

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. Siringhaus*, 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. Szysoev, 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 threshold-less 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 $0.1 \text{ cm}^2/\text{V}\cdot\text{sec}$.

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 $10^2 \text{ S}\cdot\text{cm}^{-1}$. 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

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shadow-mask patterned layers of gold, alumina and pentacene. TFT mobilities greater than 2 cm²/Vs were measured and propagation delays 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 cm x 6 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.

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 ($\tau_s > 1$ 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 Oersteds (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.

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 dioxathiophene) (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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Poster Session

OF-TuP3 Real Time Observation of Surface Stress during Dithiol Adsorption in Gas Phase, A.N. Itakura, National Institute for Materials Science, Japan; *R. Berger*, Max Planck Institute for Polymer Research, Germany; *S. Igarashi*, Japan Science and Technology Corporation, Japan; *M. Kitajima*, National Institute for Materials Science, Japan
Self-assembled monolayers (SAM) such as alkanethiol, HS-(CH₂)_n-SH on Au induce compressive surface stresses during the self-assembly, and the saturation value of the stress is proportional to the length of alkyl chain. We observed the compressive stress for dithiol HS-(CH₂)_n-SH for n=6,8,10, adsorption on Au in gas phase. Contrary to the alkanethiol adsorption, the saturation value of the compressive stress showed smaller value for longer alkyl chain. The compressive stress for dithiol adsorption may be induced by the bonding between S and Au substrate. Dithiol adsorbs on Au surface as a lie-down phase, while alkanethiol as a standing phase. Density of the S-Au bonds should be lower for longer chain of dithiol, resulting in the reduction of the stress. @FootnoteText@ @footnote 1@ A.N.Itakura, R.Berger, T.Narushima and M.Kitajima, Appl.Phys.Lett.80, 3712 (2002)

OF-TuP4 XPS Studies of Charge Transfer between Dye Molecules and Polymer Chains in Dye Molecule Doped Conducting Polymer Films, H. Kato, S. Takemura, Kanto Gakuin University, Japan

Conducting polymer polythiophene (PT) films incorporated with dye molecules such as methylene blue (MB), safranin T (ST) and brilliant green (BG) were prepared by electrochemical doping and diffuse injection methods. Polymeric structure, charge transfer and interaction between the dye molecule and PT polymer chain in the hybrid films were closely investigated by analyzing the core-level energies and spectral profiles of the atomic components. Vibrational states of the doped dye molecule and polymer backbone were also investigated by FTIR RAS and ATR in order to examine the dopant configuration into polymer chains. XPS measurements clarified the identification of doping species into the polymer chains varied with synthetic methods and conditions. Dye molecules such as MB, ST and BG were doped in polymer films as two types of states such as cation-like and salt-like. In the case of BG, XPS core-level analysis of S 2p split indicates simultaneous doping of BG cation and HSO₄⁻ in the hybrid films prepared by electrochemically reduced and dye diffused injection methods. The higher binding energy peak corresponds to HSO₄⁻ while lower binding energy peak can be assigned to the S sites of polymer backbone. Synthesized film samples were categorized into two types by the difference of S 2p core-level energy shift. In the cation-like doped sample, the energy shift of the lower peak of S 2p suggests the charge transfer between BG molecules and polymer chains creating a n-type conducting polymer state. The relation between dopant species with different configuration and dopant-chain charge transfer will be also discussed.

