effect transistors (OFETs) are of primary interest for the characterization of the transport properties of novel organic materials. At the present, a comparison between these two approaches shows that the mobility is low on the deposited thin films, which is attributed to interface and grain boundary phenomena. In the case of single crystal OFETs there are several key factors, which affect their performance (the mobility and on/off ratio). We will report on optimization of the OFET fabrication process, which allowed to reproducibly obtain the values of $\mu \sim 10 \text{ cm}^2/\text{Vs}$. To the best of our knowledge, this is the highest mobility reported for organic field-effect devices at room temperature. In addition, in contrast to the TFTs, our devices demonstrate the thresholdless operation, gate voltage independent mobility and very small subthreshold slope. Tsamouras et al. Appl. Phys. Lett. 80, 4528 (2002). Komoda et al. Jpn. J. Appl. Phys., 41, 2767 (2002).

9:20am **OF+EM-TuM4 Growth Dynamics and Electrical Properties of Pentacene Ultra-thin Films**, *R. Ruiz, A. Mayer, G. Malliaras*, Cornell University; *R.L. Headrick*, University of Vermont; *A.Y. Kazimirov, J.R. Engstrom*, Cornell University

Organic/inorganic interfaces play a crucial role in the rapidly growing field of molecular electronics. Even though huge progress has been achieved in the understanding of electronic transport in conjugated molecular materials, a complete study that relates the nucleation and growth mechanisms with charge transport properties in pentacene thin films is still missing, especially within the first few monolayers adjacent to the gate substrate where charge transport is believed to occur. Pentacene thin films were evaporated onto silicon oxide substrates and analyzed by in-situ synchrotron X-ray scattering and ex-situ atomic force microscopy (AFM). The evolution of the first monolayers was studied by monitoring the intensity of scattered X-rays at the anti-Bragg position. Layer coverages were then extracted from the X-ray intensities using a simple growth model and compared to AFM micrographs. Film evolution as a function of substrate temperature will also be discussed. Thin film transistors were also fabricated with these films for electrical characterization showing a field effect hole mobility of $0.1 \text{ cm}^2/\text{V-sec}$.

9:40am **OF+EM-TuM5 Optical and Electronics Properties of Poly(o-Methoxyaniline) (POMA) for Organic FET Applications**, *R.P. Shrestha, D.X. Yang, E.A. Irene*, University of North Carolina at Chapel Hill

The optical properties of spin coated thin films of poly(o-methoxyaniline) (POMA) was investigated using spectroscopic ellipsometry (SE) and optical absorption spectroscopy in the visible-near UV optical range. A Gaussian oscillator optical model was used to fit the data obtained from SE. Atomic force microscopy (AFM) was used to characterize film roughness and these results were also evaluated in the optical model. We have investigated the effect of different spin deposit conditions including spin rate, and concentration of solution and deposition ambient on the POMA film thickness, surface roughness, optical and electronic properties. Organic

thin film field effect transistor fabrication was carried out using POMA on a gold line structure that formed the source and drain contacts and with SiO₂ covered Si wafer as the gate dielectric and substrate, respectively. Device characteristics are presented.

10:00am **OF+EM-TuM6 An Optical and Electronic Properties Study of a Stable n-Type Organic Semiconductor: N,N'-bis(3-phenoxy-3-phenoxyphenoxy)-1,4,5,8-naphthalenetetracarboxydiimide**, *D.X. Yang, R.P. Shrestha*, University of North Carolina at Chapel Hill; *T.J. Dingemans*, Delft University of Technology, The Netherlands; *E.T. Samulski, E.A. Irene*, University of North Carolina at Chapel Hill

The use of organic semiconductors in the electronic devices typically requires stable and reliable n and p-type semiconductors. Stable p-type organic semiconductors are well known, but useful n-type organic semiconductors are rare mainly due to their relative reactivity. In this study, a novel n-type organic semiconductor: N,N'-bis(3-phenoxy-3-phenoxyphenoxy)-1,4,5,8-naphthalenetetracarboxydiimide (NDA-n2) is investigated. NDA-n2 is stable up to 200 °C in air and shows excellent solubility in THF and CH₂Cl₂. Also, its co-planar packing structure could yield high electronic mobility. NDA-n2 film was spin-cast onto SiO₂ coated Si wafer substrate. The optical properties were determined using spectroscopic ellipsometry (SE) and optical absorption spectroscopy in the visible near UV optical range. The optical properties were obtained from the experimental data using a Gaussian oscillator model and regression analyses. The results show four absorption peaks around 4.60 eV, 3.87 eV, 3.68 eV and 3.48 eV. Atomic force microscopy (AFM) was used to obtain surface roughness which was included in the optical model using the Bruggeman effective medium approximation. Electrical properties were determined from simple structures and correlated with film deposition parameters. PN junctions were formed and evaluated.

10:20am **OF+EM-TuM7 Organic Semiconducting Materials for Plastic Electronics**, *Z. Bao*, Bell Labs, Lucent Technologies
INVITED

Organic electroactive materials are now being considered as the active materials in displays, electronic circuits, solar cells, chemical and biological sensors, actuators, lasers, memory elements, and fuel cells. The flexibility of their molecular design and synthesis makes it possible to fine-tune the physical properties and material structure of organic solids to meet the requirements of technologically significant applications. In this talk, the performance of several new organic semiconducting materials will be presented. These materials are designed for high performance, long-term stability, and ease of fabrication.

11:00am **OF+EM-TuM9 Localized Deposition of Thin Films of Conducting Polyaniline on Microhotplates for Chemical Sensing**, *G. Li, S. Semancik*, National Institute of Standards and Technology

A procedure for directly processing thin films of conducting polyaniline on MEMS microhotplates is described. The method allows the fabrication of conductometric gas microsensors within microarray platforms. It combines alternating electrochemical and electroless surface polymerization steps along with the localized heating capability of microhotplates to selectively deposit strongly adhering, smooth and compact films on the hybrid (metal/SiO₂) surfaces of microhotplate sensing elements. The polyaniline films within the arrays can be deposited using different processing parameters and then further functionalized electrochemically. In this way, both the film thickness and film conductance can be efficiently fine-tuned to desirable values. Film thickness varies in the sub-micron range and the film conductivities range from insulating up to the order of magnitude 10^5 S/cm . In addition, we describe the effect of these film characteristics on the temperature programmed sensing performance of the microsensors to various gases (methanol, H₂O, CO and NH₃ etc at 1-1000 ppm concentrations in air).

11:20am **OF+EM-TuM10 Polymeric Aperture Masks for High Performance Organic Integrated Circuits**, *D.V. Muyres, T.W. Kelley, P.F. Baude, S. Theiss, M. Haase, P. Fleming*, 3M

We present here the use of polymeric aperture masks to fabricate high performance pentacene-based integrated circuits. The aperture masks are fabricated using a laser ablation process with capabilities of generating 10 micron features. A mask set consisting of 4 to 6 aligned layers has been fabricated and has been used to demonstrate functional rf-powered integrated circuits with 20 micron gate lengths. Devices consisted of shadow-mask patterned layers of gold, alumina and pentacene. TFT mobilities greater than $2 \text{ cm}^2/\text{Vs}$ were measured and propagation delays

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from 7-stage ring oscillators of less than 5 microseconds were observed. This all-additive, dry patterning method has been extended to the production of samples as large as $6 \text{ cm} \times 6 \text{ cm}$. Larger aperture masks are under investigation and continuing efforts are focused on automation of the alignment process.

11:40am **OF+EM-TuM11 Conducting Nanofibers Integrated with Surface Micromachined Structures**, *D. Czaplewski, H. Liu, J. Kameoka, R. Mathers, G. Coates, H.G. Craighead*, Cornell University

We present a non-lithographic approach to the formation of oriented polymer nanowires on patterned surfaces. We utilized MEMS structures to deposit conducting nanofibers integrated with patterned electrodes on the surface of a silicon chip. The MEMS structures, used as scanned electro-spray sources, are bulk micromachined silicon tips fabricated using microfabrication techniques. A 5 kV potential was applied between the MEMS tip and a rotating counter electrode, which was used to control the orientation of the fibers on the silicon chip containing the measurement electrodes. The nanofibers would form from the extraction of a liquid jet from the silicon tip under an applied electric field. The fibers would dry in transit to the counter electrode, thus depositing single cylindrical fibers. We deposited nanofibers made from a mixture of poly(ethylene oxide) and polyaniline on surface patterned electrodes. Fibers, with diameters ranging from 600 nm to 20 micrometers, were deposited on a set of 4 electrodes, used in a 4 point probe configuration. We measured the conductivity of the fibers, which is consistent with previous reports. We have deposited poly(ethylene oxide) fibers suspended over trenches with diameters as small as 50nm. Additionally, we have used this method to deposit fiber arrays, forming polymer junctions. This method can be used to deposit polymers of various compositions integrated with topographical and surface features.

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Electronic Materials and Devices

Room 310 - Session EM+SC-TuA

50th Anniversary Sessions: Electronic Materials

Moderator: L.J. Brillson, Ohio State University

2:00pm **EM+SC-TuA1 Electronic Materials Growth: A Retrospective and Look Forward**, *C.W. Tu*, University of California, San Diego **INVITED**

This article reviews the development of electronic materials, primarily III-V compound semiconductors, from substrates to epitaxy and in situ monitoring to heterostructures, quantum wells and superlattices, that are important to various device applications. As the current research direction leads to the immediate future, the article then summarizes some of the recent advancement in quantum wires, nanowires, and quantum dots.

2:40pm **EM+SC-TuA3 Electronic Materials Theory: Interfaces and Defects**, *C.G. Van de Walle*, Palo Alto Research Center **INVITED**

The experimental advances in electronic materials over the past decades have been accompanied by a remarkable increase in the ability to predict structural and electronic properties from first principles. Basic theory, along with modeling and simulation, has always been instrumental in understanding materials. Only recently, however, has the capability emerged to accurately predict properties based solely on the composition of the material, without any fitting to experimental quantities. Such a description must be based on a quantum-mechanical treatment, i.e., a solution of the Schrödinger equation for the system of atomic constituents. The seemingly impossible task of solving this vast many-body problem was rendered feasible by the development of density functional theory (DFT), an achievement for which Walter Kohn received the Nobel Prize in Chemistry in 1998. Other important developments that have greatly enhanced the ability to tackle large systems include pseudopotentials, the simultaneous optimization of electronic and atomic degrees of freedom as embodied in the Car-Parrinello method, and the tremendous increase in available computer power. In this talk I will focus on two areas in which these theoretical and computational advances have had a major impact, namely heterojunction interfaces and defects in semiconductors. Both are intimately connected to the high-quality growth techniques that have enabled a host of novel electronic devices. In the area of defects I will describe the effects of point defects and impurities on doping, specifically highlighting the role of hydrogen. A recently discovered universal alignment for the electronic level of hydrogen in semiconductors and insulators reveals a surprising link with the problem of heterojunction band lineup.

3:20pm **EM+SC-TuA5 Progress in Electronic Materials Characterization**, *P.H. Holloway*, University of Florida **INVITED**

Progress in characterization of electronic materials over the past 50 years will be illustrated by selected examples of determination of the atomistic reconstruction and formation of electronic states at surfaces and interfaces of semiconductors using surface sensitive characterization techniques. The same techniques have been used to characterize reactions at interfaces and determine the mechanisms by which charge carrier transport is changed from that controlled by Schottky rectifying to contacts with ohmic characteristics. Secondary ion mass spectrometry (SIMS) has been used to measure dopant profiles over dimensions <10 nm below the surface, and optical characterization techniques have been used for real time control of semiconductor growth. Finally, areas of future development in electronic materials characterization techniques will be the subject of speculation.

4:00pm **EM+SC-TuA7 Making Contact - The Evolution of Materials for Silicon Device Contacts and Interconnections**, *J.M.E. Harper*, University of New Hampshire; *S.M. Rossnagel*, *F.M. d'Heurle*, *L. Clevenger*, *C. Lavoie*, *C. Cabral, Jr.*, IBM T.J. Watson Research Center **INVITED**

The evolution of silicon device technology during the 50-year history of the AVS required not only the constant miniaturization of the transistor, but the concurrent miniaturization of contact metallurgy and interconnection structures. With decreasing area and thickness came a series of materials challenges related to deposition processes, interdiffusion, compound formation and phase stability. These challenges were overcome with a steady stream of innovations in alloy metallurgy, deposition methods, diffusion barriers and understanding of phase formation that apply far beyond the field of microelectronics. Many of these advances were developed by active AVS members and award winners, since the AVS has provided a fertile professional arena for bringing together the necessary

scientific and engineering perspectives. Examples will be taken from the development of aluminum-copper and copper interconnections and from the evolution of titanium, cobalt and nickel silicide contact metallurgy.

