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**2012 SPRING MEETING of the
AVS HUDSON MOHAWK CHAPTER**

Talks, posters, networking, pizza

3:00 – 7:00 pm

Monday, April 2, 2012

Russell Sage Dining Hall

***Rensselaer Polytechnic Institute
Troy, NY 12180.***

Parking and directions: Visitor parking is available behind the Public Safety office on 15th Street—turn left immediately after crossing the over bridge pedestrian walkway when driving south on 15th street. You will need quarters, but will need to pay only until 5 pm. The Russell Sage Dining Hall is on the right on the west side of the walkway, opposite to cream-colored CII building to your left.

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3:00 – 3:30 pm

INFORMAL MIXER

3:30 – 5:10 pm

TALKS

- T1. GOLD-SULFUR BOND BREAKING IN Zn(II) TETRAPHENYLPORPHYRIN MOLECULAR JUNCTIONS, Adam J. Simbeck, Guoguang Qian, Saroj K. Nayak, Gwo-Ching Wang, Kim M. Lewis, *Rensselaer Polytechnic Institute*. **3:30 – 3:50 pm**
- T2. BONDING-INDUCED MULTIFOLD THERMAL CONDUCTANCE ENHANCEMENT AT INORGANIC HETEROINTERFACES USING NANOMOLECULAR MONOLAYERS, Peter J. O'Brien, Sergei Shenogin, Jianxiun Liu, Philippe K. Chow, Danielle Laurencin, P. Hubert Mutin, Masashi Yamaguchi, Pawel Keblinski, Ganpati Ramanath, Rensselaer Polytechnic Institute, Institut Charles Gerhardt Montpellier, France. **3:50 – 4:10 pm**
- T3. XPS AND REELS SURFACE CHARACTERIZATION AND IMAGING OF GRAPHENE AND OTHER CARBON-BASED MATERIALS, Andrew E. Wright, Tim S. Nunnery, Richard G. White, and Brian R. Strohmeier, *Thermo Fisher Scientific*.
- T4. CHARACTERIZATION OF FEW LAYER GRAPHENE FILMS GROWN ON Cu, Cu-Ni AND SiC SUBSTRATES, P. Tyagi, J. D. McNeilan, J. Abel, F. J. Nelson, Z. R. Robinson, R. L. Moore, A. C. Diebold, V. P. LaBella and C. A. Ventrice, Jr., A. Sandin, D. B. Dougherty, and J. E. Rowe, C. Dimitrakopoulos, A. Grill, and C. Y. Sung, S. Chen, A. Munson, C. W. Magnuson, and R. S. Ruoff, *University at Albany-SUNY, North Carolina State University, IBM T.J. Watson Research Center, University of Texas, Austin*. **4:10 – 4:30 pm**
- T5. A NOVEL NANOSCALE NON-CONTACT TEMPERATURE MEASUREMENT TECHNIQUE BASED ON SCANNING ELECTRON MICROSCOPY, Xiaowei Wu, Robert Hull, *Rensselaer Polytechnic Institute*. **4:30 – 4:50 pm**
- T6. 3D CHEMICAL IMAGING OF SOLID OXIDE FUEL CELLS BY FIB-TOF TOMOGRAPHY, John S. Hammond Gregory L. Fisher and Scott R. Bryan, *Physical Electronics*. **4:50 – 5:10 pm**

