Science and Technology
of Materials, Interfaces, and Processing

2009 FALL MEETING of the AVS HUDSON MOHAWK CHAPTER

Tuesday, Oct 13, 2009
3-7pm,
CESTM auditorium
College of Nanoscale Science and Engineering
The University at Albany
257 Fuller Rd., Albany, NY

TALKS (3 to 5pm):

T1. Sputtering Behavior and Depth Resolution in Low Energy Ion Irradiation of GaAs
M.J.P. Hopstaken[1], D. Pfeiffer[1], M.S. Gordon[1], E.W. Kiewra[1], Yanning Sun[1], D.K. Sadana[1], T. Topuria[2], P.M. Rice[2], C. Gerl[3], C. Marchiori[3], M. Richter[3], M. Sousa[3], and J. Fompeyrine[3]
[1.] IBM T.J. Watson Research Center, Yorktown Heights (NY), USA
[2.] IBM Almaden Research Center, San Jose (CA), USA
[3.] IBM Research GmbH, Zurich Research Laboratory, Rüschlikon, Switzerland

T2. Photochemically Triggered Assembly of Composite Nanomaterials Through the Photodimerization of Adsorbed Anthracene Derivatives
Anthony R. Smith, David Watson
Department of Chemistry, University at Buffalo, The State University of New York
Buffalo, New York 14260-3000

T3. Influence of Aqueous Quantum Dots' Surfactant Structure on Attachment to Nanocrystalline TiO_2 Thin Films and Examining the Electron Injection Efficiency
Jeremy S. Nevins, Kathleen M. Coughlin, and David F. Watson
Department of Chemistry, University at Buffalo, The State University of New York
Buffalo, New York 14260-3000

T4. Titanium Nitride Based Durable Electrocatalysts for Proton Exchange Membrane Fuel Cells
Bharat Avasarala, Pradeep Haldar
College of Nanoscale Science and Engineering, University at Albany, Albany NY, 12203

T5. Front Metallization for Next Generation Photovoltaic Devices
Anh Nguyen[1***], Andrew Fioramonti [2], Denis Morrissey[2], Manisha Rane-Fondacaro[1], Zhouying Zhao[1], Harry Efstathiadis[1], Pradeep Haldar[1]
[1]Energy and Environmental Applications Center (E2TAC), College of Nanoscale Science and Engineering, University at Albany, State University of New York
[2]Technic, Inc., Plainview, NY

T6. Toughening Copper-Silica Interfaces Using Molecular Nanolayers
Saurabh Garg[1], Binay Singh[1], Ashutosh Jain[1], Xinxing Liu[2], P. G. Ganesan[1], L. Interrante[2], G. Ramanath[1*]
[1]*Materials Science and Engineering Dept, Rensselaer Polytechnic Institute, Troy, NY 12180.*
[2]*Chemistry Department, Rensselaer Polytechnic Institute, Troy, NY 12180*

POSTERS (5 to 7pm):

P1. Depth Profiling of Organic Electronics

John S. Hammond
Physical Electronics, 18725 Lake Drive East, Chanhassen, MN, USA 5544

P2. Chemical State Analysis of Nanotechnology Structures with Scanning Auger Microscopy

J. S. Hammond, D. F. Paul, D. Watson, P. E. Larson, R. E. Negri
Physical Electronics USA, 18725 Lake Drive East, Chanhassen, MN. 55317 USA

P3. Complete Band Offset Characterization of the $HfO_2/SiO_2/Si$ Stack using Charge Corrected X-ray Photoelectron Spectroscopy

*E. Bersch, *M. Di, **S. Consiglio, **R.D. Clark, **G.J. Leusink, and *A.C. Diebold
*College of Nanoscale Science and Engineering, University at Albany, 255 Fuller Rd., Albany, NY 12203
**TEL Technology Center, America, LLC, 255 Fuller Rd., Albany, NY 12203

P4. Programmable Nanoelectronics Using Memristor Nanomaterials

J.E. Van Nostrand[1] and B. Wysocki[1], R. Cortez[2], N. Cady[3] and M. Bergkvist[3]
[1]Information Directorate, Air Force Research Lab, Rome, NY
[2]Department of Mechanical Engineering, Union College, Schenectady, NY
[3]Nanobioscience, Albany College of Nanoscale Science and Engineering, Albany, NY