Organic Films and Devices

Room 318/319 - Session OF+EM-TuA

Molecular and Organic Films and Devices-Optoelectronics

Moderator: A.J. Makinen, Naval Research Laboratory

2:00pm **OF+EM-TuA1 OLEDs and Solid State Lighting**, *A.R. Duggal*, GE Global Research **INVITED**

OLED technology has improved to the point where it is now possible to envision developing OLEDs as a low cost solid state light source. In order to realize this, significant advances have to be made in device efficiency, lifetime at high brightness, high throughput fabrication, and the generation of illumination quality white light. In this talk, the research challenges for general lighting will be reviewed and approaches being pursued at GE to meet them will be outlined.

2:40pm **OF+EM-TuA3 Hybrid Electroluminescent Devices Based on Conjugated Polymers and CdS:Mn/ZnS Core/Shell Nanocrystals**, *H. Yang*, *P.H. Holloway*, University of Florida

Nanocrystals with a CdS:Mn/ZnS core/shell structure with a core crystal diameter of 2.3 nm and a shell thickness of 0.4 nm were synthesized via a reverse micelle route. Direct current (dc) electroluminescent (EL) devices were tested having a hybrid organic/inorganic multilayer structure of ITO//PEDOT-PSS//conjugated polymer//CdS:Mn/ZnS nanocrystal//Al, where two different conjugated polymers (poly(N-vinylcarbazole) (PVK) and poly(p-phenylene vinylene) (PPV)) were used. The poly(3,4-ethylenedioxythiophene)/poly(styrenesulfonate) (PEDOT-PSS) layer was used for enhanced hole injection from the ITO electrode. In PVK-based nanocrystal devices, only orange emission from the CdS:Mn/ZnS nanocrystal layer was observed, with no emission from the PVK. However, only green EL emission was observed from the PPV layer in PPV-based nanocrystal hybrid devices, with no emission from the nanocrystal layer. EL emission from a single layer of a multilayer structure was concluded to result from radiative electron-hole recombination occurring predominantly in that layer. All of these data will be interpreted in terms of energy levels for the PVK, PPV, and quantum-shifted CdS:Mn/ZnS structures, where a charge transport through the device depends upon the valence and conduction band offsets at the interfaces between conjugated polymer and nanocrystal layer. In addition, PPV-only EL devices showed much smaller current flow and weaker EL emission than PPV-based nanocrystal hybrid EL devices, suggesting that the CdS:Mn/ZnS nanocrystal layer serves as an electron transport layer (ETL) in the hybrid device. These observations will be shown to be consistent with the energy level diagrams of the EL devices.

3:00pm **OF+EM-TuA4 Large Magnetic Field Effects in Organic Light Emitting Diodes (OLED) based on Alq₃**, *A.H. Davis*, *K. Bussmann*, Naval Research Laboratory

A study of the spin statistics of exciton formation in organic semiconductors predicts that the amount of light produced by an organic light emitting diode (OLED) can be modulated by controlling the relative spin-polarization of the holes and electrons that combine to form excitons. Organic materials with intrinsically low spin-orbit coupling show long electron and hole spin lifetimes ($t_S > 1$ ms), allowing for the possibility of spin-coherent transport from ferromagnetic electrodes to the recombination zone of a bilayer organic LED. It is important to distinguish this spin-dependent exciton formation and luminescence from other various magnetic field effects (MFE's) observed in the photoconductivity, photoluminescence, delayed luminescence and electroluminescence (EL) of certain organic crystals. We have grown a number of OLED's with magnetic and non-magnetic electrode materials based on a conventional Alq₃/NPB organic bilayer and report two magnetic field effects that are present in all devices. The first is a low field effect (LFE) consisting of a one to seven percent increase in EL with an applied field that typically saturates below 1000 Oersted (Oe). The second is a high field effect (HFE) consisting of an EL decrease by as much as 20+% at 1.8 Tesla (T). Unlike the LFE, the HFE is dependent on temperature, current density and electrode material. This suggests that the LFE and HFE are caused by separate mechanisms and that conditions near the electrode/organic interfaces are important to the HFE. We discuss these results in terms of several possible mechanisms, some of which should be sensitive to the spin-polarization of the injected holes and electrons.

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4:00pm **OF+EM-TuA7 The Application of DLC Layer for Polymeric Electroluminescent Devices**, *S.H. Choi*, Yonsei University, Korea; *D.W. Han*, Samsung SDI; *S.M. Jeong*, Yonsei University, Korea; *H.K. Baik*, Yonsei University, Korea, South Korea; *K.M. Song*, Kon Kuk University, Korea; *S.J. Lee*, Kyungsoong University, Korea

The Polymeric electroluminescent devices (PLEDs), which are included with an diamond-like-carbon (DLC) layer between indium tin oxide (ITO) and poly(styrene sulfonate)-doped poly(3,4-ethylene dioxythiophene) (PEDOT) have been fabricated. Indium diffusion, which is due to be etched ITO surface by acidic PEDOT solution into the hole transport layer can degrade the device. It has been used X-ray photoelectron spectroscopy (XPS), and Rutherford backscattering spectrometry (RBS) to measure indium contamination in PEDOT. DLC layer was deposited between hole transport layer and ITO anode by the using the Cs⁺ ion sputtered negative ion deposition system (CsISNIDS). It was found that device stability and efficiency were seriously affected by indium contamination in HTL and DLC layer could improve device stability. In addition it has been investigated the I-V, L-V characteristics, and Quantum efficiency as a function for a set of devices with and without DLC layer.

4:20pm **OF+EM-TuA8 Photonic Crystals and Nanocomposite Materials**, *J. Ballato*, *D. Carroll*, *S. Foulger*, Clemson University **INVITED**

The promise (some fact and some fanciful) of nanotechnology has led to a well funded global race to develop new materials, components, and devices for use in a remarkably diverse range of applications. Towards the true realization of commercial- and defense-relevant devices, this talk will focus on highly promising results on passive and active photonic devices whose performance is markedly improved, with respect to traditional analogs, through the use of nanocomposite materials. Specifically to be discussed are highly efficient organic light emitting diodes (OLEDs) and photovoltaics (OPVs) fabricated using doped and undoped carbon nanotube-containing conjugated polymers. All-organic photonic crystals based on ordered arrays of nanoparticles encapsulated in elastomeric matrices also will be discussed. These nanocomposites exhibit bandstops that are highly tunable though stain generated by mechanical forces (mechano-chromism) or chemical affinity (chemo-chromism) which opens new doors for optical beam steering and chemical sensing.

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Electronic Materials and Devices

Room Hall A-C - Session EM+SC-TuP

Poster Session

EM+SC-TuP2 A New Method to Produce Silicon-on-Insulator Wafer-Ar@super +@ Implantation with H@super +@-plasma Processing, B. Chen, New Jersey Institute of Technology; *A. Usenko,* New Jersey Silicon Wafer Tech; *W. Carr,* New Jersey Institute of Technology

In this paper, we describe a new method to fabricate SOI wafer. Ar⁺ ions were implanted into Si(100) at energy ranging from 30 KeV to 200 KeV and dose from 1*10@super 15@ to 1*10@super 16@ cm@super -2@. To avoid amorphization, the samples were thermally insulated and the beam current was maintained high enough (about 3mA/cm²). After implantation, pieces of these samples were subjected to thermal annealing at temperature ranging from 200°C to 800°C. The evolution of microstructure of these samples were investigated by TEM. In the annealed samples, Argon clusters are found in either 2-D cavities (Nano-cracks) or 3D cavities (bubbles). Then, these samples were processed by H⁺ plasma. Nano-cracks and bubbles will help trapping H diffused from the surface. Then this hydrogenated wafer was bonded with the other oxidized wafer. After annealed at 600 °C, a thin layer will be transferred from the hydrogenated wafer to the oxidized one. In this way, we can get the thin layer SOI wafer.

EM+SC-TuP3 Effects of Remasking Materials and Dimensions on Sidewall Roughness of Deep Etched Waveguide, J.W. Bae, W. Zhao, J.H. Jang, I. Adesida, University of Illinois at Urbana Champaign; *A. Lepore, M. Kwakernaak, J.H. Abeles,* Sarnoff Corporation

Photonic devices and circuits based on InP/InGaAsP materials require optical waveguides with highly anisotropic and smooth sidewall profile to achieve good optical mode quality and low loss performance. In the fabrication of optical waveguides, critical factors include lithography, masking, and etching. Each factor introduces various degrees of sidewall roughness (SWR). The rough sidewall of waveguides causes scattering loss, which is one of the major sources of optical loss in deep etched waveguides. Therefore, the characterization of sidewall roughness for the various processes is required. In this study, the SWR of InP/InGaAsP heterostructures fabricated using inductively-coupled-plasma etching (ICP) was investigated as a function of the remasking materials and the dimensions of masks. Among the factors introducing SWR, lithography and etching conditions were fixed at optimum condition that was previously determined. Remasking materials including silicon dioxide and silicon nitride were deposited on NiCr (40 nm)/SiO₂@sub 2@ (600 nm) mask using plasma enhanced chemical vapor deposition. Also, the effects of thicknesses of NiCr mask layer and remasking materials on the SWR were investigated in the range from 40 to 100 nm and 25 to 100 nm, respectively. Atomic force microscopy (AFM) was utilized to directly measure the SWR of waveguides. Electron beam lithography was used to delineate specially designed line patterns that permitted AFM tips to be directly utilized to measure SWR. Results on SWR from various sources will be presented and discussed with relation to optical losses.

EM+SC-TuP4 Sub 100 nm Radius of Curvature Wide-Bandgap III-Nitride Vacuum Microelectronic Field Emitter Structures Sharpened by ICP Etching, P.B. Shah, M.D. Derenge, B.M. Nichols, T.S. Zheleva, K.A. Jones, US Army Research Laboratory

Nanometer scale tips make possible cold cathodes that when used in vacuum microelectronic (VME) devices bring together the advantages of high power that vacuum tubes provide with the advantages of instantaneous turn-on (no need for tedious warm up), miniaturization and long device lifetime. The advantage of gallium nitride (GaN) in these applications is its very small electron affinity (energy necessary to remove the electron from the material surface into vacuum.) Aluminum nitride (AlN) is even better because it may exhibit a negative electron affinity. For vacuum microelectronic devices we are developing field emitters using inductively coupled plasma (ICP) etching. This technique involves two steps, first, a fast deep etch to define columns of a given aspect ratio followed by etches to sharpen the columns. We investigate and optimized gas flow rates, etch times, gas pressures, ICP coil RF power, chuck RF power, and masking material. Advantages of this technique over other demonstrated techniques for producing GaN based field emitters such as selective area deposition are that it can be easily transferred to existing fabrication lines and that it allows for easy definition of complex VME device structures. Using an ICP etch high aspect ratio field emitters were

fabricated from MOCVD grown GaN exhibiting a tip radius of 80 nm and height of 900 nm. Currently we are optimizing the technique to achieve a smaller GaN tip radius. In parallel an etch process is being optimized to produce field emitter tips from AlN. Our presentation will discuss optimized etch chemistries and preliminary electrical performance along with surface passivation and cleanup techniques.