OF-TuP5 XPS Studies of Organic-Inorganic Interface Interaction between Conducting Polymer Chains and Si Sublayers, H. Kato, S. Takemura, Kanto Gakuin University, Japan

Conducting polymer polythiophene (PT) and polypyrrole (PP) films were grown on Si substrates. PT/Si and PP/Si interfaces were fabricated by electrochemical method. Thin polymer film growth was obtained by controlling the applied voltage to the anode Si wafer in an electrochemical cell. Obtained film thickness was thin enough to be penetrated by XPS measurement to detect the organic-inorganic interface. Polymer chain configuration was also investigated by FTIR. XPS measurements were conducted closely investigating the core-level energies and spectral profiles of the atomic components. An affinity between a deposited polymer film and a Si substrate was strong compared with the case of film growth on metal oxide substrates such as ITO and SnO₂. Si 2s and 2p core-level spectra which were basically composed of different Gaussian components reflect different valence states of Si interacting with upper polymer layers in comparison with the core-level spectra of non-deposited Si substrate expecting bonds between polymer chains and Si substrate layers. The lower binding energy peaks observed in Si 2p spectra of PT/Si correspond to the Si states with strong interaction between Si and PT suggesting Si-C and Si-F bonds created at the PT/Si interface. In addition to the organic-inorganic bonding, the polymer chain configuration was also investigated

by FTIR. The polymer chain orientation on a Si substrate will be discussed comparing with the data obtained by RAS and ATR techniques detecting ring stretching modes of the polymer chain. The polymer chain linkage which reflects symmetric and asymmetric vibration modes will be also discussed.

OF-TuP6 Vibrational Spectroscopy and Charge Transport Characteristics of Metal-Molecule-Metal Junctions, J.L. Lazorcik, J.G. Kushmerick, R. Shashidhar, Naval Research Laboratory

We report the current-voltage characteristics and inelastic electron tunneling spectra of self-assembled monolayers in a crossed-wire tunnel junction. Inelastic electron tunneling spectroscopy (IETS) enables in situ vibrational characterization of metal-molecule-metal junctions. The well defined spatial orientation of molecules in a self-assembled monolayer enables the selection rules for IETS to be explored. Results for an insulating alkane-thiol and two @pi@-conjugated molecular wires, oligo(phenylene ethynylene) and oligo(phenylene vinylene), will be presented.

OF-TuP7 Photolithographically Defined Micropatterned Organosilane Monolayer as a Template Surface for Guided Self-Assembly of Charged Microparticles, A. Takahara, T. Koga, M. Morita, H. Otsuka, Kyushu University, Japan

Two-dimensional arrangement of microparticles on the substrate surface might be a promising method to fabricate functional materials. In this study, micropatterned fluoroalkylsilane/aminosilane monolayer was prepared as a template surface for site-specific arrangement of sulfonated polystyrene (PS) microparticles. Micropatterning of organosilane monolayer was carried out by area-selective irradiation of vacuum ultraviolet-ray through the photomask. Si wafer substrates with micropatterned organosilane monolayer were then exposed to the dispersed aqueous solution of sulfonated PS microparticles. Atomic force microscopic (AFM) observations revealed that the PS microparticles were area-selectively adsorbed onto the aminosilane phase. The site-specific adsorption of PS microparticles onto the aminosilane phase was ascribed to the electrostatic interaction between sulfonic acid groups of PS microparticles and amino groups of aminosilane phase. The height of adsorbed PS microparticles is in good agreement with the diameter of PS microparticle. This result suggested that the sulfonated PS particles formed a monolayer on the substrate surface. This consideration was supported by the result of adhesion force measurements. Adhesion force measurements clearly showed the specific interaction between sulfonic acid group of cantilever tip and amino group of aminosilane patterned surface. Compared with fluoroalkylsilane phase, strong adhesion force was observed on the aminosilane phase. On the other hand, very weak adhesion force originated from repulsive interaction was observed between sulfonic acid group of cantilever surface and that of PS microparticles. It is considered that the micropatterned surface prepared by present method can be applied for area-selective arrangement of two kinds of microparticles onto the substrate surface.