P5. Characterization of Aluminum Oxide Tunnel Barrier for use in a Non-Local Spin Detection Device

J. Abel, J. Garramone, I. Sitnitsky, E. Bersch, A.C. Diebold, and V. LaBella
College of Nanoscale Science and Engineering, University at Albany, 253 Fuller Rd, Albany, NY, 12203, USA

P6. Hot Electron Transport Properties of Thin Copper Films Using Ballistic Electron Emission Microscopy

J.J.Garramone[1], J.R. Abel[1], I.L. Sitnitsky[1], L. Zhao[2], I. Appelbaum[2], V.P. LaBella[1]
[1]University at Albany*,*
[2]University of Maryland*,*

P7. Sputter Deposition of Highly Flexible ITO on Polymeric Substrates

Brian Scherer, Min (Martin) Yan, Ahmet Gün Erlat, Paul McConnelee, Anil Duggal, Thomas Feist
GE Global Research

P8. Formation of $CuInAlSe_2$ Films Using Co-sputtered Precursors and Selenization

Daniel Dwyer[1], Ingrid Repins[2], Harry Efstathiadis[1], Pradeep Haldar[1]
[1]College of Nanoscale Science and Engineering, University at Albany, State University of New York, Albany, NY 12203
[2]National Renewable Energy Laboratory, Golden, CO 80401

P9. Si/SiC Superlattice Multilayer Quantum Wells For Thermoelectric Generation

Sean Teehan, Harry Efstathiadis, , Pradeep Haldar
College of Nanoscale Science and Engineering (CNSE), SUNY Albany
Dan Krommenhoek and Norbert Elsner
Hi-Z Technology, Inc., San Diego, California.

P10. Mass Spectrometer Calibration for Measurement of Photoresist Outgassing Species Identification and Quantification

Alin O. Antohe[1], Gregory Denbeaux[1], Chimaobi Mbanaso[1], Leonid Yankulin[1], Yu Jen Fan[1], Warren Montgomery[2]
[1]College of Nanoscale Science and Engineering, University at Albany, NY
[2]SEMATECH, Albany, NY

P11. Relationship of Aluminum Grain Size to the Grain Size of Polycrystalline Silicon Produced by the Aluminum Induced Crystallization of Amorphous Silicon
Emilio Stinzianni, Kathleen Dunn, Zhao Zhouying, Manisha Rane-Fondacaro, Harry Efstathiadis, and Pradeep Haldar
Energy and Environmental Applications Center (E2TAC), College of Nanoscale Science and Engineering, University at Albany, State University of New York

P12. Aberration-Corrected HRTEM and HAADF-STEM Simulation Study of Few-Layer Graphene
F. Nelson[1], A.C. Diebold[1], R. Hull[2]
[1]College of Nanoscale Science and Engineering, University at Albany, Albany, N.Y. 12203
[2]Rensselaer Polytechnic Institute (RPI), 110 8th St., Troy, NY 12180

P13. The Relative Classification of Carbon Containing Molecules Related to the Contamination of Extreme Ultraviolet Lithography (EUVL)
Leonid Yankulin, Rashi Garg, Alin Antohe, Petros Thomas, Yu Jen Fan, Chimaobi Mbanaso, Gregory Denbeaux, - College of Nanoscale Science and Engineering, University at Albany, NY
Vibhu Jindal, Andrea Wuest, SEMATECH, Albany, NY 12203

P14. Wavelength Dependence of Carbon Contamination on Mirrors with Different Capping Layers
Petros Thomas, Leo Yankulin, Rashi Garg, Chimaobi Mbanaso, Alin Antohe, Yujen Fan, Gregory Denbeaux, CNSE, University at Albany, NY 12203
Vibhu Jindal and Andrea Wuest, SEMATECH, Albany, NY 12203

P15. Low Relaxation Rate in Epitaxial Vanadium Doped Iron Ultrathin Films
Lili Cheng, Christian Scheck, and William Bailey
Materials Science and Engineering Program, Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY 10027

P16. Two-Dimensional Computer Modeling of Single Junction a-Si:H Solar Cells
Changwoo Lee, Harry Efstathiadis, James E. Raynolds, Pradeep Haldar
Energy and Environmental Applications Center (E2TAC)
College of Nanoscale Science and Engineering
University at Albany, State University of New York