5:10 – 5:30 pm

BREAK

- P1. BI-AXIAL TEXTURE DEVELOPMENT IN AlN LAYERS DURING OFF-AXIS SPUTTER DEPOSITION, Ruopeng Deng, Daniel Gall, *Rensselaer Polytechnic Institute*.
- P2. NEAR SINGLE-CRYSTAL SEMICONDUCTORS ON TAPES OR GLASS FOR SOLAR ENERGY CONVERSION, C. Gaire, L. Chen, A. Goyal, I. Bhat, G.-C. Wang, and T.-M. Lu, *Rensselaer Polytechnic Institute, and Oak Ridge National Laboratory*.
- P3. MOLECULAR SWITCHES: TRACKING A TWO-STATE CONDUCTANCE FROM PORPHYRIN MOLECULES, Alexander Buck, Andrew Shapiro, and K. M. Lewis, *Rensselaer Polytechnic Institute*.
- P4. Au-NANOWIRE NETWORK-FILLED POLYMER COMPOSITES FOR HEAT MANAGEMENT IN NANODEVICE PACKAGING, Nikhil Balachander, Rutvik J. Mehta, Indira Seshadri, L.S. Schadler, Pawel Koblinski, Theo Borca-Tasciuc, Ganpati Ramanath, *Rensselaer Polytechnic Institute*.
- P5. CHARACTERIZATION OF THE STRUCTURAL AND OPTICAL PROPERTIES OF EPITAXIAL GRAPHENE GROWN ON VICINAL 6H-SiC SURFACES, F. Nelson, A.C. Diebold, Andreas Sandin, Daniel B. Dougherty, Jack E. Rowe, *University at Albany, North Carolina State University, Raleigh, NC*.
- P6. CHEMIREISTOR SENSOR: CHARACTERIZATION OF ELECTROSTATIC TRAPPING OF GOLD NANOPARTICLES FOR THE DETECTION OF VOLATILE ORGANIC COMPOUNDS, Hengshuo Fu, Anpu Zhu, *Rensselaer Polytechnic Institute*.
- P7. PORPHYRIN-BASED MOLECULAR MULTILAYER THIN-FILM ASSEMBLED ON GOLD ELECTRODES FOR ELECTRO-OPTICAL APPLICATIONS, Alexandra Krawicz¹, Guoguang Qian, Kim M. Lewis, and Peter H. Dinolfo, *Rensselaer Polytechnic Institute*.
- P8. FEMTOSECOND PUMP-PROBE STUDY OF ELECTRON-PHONON COUPLING IN COPPER THIN FILMS, Xiaohan Shen, Andrej Halabica, Pei-I Wang, Toh-Ming Lu, and Masashi Yamaguchi, *Rensselaer Polytechnic Institute*.
- P9. TRANSPORT CHARACTERISTICS OF Zn PORPHYRIN IN AN ELECTROMIGRATED JUNCTION, Swatilekha Saha, Guoguang Qian, Kim M. Lewis, *Rensselaer Polytechnic Institute*.
- P10. MEASUREMENT TECHNIQUES FOR CONTACT RESISTANCE BETWEEN METAL-THERMOELECTRIC MATERIALS, Devender, Theo Borca-Tasciuc, Ganpati Ramanath, *Rensselaer Polytechnic Institute*.
- P11. DEVELOPMENT OF GaInN/GaN MULTIPLE QUANTUM WELL SOLAR CELLS GROWN BY MOCVD, Liang Zhao, Christoph Stark, Shi You, Wenting Hou, Xiaoli Wang, Theeradetch Detchprohm, Christian Wetzel, *Rensselaer Polytechnic Institute*.
- P12. ENHANCED SEEBECK IN NANOSTRUCTURED Sb₂Te₃ BY ANTISITE DEFECT SUPPRESSION THROUGH SULFUR DOPING, Rutvik J. Mehta, Y. Zhang, M. Belley, E. Sachdeva, T. Borca-Tasciuc, H. Zhao, R. Ramprasad, Ganpati Ramanath, *Rensselaer Polytechnic Institute, and University of Connecticut, CT*.

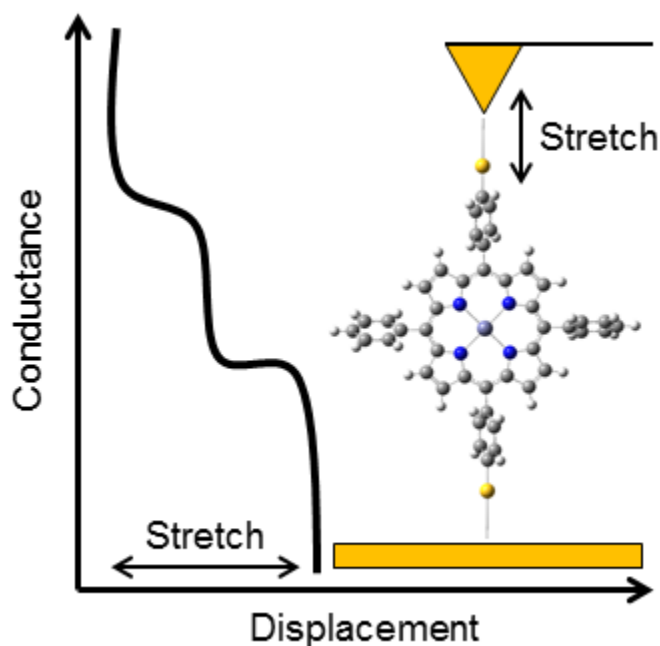
GOLD-SULFUR BOND BREAKING IN Zn(II) TETRAPHENYLPORPHYRIN MOLECULAR JUNCTIONS*

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Quantized conductance of single tetraphenylporphyrin molecules with and without a central zinc(II) [Zn(II)] atom was measured using a molecular break junction (MBJ) method [X.L. Li, H.X. He, B.Q. Xu, X.Y. Xiao, L.A. Nagahara, I. Amlani, R. Tsui, N.J. Tao, *Surf. Sci.* 573 (2004) 1]. From the conductance histograms we observed an additional 1.7 Å stretch for two-state conductance in a single Zn(II) tetraphenylporphyrin (ZnTPP) molecule as compared to single state conductance in a free tetraphenylporphyrin (TPP) molecule, i.e., no central Zn(II) atom. First-principles density functional calculations, using an electrode-molecule-electrode model, are completed to provide insight into the mechanisms behind bond stretching, and eventual bond breaking, to better understand the additional 1.7 Å of stretching observed with ZnTPP.