OF-TuP8 Electrical and Optical Characteristics of Indium Tin Oxide Thin Films Deposited by an Oxygen Beam Assisted Deposition Technique on Organic Electroluminescent Device (OLED), N.G. Cho, Y.H. Lee, J.H. Lee, Sungkyunkwan University, South Korea; *Y.W. Ko, J.H. Lee*, Electronics and Telecommunications Research Institute (ETRI), Korea; *G.Y. Yeom*, Sungkyunkwan University, South Korea

To fabricate active matrix organic electroluminescent devices (OLED), a transparent conducting material such as indium tin oxide (ITO) has to be deposited on the organic material of the devices and the organic materials are easily damaged by the oxygen atom, ion bombardment, heating, etc. during the deposition processing of ITO. Therefore, it is very difficult to deposit ITO on the OLED to form a transparent electrode. Also, it is difficult to maintain both electrical conductivity and transparency of ITO without generating damages to OLED when a conventional ITO deposition technique such as sputter deposition is used. Therefore, in this study, a dual oxygen ion, neutral beam assisted evaporator system has been used to deposit ITO films on the OLED to investigate as a possible transparent and conductive ITO deposition technique without generating damage to OLED. The characteristics of the deposited ITO on OLED was investigated using a four-point probe and a UV-spectrometer to measure the resistivity and transmittance of ITO films, respectively. The change of surface roughness after ITO deposition was investigated using an atomic force microscopy. Also, current-voltage (I-V) characteristics of the fabricated OLED with the ITO electrode were measured with HP-4145A semiconductor parameter analyzer.

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OF-TuP9 Contour TPD of N,N'-disalicylidene-1,2-propanediamine Thin-films, C.C. Chusuei, University of Missouri-Rolla; *J.A. Schreifels*, George Mason University

A simple method for obtaining a comprehensive overview of large ($m/e > 200$) molecular weight compounds desorbing from the surface during temperature programmed desorption (TPD) experiments is presented. Standard 2D TPD methods require a priori knowledge of surface reactions and typically therefore is limited to a few pre-selected mass-to-charge ratios (< 10). Our method precludes this necessity since wide mass ranges ($m/e = 25$) can be monitored in a single experiment. Desorbing organic films can be represented in the form of contour TPD (CTPD) plots. In our example, the desorption of N, N'-disalicylidene-1,2-propane -diamine, an important jet fuel additive used in aircraft, is adsorbed onto oxidized and oxide-free 304 stainless steel surfaces. The utility of CTPD for providing mechanistic insight into thermal decomposition pathways is demonstrated. Four chemical species were observed at $m/e = 107, 133, 232$ and 290 respectively, and mechanistic pathways for their formation are presented. Conventional 2D TPD spectra can be extracted from the CTPD by taking vertical slices of the contours.

OF-TuP10 Organic Electroluminescent Devices Fabricated by Ink-jet Printing, S.J. Jo, S.M. Jeong, Yonsei University, Korea; *H.K. Baik*, Yonsei University, Korea, South Korea; *S.H. Choi, W.H. Koo*, Yonsei University, Korea; *K.M. Song*, Kon Kuk University, Korea; *S.J. Lee*, Kyung Sung University, Korea

Organic Electroluminescent Devices for full color were fabricated by ink-jet printing methods. ITO used as anode was treated by atmospheric plasma for hydrophilic surface. Also polyimide as a bank was treated by atmospheric plasma for hydrophobic surface. In this experiment, we investigate characters of OLED and the influence of atmospheric plasma treatment.

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Room 318/319 - Session OF+NS-WeM

Molecular Electronics

Moderator: D. Cahen, Weizmann Institute of Science, Israel

8:20am **OF+NS-WeM1 Electronics and Mechanics with Single Molecules, P.L. McEuen, Cornell University** **INVITED**

It is now possible to make electronic and mechanical devices where an individual molecule is the active element. Examples include devices made from single-walled carbon nanotubes or single organic molecules. These molecular devices are proving to be wonderful systems for the study of the physics of materials at the nanometer scale. In this talk, I will review recent progress within our group on the electrical, electromechanical, and electrochemical properties of individual nanotubes and single molecules, as inferred from both transport and scanned probe measurements.