P17. Impact of Carbon Contamination on Patterned Extreme Ultraviolet (EUV) Masks
Yu-Jen Fan[1,1], Leonid Yankulin[1], Alin Antohe[1], Rashi Garg[1], Petros Thomas[1], Chimaobi Mbanaso[1], Andrea Wüest[2], Frank Goodwin[2], Sungmin Huh[2]
Patrick Naulleau[3], Kenneth Goldberg[3], Iacopo Mochi[3]
Gregory Denbeaux[1]
[1]College of Nanoscale Science and Engineering, University at Albany
[2]SEMATECH
[3]CXRO, Lawrence Berkeley National Lab

P18. Platinum Monolayer Electrocatalysts for O2 Reduction: Pt Monolayer on Carbon-Supported PdIr Nanoparticles
Seth L. Knupp[1], Miomir Vukmirovic[2], Radoslav Adzic[2] and Pradeep Haldar[1]
[1]College of Nanoscale Science and Engineering, University at Albany, State University of New York, Albany, New York 12203, USA
[2]Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973-5000

P19. Eutectic Mixtures of Room Temperature Ionic Liquids Electrolytes for Electric Double Layer Capacitors

Seiichiro Higashiya[1], Thamarai selvi Devarajan[1], Manisha V. Rane-Fondacaro[1], Pradeep Haldar[1]
[1]Energy and Environmental Applications Centre (E2TAC), Collage of Nanoscale Science and Technology, University at Albany, 257 Fuller Road, Albany, New York 12203, USA

P20. Porous Silicon Based Electric Double Layer Capacitors

Thamarai selvi Devarajan[1], Seiichiro Higashiya[1], Manisha V. Rane-Fondacaro[1] and Pradeep Haldar[1]
[1]College of Nanoscale Science and Engineering, University at Albany, SUNY, Albany NY, 12203

P21. Angle Resolved XPS and Its Application in Advanced High-K Gate Dielectric Research

S. Consiglio, R. D. Clark, C. S. Wajda, and G.J. Leusink
TEL Technology Center, America, LLC, 255 Fuller Road, Albany, NY, 12203, USA

P22. Chromatic White Light Profilometer

Rosalyn L. Neander and Sara G. Ostrowski,
General Electric Research and Development, Niskayuna NY, 12309, USA

ABSTRACT for TALKS

Sputtering Behavior and Depth Resolution in Low Energy Ion Irradiation of GaAs

M.J.P. Hopstaken[1], D. Pfeiffer[1], M.S. Gordon[1], E.W. Kiewra[1], Yanning Sun[1], D.K. Sadana[1], T. Topuria[2], P.M. Rice[2], C. Gerl[3], C. Marchiori[3], M. Richter[3], M. Sousa[3], and J. Fompeyrine[3]

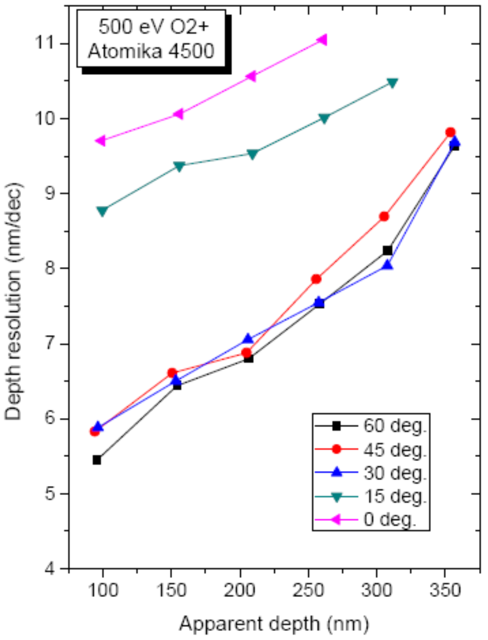
1. IBM T.J. Watson Research Center, Yorktown Heights (NY), USA
2. IBM Almaden Research Center, San Jose (CA), USA
3. IBM Research GmbH, Zurich Research Laboratory, Rüschlikon, Switzerland
Marco.hopstaken@us.ibm.com 914-945-2570

Recently, there has been renewed research interest for application of GaAs and related III-V compound semiconductors as high-mobility channel material in ultimate sub-22 nm CMOS technology [1]. To achieve extreme scaling – competitive with mainstream Si-based devices–, Ultra Shallow Junction (USJ) formation in III-V materials will be one of the key enablers for successful CMOS process integration. In the more widely established application of III-V quantum well (QW) structures for optoelectronic devices, abruptness of hetero-epitaxial interfaces is known to have large impact on device performance [2]. Successful development of above-mentioned applications requires the accurate characterization of in-depth chemical distribution with nanometric precision. Whereas Ultra-Low Energy (ULE) SIMS is a well established technique for the characterization of USJ in Silicon with sub-nm resolution, sputtering of GaAs and related III-V compound semiconductors has been reported to be very sensitive to ion-beam induced formation of topography [3, 4].