*Work supported by NSF IGERT, Grant No. 0333314

BONDING-INDUCED MULTIFOLD THERMAL CONDUCTANCE ENHANCEMENT AT INORGANIC HETEROINTERFACES USING NANOMOLECULAR MONOLAYERS

Peter J. O'Brien^{1*}, Sergei Shenogin¹, Jianxiun Liu², Philippe K. Chow¹, Danielle Laurencin³, P. Hubert Mutin³, Masashi Yamaguchi², Pawel Koblinski¹, Ganpati Ramanath¹

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Manipulating interfacial thermal transport is crucial for many technologies including nanoelectronics, solid-state lighting, energy generation, and nanocomposites. Here, we demonstrate the use of a strongly-bonding organic nanomolecular monolayer (NML) at metal-dielectric interfaces to obtain up to a fourfold increase in the interfacial thermal conductance, to values as high as $430 \text{ MWm}^{-2}\text{K}^{-1}$ in the copper-silica system. We also show that the approach of using an NML can be implemented to increase or decrease the interfacial thermal conductance in other materials systems. Molecular dynamics simulations indicate that the remarkable enhancement we observe is due to strong NML-dielectric and NML-metal bonds that facilitate efficient heat transfer through the NML. Our results underscore the importance of interfacial bond strength as a means to describe and control interfacial thermal transport in a variety of materials systems.

XPS AND REELS SURFACE CHARACTERIZATION AND IMAGING OF GRAPHENE AND OTHER CARBON-BASED MATERIALS

Andrew E. Wright¹, Tim S. Nunney¹, Richard G. White¹, and Brian R. Strohmeier²

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The application potential of graphene is currently being extensively explored by the materials science community. Its immediate potential as a transparent conductive electrode for the microelectronics industry is already being exploited and it is speculated that the unique combination of electronic, chemical, and structural properties exhibited by graphene will impact the development of thin film transistor development. In all stages of application development, from the initial research stages, through to testing of the finished devices, there is a requirement for materials characterization and analysis. Most materials need to be analyzed for compositional homogeneity across the sample surface and through the sample thickness. X-ray photoelectron spectroscopy (XPS) is a valuable technique for the surface characterization of graphene and other carbon-based materials. XPS can be used to characterize the surface chemistry of graphene and modified graphene materials, detect surface impurities, and evaluate graphene-substrate interactions. XPS can also be used to generate chemical state surface images of graphene and to determine total layer thicknesses (i.e., layer counting).

Reflection electron energy loss spectroscopy (REELS) is a complementary technique to XPS that can be performed in standard XPS instruments that utilize a variable energy electron flood gun for sample charge neutralization. The electron flood gun source together with the XPS electron energy analyzer can be used to produce high quality REELS spectra. An important advantage of REELS is the ability to detect and quantify surface hydrogen, which is undetectable by XPS. Hydrogen surface maps can also be produced by REELS to supplement XPS surface images of other elements and/or chemical states. In addition to the detection of hydrogen, REELS can also be used to examine the level of carbon unsaturation at the uppermost surface of organic materials to complement information obtained from high resolution C 1s XPS spectra. This presentation will describe several examples of XPS and REELS applications for the surface characterization of graphene and other organic materials.

CHARACTERIZATION OF FEW LAYER GRAPHENE FILMS GROWN ON Cu, Cu-Ni AND SiC SUBSTRATES

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The electronic structure of graphene depends on the number of graphene layers and the stacking sequence between the layers. Therefore, it is important to have a non-destructive technique for analyzing the overlayer coverage of graphene directly on the growth substrate. We have developed a technique using angle-resolved XPS to determine the average graphene thickness directly on metal foil substrates and SiC substrates. Since monolayer graphene films can be grown on Cu substrates, these samples are used as a standard reference for a monolayer of graphene. HOPG is used as a standard reference for bulk graphite. The electron mean free path of the C-1s photoelectron can be determined by analyzing the areas under the C-1s peaks of monolayer graphene/Cu and bulk graphite. With the electron mean free path, the graphene coverage of a film of arbitrary thickness can be determined by analyzing the area under the C-1s of that sample. Analysis of graphene coverages for graphene films grown on Cu-Ni substrates and of the thickness of both the graphene overlayer and intermediate buffer layer on SiC will be presented. This research was supported in part by the National Science Foundation (grant no. 1006350/1006411).

A NOVEL NANOSCALE NON-CONTACT TEMPERATURE MEASUREMENT TECHNIQUE BASED ON SCANNING ELECTRON MICROSCOPY

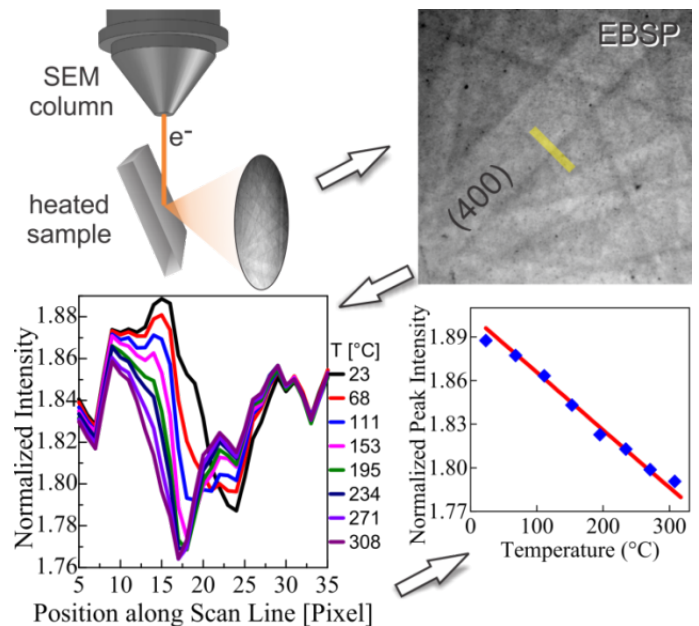
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Detecting nanoscale temperature and temperature distributions is important for studies of heat generation and transfer in a wide range of engineering systems, such as microelectronic, optoelectronic and micromechanical systems. In this presentation, a new high spatial resolution non-contact temperature measurement technique (which we call thermal scanning electron microscopy, ThSEM) is described which employs temperature dependent thermal diffuse scattering in electron backscatter diffraction (EBSD) in a scanning electron microscope (SEM). Unlike conventional scanning thermal microscopy, which uses contact probes, ThSEM provides non-contact temperature mapping. In contrast to optical temperature mapping techniques, ThSEM doesn't have the spatial resolution limitation that arises from the optical wavelength and theoretically can reach a resolution of < 10 nm. The hardware setup is very similar to the EBSD system in a SEM, which makes the integration of temperature mapping into SEM relatively straightforward. Moreover, multiple signals or contrast mechanisms, such as temperature maps, grain orientation maps, topographic images, and elemental maps could be obtained from the same sample area depending on the specific SEM capability.