9:00am **OF+NS-WeM3 Understanding Charge Transport in Molecular Electronics, J.G. Kushmerick, R. Shashidhar, Naval Research Laboratory**

We use an experimentally simple crossed-wire tunnel junction to interrogate how factors such as metal-molecule coupling, molecular structure and the choice of metal electrode influence the current-voltage characteristics of a molecular junction. Results on junctions with symmetric and asymmetric metal-molecule contacts demonstrate that a specific molecular core can act either as a molecular wire or a molecular rectifier depending on its coupling to the metal electrodes. By tuning the coupling at the two metal-molecule interfaces-through the use of different attachment chemistries and metal electrodes-we are able to control the extent of current rectification. Experimental measurements and theoretical calculations demonstrate that the conductance of a molecular wire can be directly related to how well it's π -conjugated backbone mimics an ideal one-dimensional metal. Finally, we will show that the conductance of a molecular junction scales with the number of molecules contacted, and that the π -systems of molecular wires connected in parallel are not strongly coupled. Initial results demonstrating the utility of in situ vibrational spectroscopy to characterize the molecular junction will also be presented.

9:20am **OF+NS-WeM4 Observation of Negative Differential Resistance Measured through Individual Molecules on Silicon at Room Temperature, N.P. Guisinger, R. Basu, A.S. Baluch, M.C. Hersam, Northwestern University**

In recent years, substantial progress has been made in the emerging field of molecular electronics. In particular, metal-molecule-metal junctions have been widely studied. In this paper, charge transport through molecule-semiconductor junctions is considered. The presence of the energy band gap in semiconductors provides opportunities for resonant tunneling through individual molecules, leading to interesting effects such as negative differential resistance (NDR). The ultra-high vacuum (UHV) scanning tunneling microscope (STM) allows individual molecules to be imaged, addressed, and manipulated on semiconducting surfaces with atomic resolution at room temperature. This paper considers two distinct chemistries on the Si(100) surface. Styrene reacts with Si(100) via a covalent silicon-carbon bond. On degenerately n-type Si(100), STM current-voltage characteristics on individual styrene molecules show clear NDR at negative sample biases of approximately -2.5 V and -4 V. However, at positive sample bias, the styrene is liberated from the surface via inelastic electron stimulated desorption (ESD). In an effort to minimize perturbation via ESD, individual 2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO) molecules were bound to degenerately n-type Si(100). The exceptional stability of the silicon-oxygen bond allows charge transport measurements on TEMPO at high biases up to ± 5 volts without ESD. Similar to styrene, NDR is clearly observable at negative sample biases of approximately -3 V, -4 V, and -4.5 V. These effects will be explained by considering the energy band diagram of the semiconductor-molecule junction.

9:40am **OF+NS-WeM5 Molecular Materials and Devices, C.R. Kagan, A. Afzali, R. Martel, P.M. Solomon, L.M. Gignac, A.G. Schrott, B. Ek, C. Lin, IBM T.J. Watson Research Center** **INVITED**

Efforts to fabricate devices based on active molecular components have been driven by both the fundamental interest in using chemistry to build function at the molecular level and the looming technological expectation of the end of Moore's law. In this talk, we describe the directed assembly of organic and metal-metal bonded supramolecular systems that are interesting materials for potential electronic and memory device

applications. Molecules are chosen with head groups that bind to metal or oxide surfaces and tail groups that bind to metal electrodes or that template the growth of the particular molecular system. Optical spectroscopy, atomic force and scanning tunneling microscopy, electrochemistry, and electrical measurements are used to characterize the chemistry and physics of molecular assemblies and the behavior of devices. Self-assembled organic monolayers are used to fabricate reported field-effect transistor structures and to elucidate the important requirements necessary to successfully design two- and three-terminal molecular devices. We demonstrate the layer-by-layer assembly of metal-metal bonded supramolecules and utilize this approach to fabricate molecular devices.