Here we report on the effects of sputtering of GaAs and impact on depth resolution under low (sub-keV) energy ion irradiation for different ion beams at varying impact angles. We have used an MBE grown GaAs/InGaAs QW structure, which has been well characterized by Transmission Electron Microscopy (TEM) and Rutherford Backscattering Spectroscopy (RBS). Presence of multiple InGaAs delta-layers with nearly atomic abruptness allows assessment of depth resolution and Its evolution in depth during sputtering of GaAs.

In case of O_2^+ ion beam irradiation, strong anomalies in sputtering behavior have been observed at lower impact energies near normal incidence with progressive degradation of depth resolution (see Figure). Moreover, we have observed remarkable ion yield variations as evidenced from transient changes in GaAs matrix species and their O-associated cluster ions. Results are explained in terms of altered oxide layer formation and development of surface topography.

In case of 1 keV oblique incidence Cs+ ion beam irradiation, GaAs sputtering behavior is well behaved and comparable to Si-sputtering behavior with a constant depth resolution as low as 3 nm/decade over a large depth range. Preliminary experiments reveal further improvement in depth resolution using sub-keV Cs+ ion impact energies, enabling high-resolution SIMS in III-V materials.



References:

1. S.J. Koester, E.W. Kiewra, Yanning Sun, D.A. Neumayer, J.A. Ott, M. Copel, D.K. Sadana, D. J. Webb, J.Fompeyrine, J.-P. Locquet, C. Marchiori, M. Sousa and R. Germann, *Appl. Phys. Lett.* **89**, 042104 1-3 (2006)
2. K. Muraki, S. Fukatsu, and Y. Shiraki, and R. Ito, *Appl. Phys. Lett.* **61** (5), 557 (1992)
3. A. Karen, K. Okuno, F. Soeda, and A. Ishitani, *J. Vac. Sci. Technol. A* **9** (4), 2247 (1991)
4. S.W. MacLaren, J.E. Baker, N.L. Finnegan, and C.M. Loxton, *J. Vac. Sci. Technol. A* **10** (3), 468 (1992)

Photochemically Triggered Assembly of Composite Nanomaterials through the Photodimerization of Adsorbed Anthracene Derivatives

Anthony R. Smith, David Watson

Department of Chemistry, University at Buffalo, The State University of New York
Buffalo, New York 14260-3000
ARSmith4@buffalo.edu (716)645-4193

We have exploited interfacial photodimerization reactions between adsorbed molecules to achieve the organization of nanoscale components into ordered assemblies in three dimensions and on surfaces. The combination of top-down and bottom-up assembly methods has proven useful for the patterned deposition of nanoparticles onto surfaces. However, the photochemically triggered attachment of nanoparticles to surfaces may enable the preparation of composite nanomaterials via a single photochemical reaction. We have developed a novel approach, in which photoinduced interfacial [4+4] cycloaddition reactions between adsorbed anthryl derivatives were utilized to induce the aggregation of dispersed gold nanoparticles and to attach gold nanoparticles to nanocrystalline metal oxide films. By illuminating through a photomask, patterned arrays of nanoparticles with ~ 100-μm features were deposited onto ZrO_2 surfaces. Composite materials were characterized by ultraviolet/visible/near-IR (UV/Vis/NIR) spectroscopy, transmission electron microscopy (TEM), and time-of-flight secondary ion mass spectrometry (ToF-SIMS). This presentation will focus on surface functionalization chemistry, photoinduced reactions in solution and on surfaces, photochemically triggered materials assembly processes, and the characterization of composite nanomaterials. The use of interfacial phtodimerization reactions to trigger materials assembly processes may represent an attractive fabrication strategy, in which patterned nanostructured materials, potentially including ternary and higher-order materials, are formed in one step.