EM+SC-TuP5 A Study of Silicon Carbide (SiC) Etching Characteristics using Magnetized Inductively Coupled Plasmas (MICP), H.Y. Lee, D.W. Kim, Sungkyunkwan University, South Korea; *Y.J. Sung,* Samsung Advanced Institute of Technology, South Korea; *G.Y. Yeom,* Sungkyunkwan University, South Korea

SiC is an attractive material for electronic devices operating at high power levels and high temperatures. In addition, the large Si-C bonding energy makes the components made of SiC resistant to chemical attack and radiation, and thus attractive for the applications in harsh environments. SiC is also used as a substrate for microelectromechanical system (MEMS) and GaN epitaxial devices due to its excellent electrical, thermal, and mechanical properties. However, due to its stability and inertness of SiC in conventional acid or base solutions at normal temperatures, plasma-based etching plays an important role in patterning SiC for the fabrication of electronic devices. Optimum etch strategies for the fabrication of these devices demand excellent profile control, low ion-induced etch damage, smooth etch surfaces, and high etch rates. In this article we report on the SiC etching in SF₆ based discharges and the etch selectivity of SiC over various mask materials to obtain high etch rates and low surface damages. The etch characteristics such as etch rates, etch selectivities, and etch profiles in addition to the plasma characteristics were investigated as functions of source power, and dc bias voltage to the substrate, gas mixtures and applied external magnetic field strength.

EM+SC-TuP6 Electroless Copper Deposition as a Seed Layer on TiSiN Barrier, Y.C. EE, Z. Chen, S. Xu, Nanyang Technological University, Singapore; *L. Chan, K.H. See, S.B. Law,* Chartered Semiconductor Manufacturing Ltd., Singapore

Electroless deposition of copper as a seeding technology has received considerable attention in back-end-of-line device fabrication. This work explores the effects of plasmas processing parameters such as argon gas flow rate and nitrogen plasmas treatment time on the properties of electrolessly plated Cu on TiSiN barrier layers formed by a low-frequency inductively coupled plasma process. TiSiN films have emerged as a promising candidate for the future generation barrier material because of its good adhesion to Cu. The properties of deposited electroless copper were characterized by X-ray diffraction (XRD), four-point resistivity probe, atomic force microscopy (AFM) and field emission secondary electron microscope (FESEM). Comparison is made with the Cu seed layer on TiN. It is found that the required palladium activation time is greatly reduced on TiSiN. The results also show that there is a preferred crystal orientation of Cu in (111) plane. Cu grain size is within the range of 24-33 nm. The sheet resistance of the Cu seed layer is less than 1.2 @ohm@ per square area. The roughness of plated Cu layer largely follows the one of the underlying TiSiN. Good surface coverage of electroless Cu seed layer on TiSiN is obtained in our experiments.

EM+SC-TuP8 Thermal Conductivity Analysis of Highly-Oriented Diamond Films for Silicon on Diamond Electronic Applications, N. Govindaraju, North Carolina State University; *A. Aleksov,* North Carolina State University; *F. Okuzumi, G.N. Yushin,* North Carolina State University; *S.D. Wolter, J.T. Prater,* Army Research Office / AMSRL- RO-PM; *Z. Sitar,* North Carolina State University

The extremely high thermal conductivity of diamond (~ 22 W/cmK) along with its wide bandgap (5.3 eV) and high specific resistance (~10@super 12@ @ohm@cm) make it an alluring material for incorporation as a dielectric in Silicon On Diamond (SOD) technology. SOD offers enhanced thermal transport properties in addition to the speed and power enhancing properties offered by the traditional Silicon On Insulator (SOI) technology. As the single crystal growth of diamond on silicon proves elusive, the pragmatic approach would entail the use of Highly Oriented Diamond (HOD) films. It is imperative, for the proposed SOD technology, that the thermal properties be well characterized. The current study seeks to fulfill this requirement by measuring all aspects of thermal conductivity of HOD films. Commercially available thin wire thermocouples (Type K) were used in conjunction with a thin film heater to carry out steady state measurements using the traditional heated bar technique. Preliminary results indicated an average value of ~ 8 W/cmK for measurements done on free standing HOD films. To further refine the accuracy of the measured

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thermal conductivity, measurements using a thin film heater and thin film thermocouples were implemented. Studies by Graebner¹ have shown that grain size has a great impact on the thermal conductivity of randomly oriented polycrystalline diamond. Since it is known that the size of the columnar grains varies as a function of diamond film thickness, we studied thermal conductivity as a function of thickness. This was achieved by etching away the diamond using an argon-oxygen plasma and implementing the thermal measurements recursively. All thermal conductivity data has been measured as a function of temperature. @FootnoteText¹@footnote 1@J.E. Graebner, et. al., *Diamond and Related Materials*, 2 (1993), 1059-1063.

EM+SC-TuP9 Deposition and Field-Emission Characterization of Electrically Conductive Diamond-Like Amorphous Carbon Films, H. Kinoshita, R. Ikuta, K. Sakurai, S. Murakami, Shizuoka University, Japan

Diamond-like amorphous carbon films doped with nitrogen (DAC:N) were formed using intermittent supermagnetron plasma chemical vapor deposition (CVD) technique.¹ for the fabrication of high performance field emitters. DAC:N films were deposited on Si and glass wafers using $i-C_4H_{10}/N_2$ plasma to investigate the influence of discharge-off time, at lower-electrode temperature of 100°C, upper- and lower-electrode rf powers (UPRF/LORF) of 800W/100W, and electrode spacing of 40mm. Discharge-on time was 1min, and off time (cooling time) was controlled to 15sec-10min. With decrease of cooling time, resistivity was decreased. At cooling time of 15sec, however, DAC:N film was peeled off from a wafer by its plasma heating. By reducing the electrode spacing from 40mm to 20mm, resistivity and optical band gap of DAC:N film deposited at 800W/800W rf powers and 5min cooling time decreased to 0.11 Ω /cm and 0eV, respectively. A DAC:N film of 500Å thickness was deposited on a n-Si wafer at 850W/100W, and was patterned in many island shapes of 1 μ m x 1 μ m sizes. Using it, a threshold emission current density of 0.01mA/cm² was observed at the electric field of 12V/ μ m. At the electric field of 21V/ μ m, maximum field-emission current density (IMAX) of 3mA/cm² was observed at the electric field of 21V/ μ m. A flat DAC:N film of 700Å thickness was deposited on a n-Si wafer at 800W/800W. Using the flat DAC:N film, a threshold electric field of 18V/ μ m, and IMAX of 2.2mA/cm² was observed at the electric field of 32V/ μ m. @FootnoteText¹@footnote 1@H.Kinoshita and T.Murakami, *J.Vac.Sci.Tecnol.A* 20, (2002) 403.

EM+SC-TuP10 Avalanche Ballistic Electron Emission Microscopy (BEEM) Studies of Subthreshold BEEM Current and STM Induced Photocurrent, C. Tivarus, E.R. Heller, J.P. Pelz, The Ohio State University

We present Ballistic Electron Emission Microscopy (BEEM) studies where the metal is deposited directly over an avalanche pn diode. Because the avalanche diode provides a hot electron gain of up to many millions, intrinsic BEEM current noise levels as low as 20 aA are possible. Hence, this technique can be very useful in nm-resolution studies of electronic transport in structures that otherwise show very low ballistic current for traditional BEEM measurements. Using this technique we were able to accurately study the shape of the subthreshold regions of the BEEM current-voltage curves where all the BEEM current is due to thermally excited electrons above the Fermi level in the STM tip. One of the problems encountered when interpreting the measurements for this avalanche BEEM technique is the presence of the Scanning Tunneling Microscopy induced photo current (STM-PC). Since this STM-PC resembles a normal BEEM current, [E.R. Heller and J.P. Pelz, *Appl. Phys. Lett.* to be published] it can interfere with BEEM measurements of structures with low signal and/or intrinsic BEEM threshold voltage larger than the substrate bandgap. We have characterized this low signal STM-PC effect using the high photon sensitivity and large collector solid angle of the underlying avalanche diode and will discuss methods to distinguish true BEEM current from STM-PC.

EM+SC-TuP11 Submicron MTJ Cell Selectivity and Switching Field Analysis using Scanning Probe Microscopy Technique, D.S. Kim, J. Heo, I.S. Chung, SungKyunkwan University, Korea

It has been reported that in a Synthetic Anti Ferromagnet (SyAF) deposited MTJ bit, the demagnetizing magneto static domain will be diminished regardless of its size with a very low aspect ratio. Thus, the anisotropy ratio and the size of the MTJ (Magnetoresistance Tunneling Junction) cell can be reduced more. Scanning Probe Microscopy (SPM) analysis has great advantage in submicron MTJ bit characterization, since it does not need to make a MTJ contact. We have successfully attained the H-R curve using SPM under controlling external magnetic field for submicron scaled MTJ bits. Therefore, We made to investigate the issues in selectivity characteristics and switching field characteristics in terms of various

anisotropy ratio and sizes. We can attain the asteroid curve by applying both hard axis and easy axis magnetic field simultaneously either by rotating sample in diagonal or by applying current through write line. We found the newly introduced SPM diagonal field appliance method would be more efficient than conventional ones, in investigating a MTJ bit switching field characterization.

EM+SC-TuP12 The Analysis on the Origin of High Resistivity in Polycrystalline CdZnTe Thick Films, K.H. Kim, S.Y. Ahn, M.H. Kim, Y.J. Park, K.N. Oh, Korea University; S.U. Kim, Korea University, Korea

The CdZnTe have an inherently high stopping power, an excellent carrier transport property, and relatively wide band gap energy. Therefore detectors using this materials have the potential for sufficient X-ray sensitivity and DQE at a sufficiently low leakage current.¹ Although research results have been presented on single crystal CdTe and CdZnTe detectors with small sized silicon readout devices, it would be difficult to apply these results to large area flat-panel detectors. Alternatives of single crystal, we have grown large area (10 x 10 cm²) polycrystalline CdZnTe films by thermal evaporation method. The thickness, average grain size and Zn composition was 150 μ m, 3 μ m and 4%. Resistivity of CdZnTe films is in the order of 2 x 10⁹ Ω cm which is comparable that of CdZnTe single crystal samples. In X-ray detectors, high leakage current limits the maximum integration time of the a-Si array for X-ray imaging applications so that high resistivity receptor material is required. Recent reports have identified deep level defects which are likely to be associated with semi-insulating property.² Based on multiple trapping model, the localized state distributions of high resistivity polycrystalline CdZnTe from TOF (time of flight) transient current are examined using Laplace transform and Tikhonov regularization methods.³ We found 3 different deep localized states above valence band related to the resistivity. In TOF measurements, indium was used as top electrode to form Schottky type contact to prevent carrier injection. @FootnoteText¹@footnote 1@ S. Tokuda, H. Kishihara, S. Adachi, T. Sato, Y. Izumi, O. Teranuma, Y. Yamane, and S. Yamada, *Proceedings of SPIE Vol. 4682*, 30 (2002)²@footnote 2@ A. Zumbiehl, S. Mergui, M. Ayoub, M. Hage-Ali, A. Zerrai, K. Cherkaoui, G. Marrakchi, Y. Daricim, *Material Science and Engineering B* 71, 297 (2000)³@footnote 3@ J. Weese, *Comput. Phys. Commun.* 69, 99 (1992).

EM+SC-TuP13 Electrical, Thermal, and Elastic Properties of MAX Phase Materials, S.E. Lofland, P. Finkel, J.D. Hettinger, Rowan University; M.W. Barsoum, A. Ganguly, S. Gupta, Drexel University; K. Harrell, J. Palma, B. Seaman, Rowan University

We have characterized physical properties of several materials in the MAX phase family.¹ These materials derive their name from the basic chemical formula $M_nA_{n-1}X$, where M is an early transition metal, A is an A-group element, and X is either N or C. These highly conductive ceramics are readily machinable and possess very desirable structural properties.¹ From a systematic study of the transport properties, we find most of these materials require two conduction bands, one consisting of holes and the other of electrons, to explain the electrical conductivity, Hall coefficient, and magnetoresistance. A Wiedemann-Franz analysis of the thermal conductivity suggests that, in most of the materials investigated, the mean-free-path of the entropy carriers is the same as that for the charge carriers. The Lorenz number at room temperature indicates that the thermal conductivity is mostly electronic in nature. We have also performed heat capacity and speed of sound measurements on many of the MAX phase materials allowing the extraction of the elastic moduli and Debye temperatures. We find very good agreement between the Debye temperature as determined from specific heat and that determined from elastic measurements. We find that the electronic term in the specific heat depends strongly on the transition metal element and very weakly on the A-group element. In general we find that the transition metal element impacts the electrical properties more dramatically than the A-group element. In contrast, the A-group element seems to more strongly impact the elastic properties of the materials. The justification for these statements will be presented. This work was supported by the New Jersey Commission on Higher Education, the NSF under grants DMR-0072067 and DMR-0114073 and Rowan University. @FootnoteText¹@footnote 1@M. W. Barsoum, *Prog. Solid State Chem.* 28, 201(2000).