10:20am **OF+NS-WeM7 Mediating Electronic Switching of Single Molecules Using Chemical Interactions, P.A. Lewis, The Pennsylvania State University; C.E. Inman, University of Oregon; J.M. Tour, Rice University; J.E. Hutchison, University of Oregon; P.S. Weiss, The Pennsylvania State University**

We have studied conjugated phenylene-ethynylene oligomers inserted into amide-containing alkanethiolate self-assembled monolayers using scanning tunneling microscopy in order to determine their physical and electronic properties when surrounded by a hydrogen-bonded matrix. The phenylene-ethynylene oligomers show stability in two conductance states, an ON and an OFF state. We observe fewer switching events between the ON and OFF states than previously reported for n-alkanethiolate matrices and attribute this to the rigidity due to the hydrogen bonds of the amide groups in the matrix. Furthermore, we demonstrate bias-dependent switching as a result of hydrogen bonding between the substituents of the inserted oligophenylene-ethynylene and the matrix molecules. We demonstrate that the chemical and physical environment of proposed molecular devices is crucial to their function and can be exploited to impart tunable electronic properties.

10:40am **OF+NS-WeM8 Two-Photon Photoemission Studies of Molecular Affinity Levels in Oligo-Phenylene Ethynylene Self-Assembled Monolayers, C. Zangmeister, S.W. Robey, R.D. van Zee, National Institute of Standards and Technology**

Two-photon photoemission has been used to study unoccupied electronic levels for a family of thiolated oligomeric phenylene-ethynylene self-assembled monolayers. Self-assembled monolayers of a three phenyl ring oligomer (OPE) and the same oligomer with a nitro group substituted for one hydrogen on the center ring (NO@sub2@-OPE) were formed on polycrystalline Au/Si substrates as well as [111] oriented Au on mica. This class of compounds has received attention because of measured conduction characteristics and the reported negative-differential resistance behavior of these compounds in nanometer-sized pore structures. Single-color, two photon photoelectron spectroscopy measurements were performed in the ultraviolet using frequency-doubled, subpicosecond pulses from a Ti:Sapphire-pumped optical parametric amplifier. For the OPE monolayers we have, based on the excitation energy dependence, identified an unoccupied level ca. 1 eV above the vacuum level. Using previous two-photon photoemission and inverse photoemission of condensed benzene layers as a guide we tentatively identify this as the remnant of the $e_{\text{sub}2\text{u}}$ unoccupied level for benzene localized on the carbon atoms of the phenyl ring. Results of studies on NO@sub2@-OPE layers will also be discussed.

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 $\sim 20\%$. 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 ns, 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.

Surface Science

Room 327 - Session SS+OF-WeA

Growth and Characterization of Organic Films

Moderator: L.A. Baker, Naval Research Laboratory

2:00pm **SS+OF-WeA1 Electronic and Geometric Structures of Pentacene Molecules Grown on Au(100), Y.J. Song, K. Lee, J. Yu, Y. Kuk**, Seoul National University, Korea

A pentacene molecule has attracted much interest for its possible application to organic-based electronic devices with its interesting electronic properties. Despite reported semiconducting property of the

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bulk crystal, it is hard to grow the high-quality film. Here, we report our scanning tunneling microscopy studies on the geometric and electronic structures of pentacene molecular layers on a Au(100) surface. Because of the high diffusivity of the molecule at room temperature, the STM studies were done at low temperature. At submonolayer coverage, the molecules are confined to the troughs of the reconstructed Au(100)-(5x20), forming a chain structure perpendicular to the reconstructed ridges. We resolved the HOMO and LUMO states of pentacene molecules on a Au(100) surface with atomic resolution. The DFT (density functional theory) results of the molecular layer reveal good agreement with the observed geometric and electronic structures. The electronic levels of pentacene molecules are shifted in the presence of metallic substrate. This result can be valuable when one makes metal-pentacene junctions for device applications. The electronic levels are also shifted with pentacene-pentacene interactions. At the coverages higher than 2 monolayers, a single phase was observed. The pentacene-pentacene interaction plays an important role to the growth structures. The 5 pentacene molecules work as a base unit for the multilayer film. The correlation between the growth structure and the transport property will be discussed.