Influence of Aqueous Quantum Dots' Surfactant Structure on Attachment to Nanocrystalline TiO_2 Thin Films and Examining the Electron Injection Efficiency

Jeremy S. Nevins, Kathleen M. Coughlin, and David F. Watson

Department of Chemistry, University at Buffalo, The State University of New York
Buffalo, New York 14260-3000
jsnevins@buffalo.edu (518)-232-8667

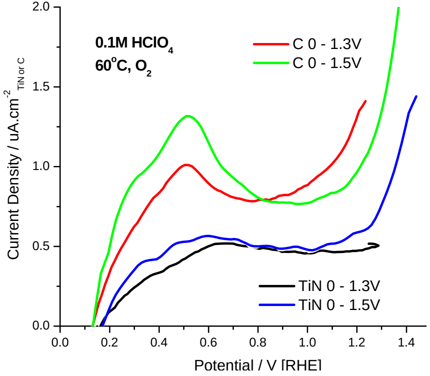
This presentation will focus on developing a 'greener' method for the attachment of quantum dots to metal oxide surfaces with the long term goal of creating efficient solar cells. CdSe nanoparticles were synthesized from aqueous solutions of cadmium sulfate and sodium selenosulfate. These precursors were mixed at room temperature in the presence of deprotonated surfactants such as L-cysteine, 3-mercaptopropionic acid (MPA), and mercaptosuccinic acid (MSA). This process yielded stable, aqueous suspensions. Cysteine-capped quantum dots exhibited sharper and more intense absorbance bands than MPA- and MSA-capped quantum dots, indicating greater monodispersity. Each surfactant's deprotonated carboxylate group allowed for the attachment of the aqueous quantum dot to the surface of nanocrystalline TiO_2 films. Equilibrium binding experiments revealed that the maximum surface coverage of cysteine-capped quantum dots was twice that of MPA-capped quantum dots. The surface adduct formation constant for cysteine-capped quantum dots was approximately an order of magnitude greater than that of MPA-capped quantum dots. Changes in pH influenced the absorbance and emission spectra of suspensions of cys-CdSe quantum dots, as well as their affinity for the TiO_2 surface. The surface coverage increased with decreasing pH, suggesting that the amine group of cysteine was involved in coordination to TiO_2. Quantum dot-sensitized solar cells (QDSSCs) with CdSe-functionalized TiO_2 working electrodes were characterized. Incident photon-to-current conversion efficiencies (IPCE) of cysteine-capped quantum dots were greater than those of MPA-capped quantum dots. Electron injection from the cysteine-capped CdSe quantum dot into TiO_2 was characterized using transient absorption spectroscopy. The influence of the structure of capping groups on the efficiency of materials assembly processes and electron-transfer processes will be discussed.

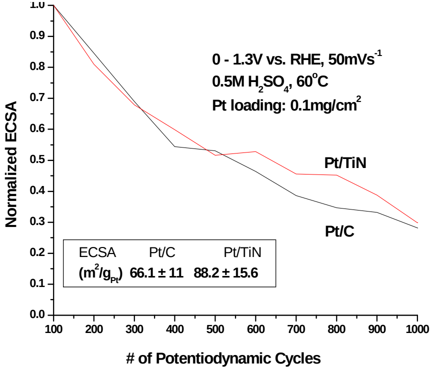
Titanium Nitride Based Durable Electrocatalysts for Proton Exchange Membrane Fuel Cells

Bharat Avasarala, Pradeep Haldar
College of Nanoscale Science and Engineering, University at Albany, Albany NY, 12203
bavasarala@uamail.albany.edu (518) 596 8616

Proton exchange membrane fuel cells (PEMFCs) are a promising power technology as stationary power sources and automotive engines. A significant challenge hindering large-scale implementation of PEMFC technology is its poor durability; which occurs due to the loss of performance through (Pt nanoparticles on C) electrocatalyst degradation[1] during extended operation and repeated cycling in the corrosive conditions of PEMFC system. An important contribution to this degradation is the carbon support corrosion in chemically and electrochemically oxidizing conditions of a PEMFC system.

In the present work, we show that titanium nitride (TiN) nanoparticles can be used as a novel catalyst support material in PEMFC and when catalyst particles are supported on TiN particles, it can outperform the conventional Pt/C electrocatalyst in terms of catalytic activity and durability. TiN has higher electrical conductivity, comparable to that of carbon and outstanding oxidation and acid corrosion resistance.[2] These unique properties can enable TiN nanoparticles to withstand the harsh operating conditions of PEMFC and has the potential to replace carbon as a support.