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EM+SC-TuP14 Photo-electronic Properties of n-ZnO:Al/p-Si Heterojunctions, F. Mohammed, A. Pontarelli, S. Bokhari, J.R. Doyle, Macalester College

We present a study of the photo-electronic properties of n-ZnO:Al/p-Si heterojunctions. Transparent conducting ZnO:Al layers having resistivities $< 1 \times 10^{-3} \text{ ohm-cm}$ and transparencies of about 80% are deposited on p-Si using reactive dc magnetron sputtering. In some devices a higher resistance ZnO:Al buffer layer was inserted between the highly conducting ZnO:Al and silicon. The junctions are characterized by dark current-voltage measurements as a function of temperature (IVT), capacitance-voltage measurements (CV), spectral response measurements, and conversion efficiency. Excellent rectification is obtained, with soft breakdown voltages typically in the range of 3-5 V reverse bias. Analysis of the IVT characteristics imply that the carrier transport is mainly tunneling limited, and the CV measurements imply a barrier height of about 1 eV. The presence of the buffer layer has no systematic effect on the dark junction characteristics. However, the buffer layer devices exhibited a significantly enhanced spectral response and efficiency, with the best devices resulting in a 3% conversion efficiency under 100 mW/cm² white light illumination. Possible roles of the buffer layer in enhancing the photoresponse will be discussed, as well as the potential application of these devices as photodetectors and solar cells.

EM+SC-TuP15 Effects of Threading Dislocations and In Composition on Structural and Optical Properties in InGaN/GaN Triangular-shaped Quantum Wells, R.J. Choi, Y.B. Hahn, H.J. Lee, Chonbuk National University, Korea

Structural and optical properties of InGaN/GaN multiple triangular quantum well (QW) structures have been studied with different threading dislocation (TD) densities and wavelengths (or In compositions). As the In composition increased, the extent of variation of the linewidth of photoluminescence (PL) measurements increased over a temperature range of 13 - 300 K. The structural quality of the quantum wells is not consistent with the PL intensity. More fluctuation of the local In composition and severer degradation of PL intensity at a higher TD density were observed, which were attributed to the stress field created by the dislocations. Observations by X-ray diffraction, transmission electron microscopy, and monochromated scanning cathodoluminescence imaging revealed that the optical property of the InGaN/GaN triangular-shaped MQWs is greatly affected by structural imperfections.

EM+SC-TuP16 Electroluminescence in the Infrared Region from Thin Film Zinc Sulfide Doped with Rare Earth Fluorides, D. DeVito, N. Shepherd, A.S. Kale, W. Glass, M.R. Davidson, P.H. Holloway, University of Florida

While electroluminescent phosphors are routinely studied for flat panel display technology, infrared emission is often ignored. A variety of applications exist for infrared emitters, including chemical analysis, infrared displays, communications and therapeutic medical treatment. Thin film electroluminescent devices could serve as highly efficient, reliable, rugged infrared emitters. Electroluminescence in high-field devices is generated by impact excitation and subsequent radiative relaxation by electronic transitions located on the luminescent centers. Rare earth elements, including erbium, terbium and holmium, are good choices for luminescent centers as they exhibit many transitions ranging from visible (550 nm) to the mid-infrared wavelengths (5 micron), as will be documented with experimental data from ZnS films deposited by RF planar magnetron sputtering. Among these, holmium is particularly interesting because of transitions at 1210 nm, 1400 nm, 2.9 micron, 4.8 micron and 5 micron. Suppression of emission at visible wavelengths and enhanced infrared emission by selective processing of sputter deposited films is achieved through proper selection of annealing temperature. Optimum luminance at characteristic wavelengths was developed by the appropriate choice of luminescent center and activator concentration, deposition temperature and annealing conditions. Low temperature device measurements are presented to evaluate the effects of room temperature on the number of energy transitions and energy transfer mechanisms in thin film devices.

EM+SC-TuP17 Visible and Near-infrared Electroluminescence from Er-doped GaN Thin Films Prepared by RF Planar Magnetron Sputter Deposition, J.H. Kim, M.R. Davidson, N. Shepherd, P.H. Holloway, University of Florida

Erbium (Er)-doped GaN thin films were prepared by radio frequency (RF) planar magnetron co-sputtering of a commercial GaN target and a metallic Er target in a pure nitrogen atmosphere. The alternating-current thin-film electroluminescent (ACTFEL) devices were fabricated using a standard half-stack configuration with an Al metal electrode, GaN:Er electroluminescent

layer, ATO (Al₂O₃-TiO₂) dielectric, and ITO (indium-tin-oxide) transparent conducting electrode. Visible and near-infrared (NIR) EL emission peaks were observed from the fabricated devices at 530, 550, 660, 1000, and 1550 nm. These emissions were attributed to the Er³⁺ 4f-4f intrashell transitions from the ²H_{11/2}, ⁴S_{3/2}, ⁴F_{9/2}, ⁴I_{11/2}, and ⁴I_{13/2} excited-state levels to the ⁴I_{15/2} ground-state, respectively. GaN host films had a wurtzite polycrystalline structure with a preferred orientation in the [0001] direction perpendicular to the film surface. Full width at half maximum (FWHM) of the (0002) wurtzite-GaN diffraction peak and the lattice constant, c both increased from 0.38° to 0.45° and from 5.18 Å to 5.205 Å, respectively, as the Er concentration in GaN host was varied from 0 to around 5 at.%, indicating that incorporation of larger Er atoms into GaN host expands the host lattice. The optimum concentration of Er was determined to be around 1 at.% for both of the green 530 nm and NIR 1550 nm emissions.

Contacts to Organic Materials Topical Conference Room Hall A-C - Session OM-TuP

Poster Session

OM-TuP1 Study of Surface Photovoltage Effects in Doped Organic Molecular Thin Films, C. Chan, W. Gao, A. Kahn, Princeton University

We investigate photoemission-induced surface photovoltage (SPV), i.e. non-equilibrium resulting from photoexcitation and separation of carriers, in organic films. We focus on electrically doped molecular films that exhibit interface depletion regions¹ and can sustain charge separation and SPV. We combine ultraviolet photoemission spectroscopy (UPS) to measure the HOMO and vacuum levels under illumination, and contact potential difference (CPD) measurement with a Kelvin probe to measure the vacuum level in the dark. Zinc phthalocyanine (ZnPc) and N,N'-diphenyl-N,N'-bis(1-naphthyl)-1,1'-biphenyl-4,4'-diamine (α-NPD) p-doped with the acceptor molecule, tetrafluorotetracyanoquinodimethane (F₄-TCNQ), are investigated.^{1,2} UPS and CPD measurements are performed as a function of film thickness deposited on Au. CPD measurements reproduce with excellent accuracy the UPS-observed shifts of the molecular energy levels, in particular through a depletion region ~30-50Å near the metal-organic interface of the doped organic films. The excellent agreement shows that: (1) efficient p-doping occurs even in the dark in these two organic systems; (2) SPV is negligible in both doped and undoped organic films. The undoped films do not have depletion regions where charge separation can occur. In the doped films, electrons separated in the interface depletion region recombine in the metal before generating significant SPV, whereas the holes readily recombine throughout the film.¹ ² W. Gao and A. Kahn, Organic Electronics 3, 53 (2002) ² W. Gao and A. Kahn, J. Appl. Phys. (accepted for publication; July 1, 2003).

OM-TuP2 Adsorption of PTDCDA on Si(100), B. Grandidier, T. Soubiron, J.P. Nys, M. Dubois, C. Delerue, D. Stievenard, IEMN-CNRS, France

Submonolayer coverages of perylene-tetracarboxylic-dianhydride (PTCDA) molecules have been investigated with scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS). At low coverage, comparisons between the STM images and calculations of the electronic structure of the molecule show that the molecule adsorbs mostly in a planar configuration with its axis parallel to the Si dimers. Different configurations are observed and associated with physisorbed and chemisorbed states of the adsorbates. At higher coverage, X-ray measurements indicate that only a fraction of the molecules are chemisorbed and that the bonding occurs through the dicarbonyl functional groups, preserving the pi-conjugation of the molecules. While PTCDA selectively reacts with the Si dimers, steric hindrance is found to be the major cause to hamper the formation of an ordered film.

OM-TuP3 Potential Imaging of Metal-organic Semiconductor Interfaces using Kelvin Probe Force Microscopy, O. Tal, Tel Aviv University, Israel; W. Gao, L. Friedman, A. Kahn, Princeton University; Y. Rosenwaks, Tel Aviv University, Israel

Understanding and improving the performance of organic electronic devices depends, to a great extent, on the elucidation of organic materials interfaces with inorganic and organic solids alike. Therefore these

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interfaces are the focus of this work. We present a study of two dimensional (2-D) potential profiles across metal-organic film interfaces (metal- Au or Al, organic film - tris(8-hydroxyquinolino) aluminum [Alq@sub 3@]) with nanometer spatial resolution provided by Kelvin probe force microscopy (KPFM) in a nitrogen environment. The contact potential difference (CPD) is measured across Al/Alq@sub 3@/Al, Au/Alq@sub 3@/Au and Au/Alq@sub 3@/Al sandwich-like structures following cleavage under the inert atmosphere. The CPD profiles are in a very good agreement with vacuum level profiles estimated by calculation, which are based on ultraviolet photoemission spectroscopy (UPS) measurements. Preliminary measurements of these structures and "device-type" structures under operating conditions will be presented and discussed. This work is the first step in providing a new and unique type of information on the electronic structure of metal-organic and organic-organic interfaces, as determined by KPFM and additional techniques.

OM-TuP4 Conductive Core-Shell Nanoparticles: An Approach to Self-Assembled Mesoscopic Wires, G. Kaltenpoth, M. Himmelhaus, Universität Heidelberg, Germany; L. Slansky, Daimler-Chrysler AG, Germany; F. Caruso, University of Melbourne, Australia; M. Grunze, Universität Heidelberg, Germany

Conductive core-shell nanoparticles were prepared by coating negatively charged monodisperse polystyrene (PS) latex spheres with a thin layer of polyethyleneimine (PEI). Subsequently, gold colloid with 3 nm in size was electrostatically adsorbed onto the PEI-coated spheres, and finally, an electroless gold plating step was repeatedly carried out to yield a high gold coverage and thus a conductive gold shell. The metallic behavior was investigated by XPS and UV-vis. In the XPS Au4f peak, a shift due to charging effects was observed at low metal coverage, which decreased with increasing gold decoration, and vanished with the formation of a conductive metal shell. The UV-vis spectra show a coverage-dependent shift and broadening of the Au plasmon resonance. The self-assembly of the metal coated spheres into continuous lines was investigated to explore the applicability of such particles to realize self-assembled electrical circuits. It was found that the particles selectively adsorb to the carboxyl-terminated areas of line patterns fabricated by microcontact printing of alternating carboxyl- and methyl terminated alkanethiolates on gold.

OM-TuP5 The Enhancement of Passivation Effect and Long Time Stability on Aluminum Cathode Deposited by Adatom Mobility Enhancing Technique in Organic Electroluminescent Display, S.M. Jeong, W.H. Koo, S.H. Choi, Yonsei University, Korea; S.J. Lee, Kyung Seong University, Korea; K.M. Song, Kon Kuk University, Korea; H.K. Baik, Yonsei University, Korea, South Korea

Highly stable and electroluminescent devices based on spin-coated PPV thin films have been achieved. The improvement of lifetime is derived from aluminum cathode deposited by adatom mobility enhancing technique. There are much less pinhole defects because of fine grain size caused by high surface mobility and contact area between Al and PPV increase. It is believed that the passivation effect and minimizing thermal degradation is induced by much less pinhole defect and large contact area between Al and PPV.

