

Electronic Materials and Processing Room 2001 - Session EM1-ThA

Contacts to Organic and Molecular Devices

Moderator: D.B. Janes, Purdue University

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

INVITED

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

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

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

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

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

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

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

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

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

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

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

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

4:40pm **EM1-ThA9 Ag Islands Decorated by C₆₀**, *C. Tao, T.J. Stasevich, T.L. Einstein, E.D. Williams*, University of Maryland, College Park

It is increasingly clear that a great challenge in nanoscale electronics will be understanding and controlling the interaction between the active nanoscale element and the conductive electrodes in devices. At nanoscale structural changes involving the displacement of even a single metal atom will be closely related to the electronic properties and reliability. Here I will introduce our study on a specific metal-molecule interface formed at Ag monolayer islands decorated by C₆₀. At room temperature, equilibrium monolayer islands on clean Ag(111) surfaces are hexagonal. At extremely low coverage of the C₆₀, C₆₀ molecules are found preferentially at sections of the island edge near corners. Individual C₆₀ is found at different position in sequential images. When more C₆₀ is deposited, C₆₀ molecules form more stable chains along the Ag island edge near the corners of the island. The shape of the islands changes at this point with smoother corners. As coverage increases further, C₆₀ chains become longer and the hexagonal islands become round. By controlling C₆₀ coverage, we can make Ag island edges fully covered by C₆₀ chains, which become closed rings. The equilibrium shape of Ag islands decorated by the surrounding C₆₀ ring is approximately circular and shows dynamic thermal fluctuations. The mechanism for C₆₀ distribution and shape change of islands will be discussed in the context of the 2D equilibrium crystal shape (ECS). By rapid STM scanning, we obtain sequential images of the C₆₀ rings and analyze the corresponding dynamic properties. The shape fluctuation of C₆₀ rings are clearly displayed by movies made of sequential images. Quantitative analysis of the shape fluctuation using correlation functions will be presented, and discussed in terms of the correlated motion of the C₆₀ molecules and underlying Ag atoms.
@FootnoteText@ --Supported by NSF, MRSEC at the University of Maryland.

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