<u>Fig1</u> (Left): cyclic voltammetry of TiN & C, at high potentials in corrosive PEMFC conditions **<u>Fig 2</u>** (Right): Accelerated Durability Test of Pt/TiN & commercial Pt/C under similar PEMFC conditions & same Pt loading.

Figure 1 shows that at higher potentials, C corrodes at much higher rate than TiN, thus degrading the Pt/C in short-term. Pt/TiN electrocatalyst, synthesized using polyol process shows comparable durability to Pt/C and has a higher catalytic performance (electro-chemical surface area). Preliminary results indicate that optimization of polyol process can increase the durability of Pt/TN.

Reference: (1). H. Gasteiger et al, Handbook of Fuel Cells, Fundamentals, Technology and Applications, John Wiley & Sons, 2003. **(2).** S. T. Oyama, The chemistry of transition metal carbides and nitrides, Springer, London, 1996.

Front Metallization for Next Generation Photovoltaic Devices

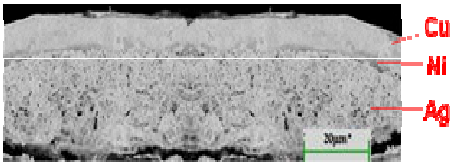
Anh Nguyen[1***], Andrew Fioramonti [2], Denis Morrissey[2], Manisha Rane-Fondacaro[1],
Zhouying Zhao[1], Harry Efstathiadis[1], Pradeep Haldar[1]

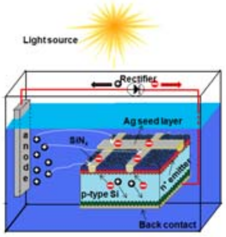
[1]Energy and Environmental Applications Center (E2TAC)
College of Nanoscale Science and Engineering
University at Albany, State University of New York
[2]Technic, Inc.
Plainview, NY
anguyen@uamail.albany.edu 518-533-8481

Currently, several metal contact fabrications techniques are commonly used for industrial solar cell front metallization, but each has its own limitations. Screen-printing is normally used for commercial silicon solar cells and allows for speedy metallization at relatively low cost. Nevertheless, there are several unwanted features such as low aspect ratio of the grid lines which creates large shading area on the front of the PV devices, and a high line resistance which lowers the final efficiency. Photolithography and metal evaporation techniques are often used for high efficiency cells since they offer improved gridline quality, however the processes are time-consuming and expensive. For the next generation of crystalline silicon solar cells when the wafer size increases from 100cm^2 to 243cm^2, a low cost metallization with low resistivity and high aspect ratio is needed.

Recently, light induced electroplating (LIP) of silver (Ag) metal on top of the front contact grid has shown promise in reducing line resistivity and increasing cell power output but received limited acceptance in the industry due to the cost of plating a precious metal layer, Ag. The feasibility of using this LIP technique to plate non-precious metals, such as nickel (Ni), copper (Cu), or tin (Sn) is well desired for PV fabrication process due to the ease of the process and the use of a lower cost material. Cu has higher electrical conductivity compared to Ag and is much cheaper material.

We developed a two-layer metallization process that deposited Cu as current-carrying electrodes by LIP technique on thin screen-printed Ag paste seed layers. A Ni layer was also deposited by LIP as the barrier and Cu adhesion layer. By optimizing the thickness of the plated Ni and Cu layers, line resistivity of 1.75µOhm-cm comparable to that of bulk Cu, 1.68µOhm-cm and bulk Ag, 1.59µOhm-cm was achieved. A 25% increase in fill factor was also achieved due to the reduction in the solar cells series resistance. We also found that Ni layer played much bigger role than being just a barrier layer to the overall line resistivity.