OM-TuP6 Hole-injection and Transport in Arylamines Films Sandwiched between Metal Contacts, G. Szulczewski, J. Li, K.-Y. Kim, J. Sun, S.C. Blackstock, University of Alabama

We have synthesized a series of electron-rich arylamines to systematically control their electronic properties, i.e. dipole moment and ionization potential. Films of these molecules were made by solution and/or vapor deposition techniques on Ag and Au substrates and characterized by cyclic voltammetry and x-ray photoelectron spectroscopy. We have measured current-voltage curves of monolayer and multilayer films to study hole-injection and transport. We find that these molecules rectify current under forward bias above a threshold voltage. A plot of the threshold voltage against the measured electrochemical oxidation potential yields a straight line with an excellent correlation coefficient, $R = 0.98$, and slope greater than unity. We will discuss how the molecular properties influence charge-injection at the metal-molecule interface. We acknowledge the National Science Foundation for support of this work through the Materials Research Science and Engineering Center grant # DMR0213985.

Electronic Materials and Devices Room 321/322 - Session EM-WeM

Multifunctional Electronic Materials

Moderator: C.J. Palmstrom, University of Minnesota

8:20am EM-WeM1 Peter Mark Memorial Award Address: Epitaxial Complex Oxide Heterostructures: Electrostatic Modulation of Correlated Electron Behavior, C.H. Ahn¹, Yale University INVITED

Complex oxide materials exhibit a tremendous diversity of behavior, including phenomena that have only been observed in oxides, such as high temperature superconductivity. An even richer spectrum of possibilities becomes available if one combines different complex oxides in epitaxial thin film form to create artificially structured, heterogeneous systems. One can use such materials to electrostatically modulate correlated electron behavior, including superconductivity and magnetism, without introducing chemical or structural disorder. It is also possible to combine complex oxides, such as ferroelectrics, with semiconductors to explore new functionality in semiconducting systems.

9:00am EM-WeM3 MBE Growth and Properties of Fe-, Cr- and Mn-doped TiO₂ Rutile and Anatase, S.A. Chambers, S. Thevuthasan, T. Droubay, S.M. Heald, C.M. Wang, A.S. Lea, V. Shutthanandan, Pacific Northwest National Laboratory; J. Osterwalder, University of Zurich, Switzerland; Y.J. Kim, Hanbat National University, Korea; R.P. Sears, B. Taylor, B.S. Sinkovic, University of Connecticut

Room temperature ferromagnetism in Co-doped anatase TiO₂ has inspired a number of experimental and theoretical efforts. A high Curie point, good electron mobility, and optical transparency are attractive for use in spin electronics and optoelectronics. A natural question concerns the use of other magnetic dopants. Combinatorial doping of anatase and rutile with Sc, V, Cr, Mn, Fe, Ni, Cu using laser ablation by Matsumoto et al. reveal that only Co-doped anatase is ferromagnetic. However, DFT calculations by van Schilfgaarde for Cr, Mn, Fe and Co in anatase predict that Co, Cr and Fe make the material ferromagnetic, whereas Mn is antiferromagnetic. We are currently exploring Fe and Cr as dopants in MBE-grown TiO₂ rutile and anatase, and plan to investigate Mn in the near future. The substrates for rutile and anatase films are rutile TiO₂(110) and LaAlO₃(001), respectively. Films were characterized with RHEED, XPS, XPD, XAS, EXAFS, XMCD, AFM, SAM, TEM and MOKE. Cr and Mn are more likely to substitute for Ti in rutile than Fe because CrO₂ and MnO₂ exhibit rutile structures that are reasonably well lattice matched to TiO₂. No such phase exists for Fe. Moreover, CrO₂ is a half-metallic ferromagnet in the bulk. Cr indeed substitutes for Ti in the rutile lattice, and assumes a +3 formal oxidation state for doping levels of a few atomic percent. The first films have been found to be antiferromagnetic. In contrast, attempting to dope rutile with Fe leads to secondary phase Fe₃O₄. Fe(II) and Fe(III) are present, as expected if Fe₃O₄ is present. In addition, these films exhibit magnetic hysteresis and circular dichroism, but these signals are presumably due to the presence of minority phase Fe₃O₄. Cr exhibits a +3 oxidation state and substitutes for Ti for doping levels of a few atomic percent in anatase. Magnetic measurements of these films are pending at the time of writing of the abstract.

9:20am EM-WeM4 Unusual Behavior of Electrical Conductivity and Thermopower Found in Mn_{1.68}X@Cu_{0.6}X+Y+Z@Co_{0.24}Y@Ni_{0.48}Z@O₄ Thin Films, F.S. Ohuchi, J.G. Moyer, D.A. Kukurznyak, M.S. Prowse, University of Washington

The thermopower, S , and electrical conductivity, σ , are measured on variations of a reference composition, Mn_{1.68}X@Cu_{0.6}X+Y+Z@Co_{0.24}Y@Ni_{0.48}Z@O₄. Doped compositions show parallel increases or decreases in conductivity and thermopower magnitude unlike typical band-gap conducting materials. This is desirable for increasing the efficiency parameter called the power factor, $S\sigma$, for thermoelectric applications. While thermopower varies by as much as 30%, the conductivity changes by up to a factor of four in the compositions explored. Conduction is attributed to small polaron hopping between neighboring Mn ions. Thin films are obtained through Metal Organic Decomposition processing. This is a low-temperature fabrication route that allows for the retention of meta-stable

Mn⁴⁺ and Cu¹⁺ ions that are essential to favorable electronic behavior. Compositional variations modify the Mn³⁺, Mn⁴⁺, Cu¹⁺, and Cu²⁺ concentrations, and in turn change the conductivity and thermopower. Supplemental XPS work defines changes in Cu oxidation states and oxygen content, and thermopower data provides Mn oxidation state information. Using the Heikes and Nernst-Einstein transport models we explain the seemingly incongruent behavior in thermopower and conductivity and identify that the discrepancy occurs in the conductivity factor. The nature of the unusual conduction behavior will be discussed.

9:40am EM-WeM5 Using Strain to Control Microwave Tunability and Loss in Barium Strontium Titanate Thin Films, S.W. Kirchoefer, W. Chang, J.A. Bellotti, J.M. Pond, Naval Research Laboratory; D.G. Schlom, Pennsylvania State University INVITED

Barium strontium titanate thin films exhibit an electric field dependent dielectric constant which can be exploited for tunable microwave devices. This technology has been of limited applicability due to the relatively high dielectric losses that typically accompany high tuning. The control of dielectric loss is of critical technological importance. Manipulation of deposition conditions and film impurities have been investigated widely as means for achieving improved films. Engineered film strain is an additional material parameter that can be controlled toward these ends, and this talk will report on experiments that demonstrate the advantages of both strain minimization and strain enhancement on the microwave properties of barium strontium titanate and strontium titanate thin films. It will be shown that the structural distortion caused by film strain results in decreased dielectric constant and tuning for compressive strain and increased corresponding values for tensional strain at room temperature. These results can be understood by examining the effects of lattice distortion on Curie temperature. A model based on thermodynamics and strain-induced polarization will be presented. The effects of strain on dielectric losses and device quality factor will also be discussed. Results from substrate mismatch strain and film annealing studies will be presented. Ongoing efforts to measure effects of extrinsic strain induced by externally-applied pressure will be discussed.

10:20am EM-WeM7 Displacive Phase Transition in SrTiO₃ Thin Films Grown on Si(001), F.S. Aguirre-Tostado, CINVESTAV-Querétaro, México, Mexico; A. Herrera-Gómez, CINVESTAV-Querétaro, México; J.C. Woicik, National Institute of Standards and Technology; R. Droopad, Z. Yu, Motorola; D.G. Schlom, Pennsylvania State University; J. Karapetrova, P. Zschack, University of Illinois and Argonne National Lab; P. Pianetta, Stanford Synchrotron Radiation Laboratory

Polarization dependent x-ray absorption fine structure and x-ray diffraction have been used to study the local structure in SrTiO₃ thin films grown epitaxially on Si(001). For films less than a critical thickness of ~ 80 Å, a splitting of the Ti-O distance perpendicular to the interface is observed: $r_{\text{Ti-O}} = 1.87 \pm 0.02$ Å and $r_{\text{Ti-O}} = 2.09 \pm 0.06$ Å, whereas only a single Ti-O distance is observed within the plane of the interface: $r_{\text{Ti-O}} = 1.95 \pm 0.01$ Å. These findings indicate that the in-plane compressive strain imposed on the SrTiO₃ layer by the Si substrate results in a tetragonal plus displacive ferroelectric distortion of the SrTiO₃ cubic unit cell. This study therefore suggests the existence of a Curie "thickness" for strained-layer, epitaxial perovskite growth.

10:40am EM-WeM8 Dielectric Response of Asymmetric KNbO₃/KTaO₃ Superlattices, J. Sigman, H.J. Bae, D.P. Norton, University of Florida; J.D. Budai, P.H. Fleming, L.A. Boatner, Oak Ridge National Laboratory

The K(Ta,Nb)O₃ perovskite is an interesting paraelectric/ferroelectric system with tunability of the dielectric response with applied electric field. Pulsed laser deposition (PLD) has been used to achieve atomic layer-by-layer growth in KTaO₃/KNbO₃ superlattices. Previously, a symmetric 1 unit cell x 1 unit cell KTaO₃/KNbO₃ was grown on KTaO₃(100) and its dielectric response and structural properties were studied. Increasing capacitance with increasing applied dc bias for temperatures just below the structural transition was observed and suggested an antiferroelectric response. We have investigated several asymmetric KTaO₃/KNbO₃ superlattices to provide further elucidation on this anomalous dielectric response. This positive tunability appears to be a function on the thickness the KNbO₃ layer. Above three unit cells of KNbO₃, the positive tunability disappears. Below three unit cells of KNbO₃, the

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positive tunability is seen in the same temperature region as the 1×1 superlattice, regardless of the Nb:Ta thickness ratio.

Electronic Materials and Devices

Room 310 - Session EM+SC+OF-WeA

Future Issues in Electronics and Optoelectronics

Moderator: C.R. Eddy, Jr., Naval Research Laboratory

2:00pm **EM+SC+OF-WeA1 Materials Issues in Solid-State Lighting, J.Y. Tsao**, Sandia National Laboratories **INVITED**

A quiet revolution is underway. Over the next 10-15 years inorganic-semiconductor-based solid-state lighting (SSL) technology is expected to outperform first incandescent, and then fluorescent and high-intensity-discharge, lighting. Nevertheless, SSL is in its infancy, and significant challenges must be met for SSL to achieve its potential for general white lighting. In this talk, we give an overview of these challenges, and of the prospects for overcoming them. We will focus especially on challenges related to the wide-bandgap AlGaInN family of materials: increasing their electrical-to-optical power conversion efficiency, and increasing their range of emitted colors. And, where possible, we will try to connect these challenges to fundamental physical properties, including: high piezoelectric coefficients, high dopant and exciton ionization energies, high microscopic internal strain and chemical immiscibility, and large differences between the bond strengths of the product materials and the chemical precursors used to grow them. @FootnoteText@ @footnote 1@J.Y. Tsao, Ed., "Light Emitting Diodes (LEDs) for General Illumination Update 2002" (Optoelectronics Industry Development Association, Washington D.C., 2002); A. Zukauskas, M.S. Shur, and R. Caska, "Introduction to Solid-State Lighting" (Wiley and Sons, New York, 2002); and M.R. Krames, H. Amano, J.J. Brown, and P.L. Heremans, Eds., Special Issue on High-Efficiency Light-Emitting Diodes, IEEE Journal of Selected Topics in Quantum Electronics, Vol. 8, Issue 2 (Mar-Apr 2002).

2:40pm **EM+SC+OF-WeA3 Organic Light Emitting Diodes as a Source of Light for General Illumination, M. Stolka**, Consultant **INVITED**

Organic Light Emitting Diodes (OLEDs) have a potential to become a technology of choice for general illumination of commercial and residential buildings. There exist no fundamental obstacles to achieve the required power efficiency (>>100 lm/W), lifetime (>50,000 hrs), and the quality of emitted white light with high rendition index. OLEDs will be ten times more energy efficient as incandescent, and twice as efficient as fluorescent lamps. Recent discovery that triplet excitons can be harvested to produce photons with nearly 100% internal quantum efficiency represents a major breakthrough towards achieving the goal. Based on a spin statistics, only 25% of excitons are singlets, which were thought to be the only excitons capable of relaxing the energy as photons, by fluorescence. The remaining 75% of the excitons in triplet states were considered ineffective since the energy, gained by recombination of charges, is typically dissipated as heat. This was thought to impose a 25% fundamental limit on the internal quantum efficiency of photon generation. It was found that phosphorescent emitters, such as complexes of Pt or Ir, enable the utilization of triplet excitons as sources of photons as well. High energy efficiency, flexibility, conformability to any shape and form, light weight, distributed nature of the light sources, and the ability to emit any color including white are the main attractive features of OLEDs. However, significant challenges still remain. The outcoupling efficiency has to be increased beyond the current ~20%. The stability, especially of blue emitters, has to be improved. Better protection against the access of moisture has to be found, etc., etc. Strategies for increasing the power efficiency, increasing the lifetime of OLEDs, and methods of obtaining white light will be discussed.