Figure 1: Summary of nanoscale temperature mapping by EBSD analysis. Top left – experimental geometry. Top right – part of typical EBSD pattern from Si(001). Bottom left – intensity scans across (400) Si Kikuchi line at different temperatures. Bottom right – calibration of normalized peak intensity vs. temperature.



3D CHEMICAL IMAGING OF SOLID OXIDE FUEL CELLS BY FIB-TOF TOMOGRAPHY

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Time-of-flight secondary ion mass spectrometry (TOF-SIMS) is a surface-sensitive chemical imaging technique in which the outermost ~ 2 nm of the surface is sampled. Characterization of materials in the range of several microns from the sample surface has become somewhat routine with the use of a sputter ion beam to remove multiple layers of material between analysis (chemical imaging) cycles. Nevertheless, there are practical limitations to the use of ion beam sputtering for probing inorganic specimens beyond the surface region. Certain matrix components do not sputter well and are susceptible to ion beam-induced damage. This accumulated beam damage gives rise to incorrect chemical distributions. Some matrix components may sputter at a different rate than others which results in a misrepresentation of the chemical distributions. Utilizing the best possible analytical conditions in order to minimize the aforementioned artifacts, the analytical time requirements can become prohibitive. Finally, the utility of sputter depth profiling for 3D TOF-SIMS imaging is limited to a few microns in the case of a favorable sample matrix and to a couple hundred nanometers in the case of an unfavorable sample matrix.

An alternative approach to achieve 3D chemical imaging is to utilize FIB milling and sectioning in conjunction with TOF-SIMS chemical imaging... what we have called FIB-TOF tomography. With FIB milling, the interior of a specimen is revealed to depths of $\geq 50 \mu\text{m}$. Additionally, 3D chemical imaging of $> 10 \mu\text{m}$ deep volumes may be achieved within reasonable analytical times. The advantage of the *in situ* FIB-TOF approach is that the artifacts caused by sputter depth profiling, such as differential sputtering and accumulated ion beam damage to matrix molecules, are avoided. The union of successive FIB sectioning and TOF-SIMS analysis cycles with the sample maintained in one analytical position to achieve 3D chemical imaging will be discussed for the analysis of solid oxide fuel cell samples. The unique capabilities of the TRIFT analyzer allow the high mass range and high mass resolution interpretation of the 3D multilayer structure. The 3D tomography reveals a highly porous structure with the segregation of key elements at the surfaces of the pores as well as at buried interfaces.