2:20pm SS+OF-WeA2 Pentacene Thin Films on Clean and Chemically Modified Si(001) Surfaces, K.P. Weidkamp, L. Fang, R.J. Hamers, University of Wisconsin-Madison

We have investigated the microstructural, chemical and electronic properties of pentacene thin films formed on Si(001) surfaces. Using FTIR and valence-band photoemission spectroscopy, we find that the initial pentacene molecules deposited onto the surface undergo a transition from sp² to sp³ bonding and partial dissociation, all indicating the formation of covalent C-Si bonds that inhibit diffusion and thereby result in poor pentacene crystal formation. In contrast films prepared by deposition on to Si(001) surfaces that were initially modified with a monolayer of pentacene molecules show no evidence for dissociation and exhibit highly reversible adsorption and desorption, demonstrating that the pentacene molecules do not form covalent bonds with the underlying organic-modified surface. In order to understand how the molecular structure of the interfacial organic layer affects that structure and electronic properties of the pentacene thin films, we have investigated pentacene thin films deposited onto silicon surfaces that were modified with several different organic molecules including cyclopentene, dodecene, and phenanthrenequinone. These three molecules are expected to differ significantly in thickness, molecular rigidity, and effective molecular conductivity. AFM images show that the each organic molecular layer induces specific changes in the microstructure of the pentacene films deposited on top. Measurements of the electrical properties through the films will also be presented.

2:40pm SS+OF-WeA3 Spectroscopic Measurements on Ultra Thin Highly Ordered Films of Organic Semiconductors, T. Fritz, TU Dresden, Germany
INVITED

Research activity on molecular solids has gathered pace in recent years as these materials have a wide range of interesting properties, emerging industrial interest with real applications at the horizon, and possible future applications that will enable electronics to move into the nanoscale. High quality samples, precise structural data, and a detailed understanding of the physical properties are essential, with special emphasis on thin films and interfaces. In this respect, the use of highly controlled growth techniques like Organic Molecular Beam Epitaxy (OMBE) is becoming more and more important, aiming at high quality thin films with controlled crystal structure and morphology, and therefore displaying well defined physical properties. In order to investigate those physical properties deeply, spectroscopy methods are required which allow to characterize films with film thicknesses down to even submonolayers. In our contribution two different spectroscopy methods will be discussed in detail. By the first one, called Scanning Tunneling Spectroscopy (STS), one can determine the energetic positions of both filled and empty states of a molecular layer on an inorganic substrate in a single measurement. Due to the high spatial resolution small domains with different ordering can be electronically distinguished. Despite electron spectroscopies, optical spectroscopy on organic materials is a very powerful tool and can even provide structural information. Given the fact that exciton confinement effects in quasi-one-dimensional organic crystals will become apparent only if the layer is sufficiently thin (usually less than 4 monolayers), a method is required which will allow to measure the optical absorption down to submonolayers coverage with a sufficient signal-to-noise ratio. The method of choice is the Differential Reflection Spectroscopy (DRS), a

variant of reflection absorption spectroscopy), carried out in situ, i.e., during the actual film growth.

3:20pm SS+OF-WeA5 Epitaxial Growth of Pentacene on Bi/Si(111) Films, G.E. Thayer, IBM T.J. Watson Research Center; J.T. Sadowski, Tohoku University, Japan; R.M. Tromp, IBM T.J. Watson Research Center