3:20pm **EM+SC+OF-WeA5 Future Issues in Spintronics, M.E. Flatté**, University of Iowa **INVITED**

Metallic spintronics, the control of electrical signals through the flow of spin-polarized current, has progressed from a research discovery in 1988 to a key information technology and commercial success. Almost every computer now contains at least one spintronic device - such as the read head for a hard disk drive. Encouraged by this success researchers have explored other material systems, especially those of semiconductors. New possibilities available from semiconductor spintronics include high-speed coupling of spin dynamics to light (optospintronics), nonlinear transport and gain (spin transistors), exceptionally long spin coherence times, and electrical control of ferromagnetism. Progress in these areas has been rapid, and has led to new perspectives on the optical and electrical manipulation or detection of information stored in magnetic systems.

Quick summary examples of such new physical and material functionality within semiconductors will be shown. Semiconductor spintronics, however, cannot do without metallic magnetism, for metals provide an exceptional combination of high conductivity and high Curie temperatures. New spintronic devices probably will depend on hybrid structures, where each component is chosen for optimal properties from metallic, inorganic semiconducting, and organic semiconducting materials.

4:00pm **EM+SC+OF-WeA7 Growth and Applications of Epitaxial Metal-semiconductor Nanocomposite Structures, A.C. Gossard, M. Hanson, D. Driscoll**, University of California, Santa Barbara **INVITED**

We explore the growth and overgrowth of nanoscale semi-metallic islands in GaAs-based semiconductors. MBE-grown ErAs and ErSb islands grow epitaxially and coherently on the semiconductor surfaces with particle dimensions that are controlled by the deposition growth parameters. The islands can be overgrown with epitaxial semiconductors, and further layers of islands and semiconductor films can be grown to form superlattices of layers of metallic islands. The distribution of islands governs the electrical and optical properties of the nanocomposites, including Fermi level position, carrier mobility, photocarrier lifetimes, plasma properties, barrier formation and carrier tunneling.

4:40pm **EM+SC+OF-WeA9 Electronic Devices from Single Crystal CVD Diamond, J. Isberg**, Uppsala University, Sweden; *D.J. Twitchen, G.A. Scarsbrook, A.J. Whitehead, S.E. Coe*, Element Six Ltd., UK **INVITED**

Diamond is well known as being the hardest of all materials making it useful in various mechanical applications. Perhaps less well known are the extreme electronic and thermal properties of diamond, which have raised considerable speculation over its usefulness as a semiconductor material in a number of applications. The high charge-carrier mobilities, dielectric breakdown field strength and thermal conductivity of high purity diamond makes it especially well suited in devices where high frequencies are required in combination with high power, high temperatures, or high voltages. Nevertheless, despite more than two decades of research, the breakthrough of diamond-based electronics has not yet happened, largely due to the difficulty of synthesising free-standing, high-quality, single crystal diamond. We will describe recent advances in growing single crystal intrinsic and boron doped diamond intended for electronic applications. The material was grown under conditions of extreme purity, resulting in films of exceptionally low defect densities. In the intrinsic material we have measured room temperature drift mobilities of 4500 cm²/Vs for electrons and 3800 cm²/Vs for holes. These mobility values were determined by using the time-of-flight technique on thick intrinsic diamond plates. The high values for the electron and hole mobility, as well as a measured carrier lifetime in excess of 2 @mu@s, indicates a huge improvement in the electronic quality of free-standing, single crystal chemical vapor deposited (CVD) diamond. At present commercially available electronic applications of diamond include UV and radiation detectors, X-ray dosimeters, photoconductive switches and surface acoustic wave (SAW) filters. These applications are mainly based on undoped diamond. We argue that even the lack of a shallow n-type dopant does not stop diamond from having an impact in high power and high frequency electronics because effective unipolar devices such as schottky diodes and MESFETs can be made. Many difficulties concerning the fabrication of diamond devices remain to be solved and a number of process technologies need to be developed such as reliable ion-implantation, etching, annealing, surface termination and contact fabrication technologies. However, the improvement in the electronic quality of diamond indicate that the potential of single crystal CVD diamond as a wide bandgap semiconductor is substantial and will eventually allow the expansion of the boundaries of device technology. @FootnoteText@ J. Isberg et al., Science, 6 Sept, 297 (2002) p1670.

Electronic Materials and Devices

Room 321/322 - Session EM-WeA

Diamond/Contacts to SiC

Moderator: J.P. Pelz, The Ohio State University

2:00pm **EM-WeA1 Electron Transport Mechanisms in Thin B-doped CVD Diamond Films, J.E. Yater, A. Shih, J.E. Butler, P.E. Pehrsson**, Naval Research Laboratory

Diamond possesses unique bulk and surface properties that can be exploited for electronic device applications. Of particular interest, diamond is a promising cold emitter material for vacuum electron devices because of

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the negative electron affinity (NEA) observed at specific surfaces. In this study, we use electron transmission measurements to examine the electron transport characteristics of NEA diamond. Specifically, we inject conduction electrons into thin CVD diamond films using a 0-20 keV electron gun, and we measure the intensity and energy distribution of low-energy electrons transmitted through the films. In measurements from films of varying thickness (0.15-5.0 microns) and B concentration, we observe two distinct transmission distributions. One distribution is consistent with emission from the diamond conduction band, with an energy spread of about 0.7 eV (although in some cases the distribution is affected by the doping properties). Transmission yields (i.e. number of transmitted electrons produced by each incident electron) are measured as high as 2-5 in this regime. The other distribution has an energy spread of about 3 eV with associated yields that are very low (~0.05). This distribution exhibits characteristics that are consistent with emission from graphitic material, and the energy distribution is relatively insensitive to the doping properties. An analysis of the data suggests that electron transport along graphite-containing grain boundaries is the primary transport mechanism when the electron escape distance is greater than 1 micron, while conduction band transport becomes increasingly dominant for transport distances less than 1 micron.

2:20pm EM-WeA2 On the Peculiarity of Depletion Layer in Diamond pn-junction, Y. Koide, National Institute for Materials Science (NIMS), Japan

The p-type Diamond has been easily obtained by doping with boron, and high-quality p-type diamond film was often grown on (100) diamond substrates by a microwave plasma-assisted chemical vapor deposition (MPCVD) technique. Recently, a growth method fabricating undeniable n-type diamond films was established by the MPCVD technique. The fabrication of the pn-junction structure widened a possibility of application of diamond to electronic and photonic devices. Therefore, understanding of characteristics of diamond pn-junction is our mandatory. Dependence of temperatures on carrier densities measured by Hall effect provided the ionization energies of P donor and B acceptor to be as large as 600 meV and 370 meV, respectively. Since both the dopants have deep nature, characteristics of the pn-junction are predicted to be very different from that of pn-junction which involves shallow dopants. The purpose of the present paper is, as a first step to understand the pn-junction physics of diamond, to analyze the deep dopant effect of the pn-junction involving deep P donor and B acceptor. The theoretical analysis will predict a limit of performance of diamond bipolar transistor, in which the deep nature of donor and acceptor will play an important role. The analysis of space charge and carrier profiles in the pn-junction was simply carried out by solving one-dimensional Poisson equation including compensation and carrier distribution. Profiles of ionized dopants and carriers in pn-junction of diamond with deep phosphorus donor and boron acceptor were calculated. Widths of depletion layer were around two times longer than those of space charge layer since there existed a transition region at the depletion layer edge. The difference between both the widths was reduced with increasing temperatures. It was predicted that a static saturation property of bipolar pnp-junction transistor was affected by the deep nature of dopants.

2:40pm EM-WeA3 Highly Conductive N-type Ultrananocrystalline Diamond: Materials Properties and Devices, J.E. Gerbi, O. Auciello, J. Birrell, Argonne National Laboratory; S. Curat, University College London, UK; D.M. Gruen, Argonne National Laboratory; R.B. Jackman, O.A. Williams, University College London, UK; J.A. Carlisle, Argonne National Laboratory

Ultrananocrystalline diamond (UNCD) is a fine-grained (3-5 nm) diamond material. Synthesized by MPECVD using Ar-rich Ar/CH₄ plasmas, the electronic, structural, and tribological film properties of UNCD can be tailored by doping with a controlled amount of N₂. These changes correspond with clear transformations in the film structure, as both the grain size and grain boundary width of the UNCD films increase with nitrogen doping. In addition, we hypothesize that modifications in the bonding of the grain boundaries themselves occur. Together, these changes result in an n-type, highly conductive film that can retain the excellent tribological and structural properties of undoped UNCD. The conduction mechanism of nitrogen-doped UNCD is different than that of single-crystal diamond, with specific nitrogen-carbon and dangling bond complexes in the grain boundaries playing a crucial role. In this work, we discuss this unique conduction mechanism in the context of the UNCD film structure and growth process. We present recent device fabrication results and new Hall measurement results, performed with a field switching setup at variable temperatures, which provide incontrovertible evidence of the n-type conduction and significant mobilities of this material. For example, a

film grown with the relatively low nitrogen doping level of ~ 0.2 at.% displays an electron carrier concentration of ~ 5 x10¹⁷ cm⁻³ and a mobility of greater than 6 cm²/Vs, while retaining the excellent tribological, chemical, and structural characteristics necessary for conductive MEMS/NEMS and bioelectronics applications. Films with much higher conductivities and doping concentrations can also be produced; doping levels as high as 1.1 at. % N will also be discussed in the context of thin-film diamond electronics. This work was supported by the DOE-Office of Science-Materials Science under Contract No. W-31-109-ENG-38.

3:00pm EM-WeA4 Raman Spectroscopy of Ultrananocrystalline Diamond Thin Films, J. Birrell, J.E. Gerbi, O. Auciello, Argonne National Laboratory; J. Johnson, X. Xiao, Argonne National Laboratory, U.S.; J.A. Carlisle, Argonne National Laboratory

Raman spectroscopy is often used as an efficient and non-destructive way of determining the bonding structure of diamond thin films. However, interpretation of the Raman spectrum of carbon materials with small grain sizes and a large number of grain boundaries, such as in nanocrystalline, ultrananocrystalline (UNCD), and amorphous diamond, is not straightforward. In order to correctly interpret the Raman spectral features of UNCD thin films, a series of films spanning the range of structures from microcrystalline to UNCD was studied using visible and UV Raman spectroscopy, as well as scanning and transmission electron microscopy. For UNCD, we find that although the sample has been found to be composed of ~95% sp³-bonded carbon by other techniques including near-edge adsorption fine structure (NEXAFS) and TEM, none of the spectral features observed using visible Raman spectroscopy can be attributed to sp³-bonded carbon. As the UNCD grains appear purely crystalline in TEM, we identify the disordered carbon at the grain boundaries of UNCD as responsible for all spectral features observed. This enables us to probe the grain boundary structure of UNCD specifically, which is of great utility for understanding the electronic and structural properties of the material. Finally, we interpret the changes in the Raman spectra of UNCD grown under various growth conditions, including low temperature growth; as well as with nitrogen doped UNCD, which results in a large increase in the conductivity of UNCD films. This work was supported by the DOE-Office of Science-Materials Science under Contract No. W-31-109-ENG-38.