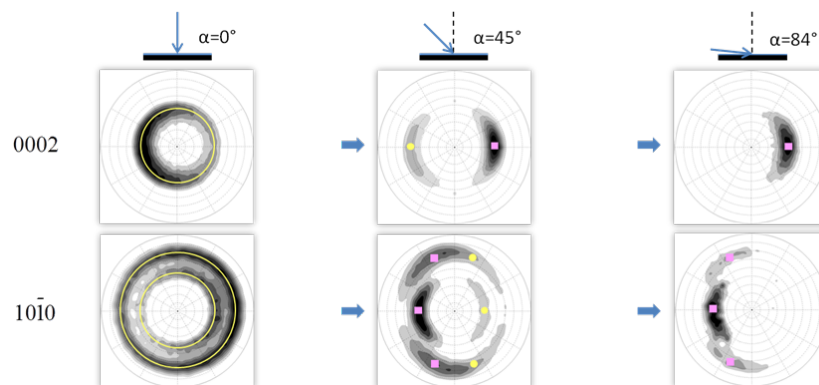
BI-AXIAL TEXTURE DEVELOPMENT IN AlN LAYERS DURING OFF-AXIS SPUTTER DEPOSITION

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Polycrystalline AlN layers were deposited by pulsed-DC reactive magnetron sputtering from a variable deposition angle $\alpha = 0\text{-}84^\circ$ in 5 mTorr pure N_2 at room temperature. X-ray diffraction pole figure analyses show that layers deposited from a normal angle ($\alpha = 0^\circ$) exhibit fiber texture, with a random in-plane grain orientation and the c-axis tilted by $42\pm 2^\circ$ off the substrate normal, yielding wurtzite AlN grains with the $\{10\bar{1}2\}$ plane approximately parallel ($\pm 2^\circ$) to the substrate surface. However, as α is increased to 45° , two preferred in-plane grain orientations emerge, with populations I and II having the c-axis tilted towards and away from the deposition flux, by $53\pm 2^\circ$ and $47\pm 1^\circ$ off the substrate normal, respectively. Increasing α further to 65 and 84° , results in the development of a single population II with a $43\pm 1^\circ$ tilt. This developing bi-axial texture is attributed to a competitive growth mode under conditions where adatom mobility is sufficient to cause inter-grain mass transport but insufficient for the thermodynamically favored low energy $\{0001\}$ planes to align parallel to the layer surface. Consequently, AlN nuclei are initially randomly oriented and form a kinetically determined crystal habit exposing $\{0001\}$ and $\{11\bar{2}0\}$ facets. The expected direction of its highest growth rate is $49\pm 5^\circ$ tilted relative to the c-axis, in good agreement with the $42\text{-}53^\circ$ measured tilt. The in-plane preferred orientation for $\alpha > 0^\circ$ is well explained by the orientation dependence in the cross-section of the asymmetric pyramidal nuclei to capture off-normal directional diffusion flux. The bi-axial texture of AlN is helpful in shear mode acoustic devices due to its tilted c-axis and good grain alignment.



NEAR SINGLE-CRYSTAL SEMICONDUCTORS ON TAPES OR GLASS FOR SOLAR ENERGY CONVERSION

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Most high performance semiconductor devices are made out of single crystal semiconductor films grown on single crystal substrates. However, single crystal substrates are too expensive for large area applications such as display and solar cells. Most low-cost commercial large area devices are either polycrystalline or amorphous semiconductors on glass or metal substrates with less than ideal efficiency and long term stability problems. Therefore a key issue is whether it is possible to grow a single crystal film on glass at all. In this poster we present examples that demonstrate the possibility of growing single crystal-like CdTe and Ge films on glass using biaxially textured CaF₂ buffer layer or directly on biaxially textured Ni sheet. We characterize these films using x-ray pole figure, transmission electron microscopy (TEM) and scanning electron microscopy.

Our results show that single crystal-like CdTe thin film grown by MOCVD on biaxial Ni sheet has the epitaxial relationship of $\{111\}_{\text{CdTe}} // \{001\}_{\text{Ni}}$ with $[1\bar{1}0]_{\text{CdTe}} // [010]_{\text{Ni}}$ and $[11\bar{2}]_{\text{CdTe}} // [100]_{\text{Ni}}$. The 12 diffraction peaks in the (111) pole figure of CdTe film and their relative positions with respect to the four peak positions in the (111) pole figure of Ni substrate are consistent with four equivalent orientational domains of CdTe with three to four superlattice match of about 0.7% in the $[1\bar{1}0]$ direction of CdTe and the $[010]$ direction of Ni. The TEM and electron backscattered diffraction (EBSD) images show that the CdTe domains are 30 degrees orientated from each other [1].

A direct growth of Ge on Ni resulted in Ni-Ge alloy formation. Therefore, a thin layer of CaF₂ was grown epitaxially on Ni followed by a heteroepitaxial Ge film on CaF₂. The epitaxial relation in the out-of-plane direction of this multilayer system was observed to be $\text{Ge}[111] // \text{CaF}_2[111] // \text{Ni}[001]$. In addition, the Ge consisted of four equivalent in-plane oriented domains such that two mutually orthogonal directions: $\text{Ge}\langle\bar{2}11\rangle$ and $\text{Ge}\langle 0\bar{1}1\rangle$ are parallel to mutually orthogonal directions: $\text{Ni}\langle\bar{1}10\rangle$ and $\text{Ni}\langle\bar{1}\bar{1}0\rangle$, respectively of the Ni(001) surface. This was shown to originate from the four equivalent in-plane oriented domains of CaF₂ created to minimize the mismatch strain between CaF₂ and Ni in those directions [2]. On CaF₂ buffered glass substrates, Ge film could be grown through thermal evaporation at a low temperature of ~400 °C. TEM revealed that the Ge(111) heteroepitaxial films possessed a single crystal-like structure with small angle grain boundaries of $\leq 2^\circ$ misorientation [3].

1. Epitaxial growth of CdTe thin film on cube textured Ni by metal organic chemical vapor deposition, C. Gaire, S. R. Rao, M. Riley, L. Chen, A. Goyal, S. Lee, I. Bhat, T.-M. Lu and G.-C. Wang, Thin Solid Films 552(6), 1862 (2012).
2. Low temperature epitaxial growth of Ge on CaF₂ buffered cube-textured Ni, C. Gaire, J. Palazzo, I. Bhat, A. Goyal, G.-C. Wang and T.-M. Lu, J. of Crystal Growth 343, 33 (2012).
3. Small angle grain boundary Ge films on biaxial CaF₂/glass substrates, C. Gaire P. C. Clemmer, H.-F. Li, T. C. Parker, P. Snow, S. Lee, G.-C. Wang and T.-M Lu, J. of Crystal Growth 312, 607 (2010).