Electrical contacts between organics and metals have been known to limit charge injection in organic electronic devices. Thus it is not surprising that there is a considerable amount of current work modifying metal surfaces and interfaces in an effort to align conduction with organic molecular levels. The solution to this problem begins with understanding the fundamental mechanisms that control both the morphology and electronic structure at the interface between metal and organic materials. Although the interfaces of organic films grown on many clean substrates (semiconductors, insulators, and metals) are found to be poorly ordered, our work has revealed that pentacene grows epitaxially on Bismuth (a semimetal). Using LEEM, PEEM, LEED, AFM, and STM our efforts have focused on understanding how pentacene molecules order in Pn/Bi/Si(111) thin films (1ML-10MLs). In contrast to the frequently used Pn/Au system, in the first ML of Pn/Bi the pentacene molecules stand up and are highly ordered as seen by the sharp LEED patterns that we observe. Our LEED analysis finds that the structure of Pn/Bi/Si(111) thin films is similar to the bulk structure of Pentacene with lateral 2D cell dimensions of a=7.8Å, b=6.2Å, and $\gamma=84.9^\circ$. In one dimension, this structure is 1:1 commensurate in the $\sqrt{3}$ direction of the underlying hexagonal Bi surface structure. However, in the other direction it is rotated by a small angle and is incommensurate with the Bi lattice. Control of Pn crystal orientation on metal electrodes will enable the fabrication of organic FET's whose electrical characteristics are not degraded by large angle grain boundaries at the source and drain junctions.

3:40pm SS+OF-WeA6 AFM Study of Carboxylic-Acid Functionalized Pentathiophenes on Mica Surfaces, J. Chen, Lawrence Berkeley National Laboratory; A.R. Murphy, University of California; D.F. Ogletree, M. Salmeron, Lawrence Berkeley National Laboratory; J.M.J. Frechet, Lawrence Berkeley National Laboratory and University of California

We studied SAM films of the oligothiophene derivative (D5TBA @footnote 1) with AFM to determine its growth and structure and its response to mechanical excitations. We found that self-assembled films formed on mica substrates from hydrophilic (THF) and hydrophobic (chloroform) solutions were totally different in their structure and mechanical properties. In one case methyl groups were exposed while in the other carboxylic groups (COOH) were exposed, resulting in very different friction properties. Friction anisotropy was observed between domains of different orientations. Scanning polarization force microscopy (SPFM) was used to obtain contact potential maps (Kelvin Probe mode) to confirm film structures deduced from contact mode imaging. Generally, deposition from THF solutions produced stable monolayer aggregates with exposed methyl groups. Multilayer regions were sometimes observed, with alternate methyl and carbonyl group terminations. During contact AFM imaging the third and higher layers could be progressively peeled off by increasing the load applied to the tip, however the second layer was found to incorporate into the first layer in a densification process. Deposition from chloroform solutions usually produced unstable multilayer films with methyl groups contacting the mica surface. @FootnoteText@ @footnote 1@ D5TBA, or 4-(5'-Decyl-[2,2'; 5', 2"; 5", 2"; 5", 2"] pentathiophen-5-yl)-butyric acid, was prepared by Stille cross-coupling methods using functionalized thiophene monomers.

4:00pm SS+OF-WeA7 Surface Polymerization by Ion Assisted Deposition for Polythiophene Film Growth, S. Tepavcevic, Y. Choi, L. Hanley, University of Illinois at Chicago

Cationic polymerization is induced at the gas-solid interface by hyperthermal organic cations coincident on a surface with a thermal beam of organic monomers. @footnote 1@ This process, termed surface polymerization by ion assisted deposition (SPIAD), produces films that maintain the chemical structure of the monomer. @footnote 2@ A polythiophene film is produced here by SPIAD with 100 eV thiophene ions and terthiophene monomers coincident on Si and indium tin oxide (ITO) substrates held under vacuum. X-ray photoelectron spectroscopy observes enhancement in film growth for SPIAD compared with either thiophene ion or terthiophene exposure alone. Polythiophene films grown by both mass-selected @footnote 1@ and non-mass-selected ions @footnote 3@ with coincident terthiophene dosing both display similar fluorescence intensity at two wavelengths characteristic of emission from films of the terthiophene monomer. Raman spectra of films from non-mass-selected

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ions display several vibrations also observed in terthiophene films. Ions therefore play a critical role in film growth from non-mass-selected ions, in addition to any radical or photochemically driven processes that may also occur. @FootnoteText@ @footnote 1@L. Hanley and S.B. Sinnott, Surf. Sci. 500 (2002) 500. @footnote 2@S. Tepavcevic, Y. Choi, and L. Hanley, J. Amer. Chem. Soc. 125 (2003) 2396.@footnote 3@L. Hanley, Y. Choi, E.R. Fuoco, F.A. Akin, M.B.J. Wijesundara, M. Li, A. Tikhonov, and M. Schlossman, Nucl. Instr. Meth. Phys. Res. B 203C (2003) 116.