3:20pm EM-WeA5 Silicon on Diamond Technology, A. Aleksov, N. Govindaraju, F. Okuzumi, G.N. Yushin, North Carolina State University; S.D. Wolter, J.T. Prater, Army Research Office / AMSRL- RO-PM; Z. Sitar, North Carolina State University

The roadmap for the development of Si-based high-speed low-power electronics for digital applications shows that Moore's law predicting an exponential increase in the speed operation of digital ICs will remain valid in the near future, yielding ever shrinking devices and larger integration scales, necessitates a decrease of the supply voltage to limit the loss power and an increase in the complexity of heat management. Silicon on Diamond (SOD) is proposed as an alternative to SOI to overcome the severe thermal limitations imposed by SOI, but at the same time retain the advantages of SOI in respect to increased device speed and carrier confinement. SOD technology is beneficial for both digital Si-applications as well as for high-power high-frequency Si-devices. This technology utilizes the unique physical properties of diamond i.e. the highest thermal conductivity (up to 22 W/cmK) and a high specific resistance (10¹² Ωcm range). In our SOD approach, the insulating layer is a highly-oriented diamond (HOD) film with bulk-like properties, which can be grown on large area Si substrates. Following the diamond growth, another Si wafer is bonded to the diamond in UHV at a pressure of around 32 MPa and a temperature of 950°C. The bonded Si wafer is then thinned to the desired thickness. The bonded interface has been studied by TEM and EELS to assess structural and chemical character of the interface, respectively. Metal strip heater devices fabricated on SOD samples confirm the heat spreading efficiency of the diamond layer and benefits of SOD. For comparison, the same device structures have been fabricated on a SOI wafer. The experimental results are accompanied by finite element thermal simulations of the experimental set ups enabling the direct comparison of theoretical and experimental data.

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3:40pm **EM-WeA6 Metallizing a Semiconductor Surface with Hydrogen**, *P.G. Soukiasian, V. Derycke*, Commissariat à l'Energie Atomique, France; *F. Amy, Y.J. Chabal*, Agere Systems; *M. D'angelo, H. Enriquez, V.Yu. Aristov, M. Silly*, Commissariat à l'Energie Atomique, France; *M. Pedio, P. Perfetti*, Istituto di Struttura della Materia, Italy

Passivation of semiconductor surfaces against chemical attacks can be achieved by terminating the surface-dangling bonds with a monovalent atom such as hydrogen. Such passivation has invariably leads to the removal of all surface states in the band gap, and thus to the termination of non-metallic surfaces. Here, the first observation of semiconductor surface metallization induced by atomic hydrogen is reported. This surprising result, established using atom resolved scanning tunneling microscopy (STM) and spectroscopy (STS), core level and valence band photoelectron spectroscopy (XPS,UPS) and multiple reflection infrared absorption spectroscopy (MR-IRAS) is achieved on the Si-terminated 3C-SiC(100) 3x2 cubic silicon carbide surface. The metallization is evidenced through band gap closing in STS, Fermi level built-up in UPS and specific related spectral features in MR-IRAS. In addition, core level photoemission spectroscopy using synchrotron radiation gives fine details about interatomic charge transfers within the surface and sub-surface regions. The metallization process results from competition between hydrogen termination of surface dangling bonds and hydrogen-generated steric hindrance below the surface. Understanding the ingredient for hydrogen-stabilized metallisation directly impacts the ability to eliminate electronic defects at semiconductor interfaces critical for microelectronics, provides means to develop electrical contacts on high band-gap chemically passive materials, particularly exciting for interfacing with biological systems, and gives control of surfaces for lubrication, e.g. of nanomechanical devices. @FootnoteText@ @footnote 1@ V. Derycke, P. Soukiasian, F. Amy, Y.J. Chabal, M. D'angelo, H. Enriquez and M. Silly, Nature Materials 2, 253 (2003).

4:00pm **EM-WeA7 Macroscopic and Microscopic Electronic Behavior of Cubic Inclusions in 4H-SiC**, *K.-B. Park, Y. Ding, J.P. Pelz*, The Ohio State University; *K.C. Palle, M.K. Mikhov, B.J. Skromme*, Arizona State University; *A. Los, M.S. Mazzola*, Mississippi State University

Double-stacking-fault cubic inclusions in n-type 4H-SiC@footnote 1@ were studied with ballistic electron emission microscopy (BEEM) in ultra high vacuum where the inclusions intersect a Pt/SiC Schottky barrier (SB) interface. We confirmed prior proposals@footnote 2@ that the inclusions behave as quantum wells, and found a propagating two-dimensional quantum well conduction band minimum (CBM) at ~0.53 eV below the CBM of the bulk 4H-SiC host. This agrees well with calculations of the quantum well state@footnote 3@ and is close to the SB height lowering found with macroscopic I-V and C-V measurements.@footnote 4@ The macroscopic C-V SB heights were found to be quite similar to macroscopic I-V measurements, which is interesting because less than 5% of the Pt/SiC interface is on the low-barrier-height inclusions. We believe this similarity between C-V, I-V, and BEEM measurements can be explained by the actual SBH of the inclusions at the Pt/SiC interface, along with changing occupation of the quantum well states away from the interface during C-V measurements. We are currently developing electrostatic modeling to quantify this hypothesis. We will also discuss the first "hole BEEM" measurements of SiC on a Pt/p-type 4H-SiC (presently without inclusions) SB interface. We found a 1.40 eV p-type SB height, compared with 1.54 eV of Pt on n-type 4H-SiC, as well as a double threshold, suggesting a possible second valence band maximum. @FootnoteText@@footnote 1@R. S. Okojie, M. Zhang, P. Pirouz, S. Tumakha, G. Jessen, and L. J. Brillson, Appl. Phys. Lett. 79, 3056 (2001).@footnote 2@T. A. Kuhr, J. Q. Liu, H. J. Chung, M. Skowronski, and F. Szmulowicz, J. Appl. Phys. 92, 5863 (2002).@footnote 3@H. Iwata, U. Lindefelt, S. Oberg, and P. Briddon, J. Phys. C 14, 12733 (2002).@footnote 4@B. J. Skromme, K. Palle, C. D. Poweleit, L. R. Bryant, W. M. Vetter, M. Dudley, K. Moore, and T. Gehoski, Mater. Sci. Forum 389-393, 455 (2002).

4:20pm **EM-WeA8 Improved Titanium / Nickel Ohmic Contacts on N-Type 4H Silicon Carbide**, *J.H. Park, P.H. Holloway*, University of Florida

Nickel (Ni) contacts are the most commonly used ohmic contacts to n-type silicon carbide (SiC). Unfortunately, the Ni contacts exhibit rough interface morphology after high temperature annealing. In addition, the reaction to form the silicide liberates carbon, which can segregate to the metal-semiconductor interface. These two factors limit the reliability of the Ni contacts to n-SiC for high temperature and power applications. The electrical and structural properties of electron-beam evaporated nickel/titanium metal contacts to n-type 4H SiC were studied by current-voltage (I-V), Auger electron spectroscopy (AES), secondary ion mass

spectrometry (SIMS) and X-ray diffraction (XRD) techniques. Nickel/titanium metal contacts on the 4H SiC were rectifying as deposited but turned to ohmic after rapid thermal annealing (RTA) at 1000°C for 2 minutes in nitrogen. The nickel/titanium contacts were converted to the layer sequence of titanium carbide/nickel silicide/SiC by annealing. This structure had a low specific contact resistance of $10 \times 10^{-5} \text{ @ohm@cm@super 2@}$. A shallower and smoother nickel silicide/SiC interface was obtained as compared to the conventional only-nickel contacts. The nickel silicide layer was formed on SiC by a nickel-SiC reaction during high temperature annealing which left excess carbon at the interface between the silicide and SiC. Titanium reacted with the carbon to form a titanium carbide layer on the nickel silicide, which led to reduced carbon excesses at the interface and lower resistance of the ohmic contacts. The phase inverting mechanisms and the effects of nickel/titanium thickness on this process have been studied. Phase analysis of the nickel silicides and titanium carbides using XRD and TEM will be reported.

4:40pm **EM-WeA9 Correlation Between Electrical and Microstructural Properties of Low Resistance TiAl-based Ohmic Contacts to p-type 4H-SiC**, *S. Tsukimoto, K. Nitta, M. Moriyama, M. Murakami*, Kyoto University, Japan

In order to understand a contact formation mechanism for TiAl-based contacts, the electrical properties and microstructure of conventional Ti/Al and recently developed Ni/Ti/Al ohmic contacts to p-type 4H-SiC were correlated. The Ti/Al and Ni/Ti/Al ohmic contacts were prepared by depositing sequentially Ni, Ti, and Al on the SiC substrates doped with Al at $4.5 \times 10^{18} \text{ @cm@super -3@}$, and subsequently annealing in an ultra high vacuum at 1000°C for 2min and 800°C for 10min, respectively. These contacts provided the lowest contact resistances of $1 \times 10^{-5} \text{ @ and } 7 \times 10^{-5} \text{ @ohm@-cm@super 2@}$, respectively. X-ray diffraction and cross-sectional transmission electron microscopy were used to identify reacted layers formed at the ohmic contacts/SiC interfaces. For the Ti/Al contacts, ternary $\text{Ti}_{0.3}\text{SiC}_{0.2}$ compound layers with a hexagonal structure were formed to grow epitaxially on the substrates. For the Ni/Ti/Al contacts, hexagonal $\text{Al}_{0.4}\text{C}_{0.3}$ compound layers were also formed to grow epitaxially on the SiC in addition to other binary compounds. The formation of these epitaxial carbide layers was found to have a strong influence on the contact resistances to the SiC, and was essential to prepare low resistance TiAl-based contacts. The present experiment indicated that both the $\text{Ti}_{0.3}\text{SiC}_{0.2}$ and the $\text{Al}_{0.4}\text{C}_{0.3}$ layers played a role of intermediate semiconductor layers (ISL) between p-type SiC and the contact metals, which reduced the barrier height and/or depletion region.

Electronic Materials and Devices Room 321/322 - Session EM-ThM

Materials for Interconnects and Contacts to Semiconductors

Moderator: S.E. Mohnhey, The Pennsylvania State University

8:20am **EM-ThM1 Self-aligned Silicides for Ohmic Contacts in CMOS Technology: TiSi@sub 2@, CoSi@sub 2@ and NiSi, S.-L. Zhang, KTH, Sweden**
INVITED

Metal silicides have played an indispensable role during the remarkable developments of microelectronics since PtSi was first used to improve the rectifying characteristics of diodes in early 1960's. Along with several other technological innovations, the implementation of the self-aligned silicide (SALICIDE) technology has paved the way for rapid and successful miniaturization of device dimensions for metal-oxide-semiconductor field-effect transistors (MOSFETs) keeping in pace with the Moore's law. The primary use of silicides has also evolved from creating reliable contacts for diodes, to generating high-conductivity current paths for local wiring, and lately to forming low-resistivity electrical contacts for MOSFETs. With respect to the choice of silicides for CMOS technology, a convergence has become clear with the self-alignment technology using only a limited number of silicides, namely TiSi@sub 2@, CoSi@sub 2@ and NiSi. The present work discusses the advantages and limitations of TiSi@sub 2@, CoSi@sub 2@ and NiSi with the development trend of CMOS technology as a measure. Specifically, the reactive diffusion and phase formation of these silicides in the three terminals of a MOSFET, i.e. gate, source and drain, are analyzed. This work ends with a brief discussion about future trends of metal silicides in micro/nanoelectronics with reference to the potential material aspects and device structures outlined in the International Technology Roadmap for Semiconductors.

9:00am **EM-ThM3 Ni-Si Thin Films Reactions at Low Temperatures: Phase Identification and Sequence Characterization, C. Coia, École Polytechnique de Montréal, Canada; C. Lavoie, IBM Research; M. Tremblay, École Polytechnique de Montréal, Canada; C. Detavernier, F.M. d'Heurle, IBM Research; P. Desjardins, École Polytechnique de Montréal, Canada**

The phase formation sequence upon thermal annealing of 5 to 20-nm-thick Ni layers on Si(001) has been investigated using a combination of in-situ synchrotron x-ray diffraction (XRD), diffuse elastic light scattering, and electrical resistance complemented by post-annealing transmission electron microscopy and XRD analyses. In addition to the generally reported Ni@sub 2@Si, NiSi, and NiSi@sub 2@ phases, we observe the formation of several metal-rich silicide compounds at low temperatures. The complete sequence is identified as Ni-Ni@sub 31@Si@sub 12@-Ni@sub 2@Si-Ni@sub 3@Si@sub 2@-NiSi-NiSi@sub 2@ with the possible brief appearance of Ni@sub 3@Si preceding Ni@sub 31@Si@sub 12@. The sequence observed for Ni reaction with B- and P-doped Si(001) starts at higher temperatures and occurs over a narrower range in temperature than for undoped Si(001), n-doping having a stronger influence thus showing the larger increase in temperature. Quantitative analyses of XRD peak intensities during isothermal anneals are used to determine rate limiting mechanisms and reaction kinetics. In complementary experiments, 200-nm-thick single-phase layers were obtained for each of the stable phases present in the Ni-Si binary phase diagram in order to determine their physical and chemical properties. The phase formation sequence in these thicker layers of fixed composition suggests that the phases still grow sequentially with the first phase being the Ni@sub 31@Si@sub 12@.