MOLECULAR SWITCHES: TRACKING A TWO-STATE CONDUCTANCE FROM PORPHYRIN MOLECULES

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Our research aim is to exploit iron porphyrin molecules to build a molecular switch. Such a switch could become the basis for any molecular electronics system, from nanoscale sensors to the next generation of supercomputers. To achieve this, we will identify the conductance switching properties of a single iron porphyrin (FeP) molecule. We employ a molecular break-junction (MBJ) technique with scanning tunneling microscopy (STM). An electrochemical etching technique is used to fabricate an STM tip from gold wire. The STM tip contacts a monolayer of iron porphyrin molecules self-assembled on a gold-mica substrate. As the probe is retracted at a rate of ~ 50 nm/sec, a plot of the current through the molecule as a function of the tip-sample separation is recorded. With constant applied voltage and the recorded current, the current is converted to the conductance of the molecule. Preliminary results suggest that iron porphyrin exhibits sequential steps in its conductance, which represents a switch from a high conductance state to a low conductance state. We identify these steps as a two-state conductance.

Au-NANOWIRE NETWORK-FILLED POLYMER COMPOSITES FOR HEAT MANAGEMENT IN NANODEVICE PACKAGING

Nikhil Balachander¹, Rutvik J. Mehta¹, Indira Seshadri^{1,2}, L.S. Schadler¹, Pawel Koblinski¹, Theo Borca-Tasciuc², Ganpati Ramanath¹

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We report the synthesis of a polymer composite filled with a metal nanowire network and investigate its thermal and mechanical properties for exploring the use of the composite for heat management applications in nanoelectronics packaging. While polymeric composites filled with nanoparticles and carbon nanotubes have been widely studied, the use of high-aspect ratio metal nanostructures and their assemblies is new. We expect the interconnected mesh of metal nanowires to be more effective thermal channels due to inherent continuity, connectivity that can lead to percolation at lower filler loadings. Gold was chosen due to its high bulk thermal conductivity, high corrosion resistance, ease of nanostructure synthesis and its relatively low stiffness conducive for conformability at rough surfaces and interfaces.

In this work, we report up to thirty fold higher thermal conductivity values of $k=5 \text{ Wm}^{-1}\text{K}^{-1}$ in a polydimethylsiloxane nanocomposite by using <5 vol. % gold nanowire network fillers. Electron microscopy and effective medium approximation modeling show that such remarkable k enhancement for such low nanofiller loadings is unprecedented, and arises due to the high aspect ratio of the thermally conductive gold nanostructures and low thermal boundary resistance at the gold-polymer interface. The measured elastic modulus values agree well with the predictions assumed about the bonding at the interface of the filler and matrix. The addition of fillers does not modify the mechanical properties of the composite noticeably as is evident by the constancy in hardness and modulus values. These nanowire-filled polymer composites showing a combination of high k and mechanical stability are attractive for use as thermal interface materials in electronic device packaging.

CHARACTERIZATION OF THE STRUCTURAL AND OPTICAL PROPERTIES OF EPITAXIAL GRAPHENE GROWN ON VICINAL 6H-SiC SURFACES

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Epitaxial graphene is of interest for “post-CMOS” device research due to its scalability and the ability to produce films resting on a semi-insulating substrate for device fabrication. Thermal annealing of SiC results in Si sublimation from the step edges. In the present study, vicinal surfaces of 6H-SiC mis-cut by 3.5° with respect to the [0001] direction were used for the growth in order to provide a high density of step edges, thought to greater facilitate the graphenization process. These vicinal surfaces actually required a higher growth temperature than on-axis samples. The growth morphology was investigated using Auger Spectroscopy and STM. Spectroscopic Ellipsometry was used to extract the optical properties of both the graphene layers as well as the “buffer” layer that sits as an interface between the SiC substrate and the graphene region. This buffer layer is thought to consist of a combination of sp^2 and sp^3 -bonded carbon and shows different spectral features when compared to that of the purely sp^2 -bonded graphene. While we still observe a strong UV absorbance peak in the former, its position has red-shifted to $\sim 4\text{eV}$ in comparison to its position at $\sim 4.5\text{eV}$ in graphene which we attribute to the additional sp^3 bonded carbon. Such information is important for optical in-line thickness metrology.

CHEMIRESISTOR SENSOR: CHARACTERIZATION OF ELECTROSTATIC TRAPPING OF GOLD NANOPARTICLES FOR THE DETECTION OF VOLATILE ORGANIC COMPOUNDS

Hengshuo Fu¹, Anpu Zhu²

¹*Department of Applied Physics and Electrical Engineering, and*

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There is growing interest in the study of nanosized particles for electronic devices. One of the studies of interest by researchers in the area of organic devices is to position conducting nanoparticles in gaps of nanometer scale. Devices, such as molecular switches, transistors, or chemical sensors can be built based on this study. Our project goal is to build a chemical sensor with a single nanoparticle positioned in a nano-sized gap covered by chemical ligands. To accomplish this goal, the first part of our project is to build an AC circuit to trap gold nanoparticles with sizes of 20nm, 40nm and 60nm to a nanometer-level gap. The sizes of the gaps will be from 20nm to 60nm. The nanogaps are coated with octanethiol which act as the sensing element. We will analyze the relationship among various parameters such as voltage, frequency, and the size of nanoparticles. The nanogaps will be characterized by measuring the resistance and capacitance before and after trapping the nanoparticles. We will determine whether the particles are trapped by inspecting the device by scanning electron microscopy and by observing the decrease in voltage during trapping experiments. Based on this study the system can work as a chemical sensor that can be used as a platform to build a chemical sensor array to detect multiple volatile organic compounds.