4:40pm **SS+OF-WeA9 Molecular Dynamics Simulation Study of Continuous C@sub 3@F@sub 5@@super +@ and CF@sub 3@@super +@ Ion Depositions on Polystyrene Surfaces, I. Jang, S.B. Sinnott, University of Florida**

Fluorocarbon plasma treatment is widely studied and used to change surface properties and to grow thin polymer films. However, it is difficult to determine the detailed mechanisms responsible for the surface reactions that lead to thin film growth due to the complexity of plasma systems. Computer simulations of the deposition of mass selected fluorocarbon ions have been used to isolate the effects of polyatomic ions in low energy plasma deposition of thin films. In this study, the continuous deposition of a beam of polyatomic fluorocarbon ions (C@sub 3@F@sub 5@@super +@ and CF@sub 3@@super +@) on polystyrene surfaces is performed using classical molecular dynamics simulations. The forces are determined using the reactive empirical bond order method for short-range interaction and Lennard-Jones potential for long-range van der Waals interaction. The incident energy of the ions is 50 eV/ion and they are deposited normal to polystyrene surface. The simulations allow us to determine the mechanisms responsible for thin-film growth and surface modification by the ion beam deposition. Specifically, they show how fluorocarbon polymer precursors are formed and react with one another. Overall, the simulations predict that CF@sub 3@@super +@ depositions are more effective in fluorination of polystyrene surface than C@sub 3@F@sub 5@@super +@ depositions. This work is supported by the NSF under grant CHE-0200838.

5:00pm **SS+OF-WeA10 Exploring the Reactivity of Atomic Oxygen with Organic Surfaces, G.M. Wolfe, A.J. Wagner, J. Torres, C.C. Perry, D.H. Fairbrother, Johns Hopkins University**

Atomic oxygen is a major component in oxygen and air-based plasmas and also plays a major role in the erosion and degradation of polymeric coatings in spacecrafts as they pass through Low Earth Orbit (LEO). Through the use of self-assembled monolayers and well-defined polymeric substrates an understanding of the fundamental molecular level surface reactions of atomic oxygen with organic surfaces can be determined. Our work explores the interactions of O radicals, with a series of self-assembled monolayers (SAMs), employed as models for polymer surfaces. In situ X-ray photoelectron spectroscopy (XPS) is used to elucidate the mechanism of radical reactions occurring with dodecane, hexadecane, and X-ray modified hexadecane SAMs, as well as a semi-fluorinated SAM (CF-SAM). In the hydrocarbon SAMs, the reaction with atomic O progresses through three stages. Initially, reactions at the vacuum/film interface generate a steady state concentration of C-O, C=O and O-C=O groups. Sustained atomic oxygen exposure on hydrocarbon-based SAMs promotes the formation of volatile oxygen-containing carbon species, e.g. CO@sub 2@, leading to the development of a steady state etch front. Ultimately, oxygen penetrates to the film/substrate interface to form sulfonate and Au@sub 2@O@sub 3@ species. Experiments on the CF-SAM reveal an induction period of ~90 minutes prior to oxygen incorporation, an effect ascribed to the inertness of C-F and C-C bonds towards atomic oxygen and the well-ordered structure of the CF-SAM. In contrast to the hydrocarbon SAMs, reactivity within the CF-SAMs are initiated by O atom reactions at the film/substrate interface leading to desorption of intact adsorbate chains. Results on the interaction of atomic O with phosphorous ion-implanted poly(ethylene) will also be presented.

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