9:20am **EM-ThM4 Development of Ohmic Contact Materials for Compound Semiconductors, M. Murakami, M. Moriyama, S. Tsukimoto, Kyoto University, Japan**
INVITED

Compound semiconductors have been extensively used in a variety of devices which Si semiconductor cannot function. Although wide gap compound semiconductors are attractive for light emitting diodes, ultraviolet laser diodes, and high frequency and/or high power devices, lack of reliable, low resistance ohmic contact materials for these compound semiconductors hinders development of these devices. Our studies on ohmic contacts for GaAs, SiC, and diamond (although not compound semiconductor) indicated that formation of an intermediate semiconductor layer (ISL) which reduced the barrier height and/or the width of the depletion region (formed at an interface between the contact metal and the semiconductor) was essential to prepare low resistance ohmic contacts. Thus, once key materials for ISL formation was found, reduction

of the contact resistance was obtained in these contacts by annealing at an optimum temperature. However, materials to form ISL could not be found for InP, ZnSe, GaN, and InGaN. For these semiconductors, not only search of materials to form ideal ISL's by reacting with these compound semiconductors should be continued, but also another contact formation mechanism should be explored. Our recent activities for ohmic contact formation mechanisms for various compound semiconductors will be reviewed.

10:00am **EM-ThM6 Indium-Based Ohmic Contacts to n-Type Gallium Antimonide, J.A. Robinson, S.E. Mohnhey, The Pennsylvania State University**
Antimonide based compound semiconductors are promising for a variety of optoelectronic and electronic devices. For some of these devices, shallow ohmic contacts to n-type GaSb are required. Among the ohmic contacts that have been developed for this semiconductor, indium-bearing contacts have provided the lowest specific contact resistances. These contacts offer the possibility of lowering the band gap of the semiconductor and the barrier height at the metal/semiconductor interface through the formation of InGaSb near the metal/semiconductor interface. However, no studies have been reported demonstrating indium-bearing contacts that remain very shallow, penetrating only tens of nanometers into the semiconductor. Furthermore, the surface morphology of these contacts can be poor due to In agglomeration. Using Pd and In, we are engineering shallow In-based contacts with improved surface and interfacial morphology. To achieve this goal, we are combining an investigation of the phase equilibria in the relevant multi-component systems and an understanding of the kinetics of reaction at the Pd/GaSb interface. In this presentation, we describe the formation of newly identified ternary phases in the Pd-Ga-Sb system, the kinetics of reaction at the Pd/GaSb interface, and the formation of ohmic contacts containing Pd and In on n-type GaSb ($n = 2.8 \times 10^{18} \text{ cm}^{-3}$). By choosing the proportions of Pd and In with guidance from multi-component phase diagrams and by minimizing the sheet resistance of the metallization itself, we have achieved to date contact resistances as low as .085 ohm-mm and specific contact resistances as low as $2 \times 10^{-6} \text{ ohm-cm}^{-2}$.

10:20am **EM-ThM7 Long and Short Term Thermal Stability of Gate Metallizations on GaN/AlGaIn/GaN Heterostructures, E.D. Readinger, S.E. Mohnhey, Penn State University; R. Therrien, Nitronex Corp.**

The III-nitride family of semiconductors is expected to provide devices for a variety of high power/high temperature applications, but only a few reports have addressed the thermal stability of gate metallizations for high electron mobility transistors (HEMTs) designed for these applications. This study examines two different forms of thermal stability. First, high temperature rapid thermal processing (RTP) commonly used for ohmic contact formation is used to identify candidates for gate metallizations that could be deposited prior to the anneal of source and drain ohmic contacts. Second, long-term anneals at moderate temperatures to accelerate the aging of HEMTs have been performed. A GaN capped Al@sub 0.23@Ga@sub 0.77@N/GaN heterostructure was used; the metallizations Re, Pt, Au, Ni, Ni/Au, Ni/Ga/Ni and Co were tested; and current-voltage curves were evaluated. Aside from Au and Pt which begin degrading above 400°C, the contacts exhibited neither improvement nor degradation after annealing for 60 s at 600°C. All the metallization schemes degrade above 600°C; however, Re showed marked improvement at 800°C for 60 s, returning to the as-deposited condition. The same metals were evaluated for long times at 425°C and 550°C. Although the commonly used Ni/Au contacts did not provide the lowest reverse currents among the metals tested, they do provide great stability at either temperature for at least 4 weeks. Rhenium exhibits improvement with respect to reverse currents after long times at 425°C, whereas most other contacts either degrade or remain stable. Materials characterization of the contacts will also be presented.

10:40am **EM-ThM8 Compositional Shift in Al@sub x@Ga@sub 1-x@N Induced by Reaction with Metallic Thin Films, B.A. Hull, E.D. Readinger, S.E. Mohnhey, The Pennsylvania State University; U. Chowdhury, R.D. Dupuis, The University of Texas at Austin**

The increasing use of AlGaIn in group III nitride devices calls for further advances in our understanding of the chemistry of contacts to this alloy semiconductor. Interfacial reactions between the metals Ni, Pd or Au and Al@sub x@Ga@sub 1-x@N ($0.15 < x < 0.6$) have been studied for annealing temperatures of 250 to 900°C. X-ray photoelectron spectroscopy indicates that the Al to Ga ratio within the Al@sub x@Ga@sub 1-x@N directly beneath the contact metal increases, in some cases dramatically. Elemental profiles across the interfaces of annealed Ni/Al@sub 0.47@Ga@sub

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0.53@N samples obtained by scanning transmission electron microscopy confirm the Al-enrichment near the interface. The Al-enrichment is consistent with thermodynamic modeling, which indicates that the AlGa_N composition is favored to shift towards the more stable of the two binary nitride components (AlN). Less severe annealing conditions result in smaller compositional shifts; however, a very narrow annealing temperature range (750°C to 825°C) was required to induce extensive compositional shifts (greater than 5% increase in x), regardless of the initial Al_xGa_{1-x}N composition, indicating that extensive reaction is limited by the slow diffusion of Ga and Al within the AlGa_N rather than the thermodynamic driving force for reaction. These compositional shifts can be expected to significantly impact the electrical properties of contacts annealed at high temperature due to the strong dependence of the band gap and Schottky barrier height on the AlGa_N composition. We have correlated these reactions to the electrical characteristics of annealed ohmic contacts to p-type AlGa_N as well as the thermal stability of Schottky contacts to n-type AlGa_N.

11:00am **EM-ThM9 Low Temperature Chemical Vapor Deposition and Characterization of Ultra-thin Ruthenium for Copper Diffusion Barriers in ULSI Interconnects**, *Q. Wang, Y.-M. Sun, D. Gay, J.M. White, J.G. Ekerdt*, University of Texas at Austin

Ultra-thin ruthenium (Ru) films covering Ta were investigated as part of a Cu diffusion barrier with enhanced adhesion of Cu that potentially enables seedless Cu plating on the barrier surface in ULSI interconnect processes. A low temperature thermal chemical vapor deposition (CVD) of ultra-thin Ru films on Ta and SiO₂ surfaces using ruthenium carbonyl [Ru₃(CO)₁₂] as a precursor was developed. Films deposited at substrate temperatures between 423 and 593 K were characterized using in-situ X-ray photoelectron spectroscopy (XPS), atomic force microscopy and in-situ four-point probe resistance measurements. A pure Ru ultra-thin film with low resistivity of ~50 μΩ/cm was deposited without any reactive gas at temperatures as low as 423 K. In-situ ion scattering spectrometry and Ta 4f XPS peak attenuation indicated that the minimum thickness to form a continuous Ru film on Ta is ~2.5 nm. The pure Ru film also showed good thermal stability at elevated temperatures (up to 593 K). This Ru film also inhibited oxidation of the Ta film when the sample was exposed to air. Compared with poor wettability of Cu on Ta, only ~0.3 nm of Cu fully covers Ru indicating excellent wetting.

11:20am **EM-ThM10 Evaluating Ruthenium Thin Film Deposited on Silicon as a Directly Plate-able Cu Diffusion Barrier**, *O. Chyan*, University of North Texas; *T.G. Hurd*, Texas Instruments; *R.M. Wallace, M.J. Kim, R. Chan, T. Arunagiri*, University of North Texas

Tantalum (Ta) and tantalum nitride (Ta_N) bilayer diffusion barrier is currently used in the fabrication of 130 nm integrated circuits to ensure the electrical integrity of the copper interconnects. Thin Ta/Ta_N are too resistive to plate Cu effectively, additional Cu-seed layer is deposited on Ta/Ta_N to carry the required current for copper electrofill. However, the Cu-seed/Ta/Ta_N tri-layer configuration will encounter severe scaling difficulties at the 45 nm node where ultra-thin barrier is need to minimize effects on interconnect resistivity. In this paper, we explore using ruthenium (Ru) as a new Cu diffusion barrier to afford direct Cu plating without the additional Cu-seed layer. Ru is an air stable transition metal with high melting point (2310 C) and is nearly twice as thermally and electrically conductive as Ta. More importantly Ru, like Ta, shows negligible solid solubility with Cu even at 900 C. The preparation and interfacial characterization of Cu thin film on both Ru metal surface and Ru thin film (<10 nm) sputtered on silicon wafer substrate will be discussed. Both dry (magnetron sputtering) and wet (electrodeposition) preparation routes were employed to deposit Cu on Ru. We will present un-published results that demonstrate efficient Cu plating (over 95% efficiency) was achieved on a ~8 nm an ultra-thin film of Ru metal deposited on silicon wafer. The nucleation and growth of Cu deposited layer on Ru was studied by the current transient techniques. The Cu deposited Ru thin film samples (Cu/Ru) were characterized by XPS, SEM, AFM. XRD and SIMS depth profiling. The observed direct Cu-plating on the ultra thin Ru film with excellent adhesion and the effective barrier performance properties based on SIMS depth-profiling and sheet resistance measurements underscores the potential of Ru as an effective direct plate-able Cu diffusion barrier for the advanced 65 and 45 nm nodes.

11:40am **EM-ThM11 ZrB₂ Diffusion Barriers: Conformal CVD Below 400 °C**, *E.J. Klein, D.-Y. Kim, S. Jayaraman, G.S. Girolami, J.R. Abelson*, University of Illinois at Urbana-Champaign

Transition metal diborides are classified as "metallic ceramics" due to their high mechanical hardness, chemical stability, melting temperature > 3000 °C and low electrical resistivity. This combination of properties makes them attractive as diffusion barrier materials for the contact metallization in next-generation microelectronics or to wide bandgap semiconductors. We report the low temperature and fully conformal chemical vapor deposition of ZrB₂ thin films with essentially bulk properties. The ZrB₂ films are deposited at substrate temperatures of 200-500 °C using the single-source precursor Zr(BH₄)₄ and a concurrent flux of atomic hydrogen produced by a remote hydrogen plasma source. The films have a B/Zr atomic ratio of 2 and electrical resistivity < 40 μΩ/cm; those produced at < 400 °C appear amorphous in X-ray diffraction. By contrast, films grown without the use of atomic hydrogen are B-rich, oxidize rapidly in air, and have high resistivity; these problems were typical of previous attempts to deposit ZrB₂ films reported in the literature. In this work, we study the diffusion barrier characteristics of ZrB₂ by annealing a sandwich structure of evaporated Cu (50 nm) / amorphous ZrB₂ (20 nm) / c-Si(100) [both n- and p-type]. For various annealing temperatures, we report the contact resistivity, stress, and micromorphology. Initial results show that no Cu diffuses into Si during annealing up to 650 °C for 30 minutes; the onset of Cu in-diffusion correlates with the appearance of crystalline X-ray diffraction peaks for ZrB₂. We will discuss the failure mechanism of the barrier material.

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