PORPHYRIN-BASED MOLECULAR MULTILAYER THIN-FILM ASSEMBLED ON GOLD ELECTRODES FOR ELECTRO-OPTICAL APPLICATIONS

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We have developed a Layer-by-Layer (LbL) method for the fabrication of thin-film molecular multilayers on gold electrodes. Copper(I) catalyzed azide-alkyne cycloaddition (CuAAC) coupling reactions were used for initial surface attachment and subsequent LbL deposition of porphyrin building blocks. The electrochemical and photophysical properties of the thin-films can be tuned through synthetic modification of the individual building blocks, resulting in new porphyrin multilayers for applications in light harvesting and molecular electronics.

Herein, we demonstrate the reproducible growth trends and optical properties of these porphyrin structures. Multilayer growth was followed by UV-Vis absorption and specular reflectance spectroscopy. Film thickness and optical constants were obtained from spectroscopic ellipsometry. Topology and surface roughness was examined by TM-AFM, while the copper content of the resulting films was quantified by XPS. The electrochemical characteristics of the films were studied by electrochemical techniques, whereas the conductance of individual porphyrin constructs has been examined by STM using the molecular break junction method.

The multilayers show consistent linear growth in absorbance and film thickness over tens of layers as well as continuity and moderate ordering in their molecular structure. This flexible molecular LbL technique has the potential to control the nanoscale structure and function of the thin film materials for a variety of electro-optical applications.

FEMTOSECOND PUMP-PROBE STUDY OF ELECTRON-PHONON COUPLING IN COPPER THIN FILMS

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With continuing size reduction and operation frequency increase in nanoscale electronic device, the heat generation and the rapid increase of the electrical resistivity becomes critical issue in these devices. Electron-phonon coupling is a major scattering mechanism of the electrons, and contribute to the electrical resistance. Surface scattering mechanism has been discussed intensively as a source of the increase of the electrical resistive in confined structure, however, the contribution of the electron-phonon coupling to the increase of the resistivity is studied, much less extent. Therefore, it is crucial to carry out an in-depth investigation on the electron-phonon coupling in nanostructures.

In our experiment, we use ultrafast pump-probe technique to investigate the electron-phonon coupling of several epitaxial grown single crystal thin copper films. We used 800 nm pump wavelength, 595 nm probe wavelength, and the pump power we used here was within low power limit for different copper samples to avoid the nonlinear dependence of reflectivity change due to the temperature raise. The electron-phonon coupling constant, λ is extracted by using two-temperature model (TTM). The results show that the increase of the electron-phonon coupling constant on the film thickness.

TRANSPORT CHARACTERISTICS OF Zn PORPHYRIN IN AN ELECTROMIGRATED JUNCTION

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Incorporation of molecules as circuit elements in microelectronics is an attractive option due to their small size and the new functions that molecules can bring to the existing electronic devices. To realize such devices, we have fabricated nanogaps from gold nanowires and positioned a few porphyrin molecules in the gap. The conductance through the molecules is studied through two terminal current versus voltage (I-V) measurements and inelastic electron tunneling spectroscopy (IETS). I-V characteristics have shown signatures of molecular junction. We have measured dI/dV and d^2I/dV^2 (IETS measurements) from the molecular junctions at 4.2 K. Measurements at low temperature give insight to the inelastic tunneling of the electron through the confined zinc porphyrin molecule. The inelastic tunneling can excite the vibrational modes and by comparing these modes obtained from Raman spectra, it can be unambiguously proved if a molecular junction has been formed. IETS can also provide valuable insight to the electrode metal-molecule coupling and the role central atoms ligated to porphyrin can play in electron transport properties.

MEASUREMENT TECHNIQUES FOR CONTACT RESISTANCE BETWEEN METAL-THERMOELECTRIC MATERIALS

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Thermoelectric materials can provide solution to the problem of on-demand localized cooling sought by semiconductor and electronics industries. Contact electrical resistance becomes critical to the efficiency of thermoelectric devices with dimensions in the range of few hundreds of μm required by electronics and semiconductor industries. Effects of factors like diffusion across interface, contact parasitics, annealing conditions and material selection are yet to be completely understood in the case of metal-thermoelectric contacts. We deposited thin films of 100 nm of metals using sputtering on the top of nanostructured-bulk bismuth telluride fabricated using novel micro-wave technique. Contact electrical resistance was measured using the 3-probe technique and Transmission Line Mode (TLM) methods and both the techniques were compared.

DEVELOPMENT OF GaInN/GaN MULTIPLE QUANTUM WELL SOLAR CELLS GROWN BY MOCVD

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We have investigated the performance of GaInN/GaN multiple quantum well (MQW) solar cells grown by metal-organic chemical vapor deposition (MOCVD) on *c*-plane (0001) sapphire substrate. The active region contains 30 pairs of 3 nm thick quantum well and 9 nm thick quantum barrier, which is sandwiched between Si doped *n*-GaN layer and Mg-doped *p*-GaN layer.

Figure 1(a) shows the External Quantum Efficiency (EQE) calculated by illuminating the fabricated device with a power calibrated and monochromatized light from a Xenon lamp and measuring the short circuit photocurrent. The electroluminescence spectrum is measured by driving the fabricated die with 20 mA current as a reference. Around 10% EQE is obtained for the wavelength between 350 nm and 400 nm. Figure 1(b) shows that under standard 1-sun AM1.5G illumination, the fabricated device has an open circuit voltage (V_{oc}) of 0.81 V, a short circuit current density (J_{sc}) of 1.35 mA/cm² and a fill factor of about 57.3% at room temperature under standard 1-sun AM1.5G illumination. The peak output power density is calculated to be 0.63 mW/cm².

Further optimization is still being carried out to increase the quantum efficiency as well as the power output.

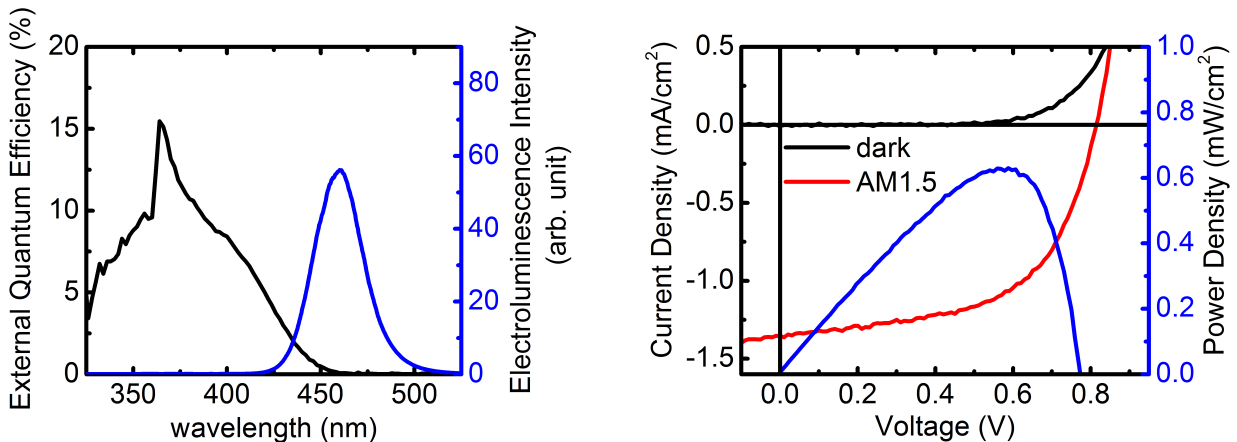


Figure 1 (a) External Quantum Efficiency of the solar cell and Electroluminescence spectrum measured at room temperature. (b) *I-V* curves of solar cell under dark condition and AM1.5G illumination, along with calculated *P-V* characteristic of the AM1.5G case.

ENHANCED SEEBECK IN NANOSTRUCTURED Sb_2Te_3 BY ANTISITE DEFECT SUPPRESSION THROUGH SULFUR DOPING

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Sculpting nanoscale building blocks with novel properties and retaining the nanostructuring-induced properties in larger scale assemblies are key to obtaining bulk nanomaterials with properties otherwise not attainable in non-nanostructured bulk materials. We have demonstrated a new class of both p- and n-type bulk nanomaterials with room-temperature thermoelectric figures of merit ZT as high as 1.1 from assemblies of pnictogen chalcogenide nanoplates obtained by a scalable (10 g/min) bottom-up approach. A unique aspect of our work is that our binary nanobulk thermoelectrics exhibit $ZT \sim 1$ by a combination of doping and nanostructuring, without any alloying additions, resulting in multi-fold ZT improvements over non-nanostructured non-doped counterparts. For example, antimony telluride is a low figure-of-merit ($ZT < \sim 0.3$) thermoelectric because of a low Seebeck coefficient α arising from degenerate carrier concentrations $\sim 10^{20} \text{ cm}^{-3}$ generated by antisite defects. Here, we report 10-25% higher α in sub-atomic percent sulfur doped nanocrystalline antimony telluride having up to hundred-fold lower carrier concentrations due to the suppression of antimony antisite defects.

High resolution X-ray photoelectron spectroscopy (XPS) using synchrotron radiation reveals lattice site-occupancy of the sulfur dopant atoms, and combined with Hall and Nernst coefficient measurements and a defect model for chalcogenides allows correlating the sulfur doping with observed electronic structure and defect chemistry changes. We show the presence of sulfur raises the lattice bond-polarity and increases the activation energy for formation of antisite defects, strongly suppressing their concentration. XPS of valence bands of the nanostructured antimony telluride reveal sulfur-induced density of states modification. The α increase, together with the nanostructuring-induced thermal conductivity decrease, in our *binary* antimony telluride yields a factor-of-three higher $ZT \sim 1$ at 423 K, thus also shifting the peak ZT to higher temperatures, outperforming state-of-art alloys. We conclude by presenting high-resolution XPS for p-type antimony telluride based alloys and n-type bismuth telluride providing insights for raising the power factors of pnictogen chalcogenides over bulk ceilings. Tuning the electron-crystal phonon-glass behavior by adapting our bottom-up approach for designing nanoscale building blocks should enable nanobulk thermoelectrics with further increases in ZT for transforming thermoelectric refrigeration and power harvesting technologies.