Toughening Copper-Silica Interfaces Using Molecular Nanolayers

Saurabh Garg[1], Binay Singh[1], Ashutosh Jain[1], Xinxing Liu[2], P. G. Ganesan[1], L. Interrante[2], G. Ramanath[1*]

[1]Materials Science and Engineering Dept, Rensselaer Polytechnic Institute, Troy, NY 12180.
[2]Chemistry Department, Rensselaer Polytechnic Institute, Troy, NY 12180

We demonstrate a novel strategy for toughening metal-dielectric interfaces by catalyzed fissure of low-polarizability moieties in an organosilane monolayer. Photoelectron spectroscopy and ab initio calculations show that sevenfold toughening of Cu-silica interfaces is due to Cu-catalyzed disilacyclobutane ring opening and siloxane bridging. Our findings open up possibilities for directly integrating metals with molecularly-derived low permittivity dielectrics for applications without using an intermediary glue layer, e.g., by incorporating strained moieties into precursors. Low-k dielectrics derived from cyclolinear polycarbosilanes with 1,3-Disilacyclobutane (DSCB) rings offer promise for realizing this exciting possibility because Cu immobilization through strong ring opening and bonding could conceivably enhance adhesion as well as inhibit metal transport. Such chemically-induced interfacial toughening through interaction of copper with carbosilane rings confirms the possibility of, and paves the way for, realizing the direct integration of Cu with molecularly tailored low-k dielectric materials.

We synthesized DSCB ring-terminated organosilanes and assembled them on silica substrates to form a 0.7 nm thick molecular nanolayer, verified by variable take-off angle X-ray photoelectron spectroscopy (XPS) and ellipsometry. Four-point bending fracture tests on as-prepared Cu/DSCB/SiO_2 sandwiches revealed a very low interface toughness of 2.1 J/m^2, comparable to that exhibited by pristine Cu/SiO_2 structures, consistent with core-level XPS spectra indicating Cu/DSCB interface fracture due to the lack of any significant bond formation. Upon annealing to 250 ºC fracture occurs at the DSCB/SiO_2 interface, indicative of Cu-DSCB interface strengthening. The interfacial toughness increases monotonically with annealing temperature, yielding values as high as 21.3 J/m^2 for T_{anneal} = 600 ºC. Interfaces with a methyl terminated monolayers (i.e., without the DSCB ring) showed 50% lower toughness values for the same deposition and annealing conditions, underscoring the crucial role of the DSCB rings. XPS fracture surface analysis combined with infrared analyses of the annealing behavior of DSCB-containing molecules on different surfaces shows that annealing-induced Cu-catalyzed ring opening of DSCB and strong siloxane bonding at the DSCB/SiO_2 interface are the main mechanisms of interfacial toughening. Our results demonstrate that carbosilane rings could be useful to enhancing toughness of metal-dielectric interfaces either directly in a polymeric material or through use in a molecular nanolayer.

ABSTRACT for POSTERS

Depth Profiling of Organic Electronics

John S. Hammond

Physical Electronics, 18725 Lake Drive East, Chanhassen, MN, USA 5544
jhammond@phi.com   952-828-6469

The research and development of organic electronic devices, particularly organic photovoltaic devices and organic light emitting diodes, has recently drawn considerable interest due to the potential for unique fabrication configurations and the potential for highly efficient, yet low cost devices. In addition to the macro-properties of these potential devices which can be characterized by electrical testing of the photon conversion efficiency or photon generation efficiency, chemical and physical characterization on nanoscale is needed to elucidate and control device fabrication parameters, efficiencies, and ultimately degradation and lifetime parameters.

The combination of mono-atomic ion sputter depth profiling with surface analysis techniques such as X-ray Photoelectron Spectroscopy (XPS) and Secondary Ion Mass Spectrometry (SIMS) have been widely used to elucidate nanoscale properties of inorganic photovoltaic and photonic devices. However, this approach has been completely unsuccessful for characterizing organic thin film structures. The recent development of C_{60} cluster ion sources has opened a revolutionary approach to the characterization of organic electronic devices.

A basic understanding of cluster ion sputter depth profiling will first be presented. Examples of multi-layer organic profiling will then be discussed to illustrate the differences between thermal deposition and solvent deposition of organic devices, as well as the elucidation of degradation mechanisms or these organic devices. Multi-layer chemical profiles of organic photovoltaics as well as organic light emitting diodes will be presented.

Chemical State Analysis of Nanotechnology Structures with Scanning Auger Microscopy

J. S. Hammond, D. F. Paul, D. Watson, P. E. Larson, R. E. Negri
Physical Electronics USA, 18725 Lake Drive East, Chanhassen, MN. 55317 USA

Scanning Auger Microscopy is a powerful compositional analysis technique for nanotechnology structures. Modern field emission Auger systems that are designed for long term image stability and incorporate a CMA analyzer for Auger imaging with minimal topographical shadowing, can provide quantitative Auger elemental information with a spatial resolution better than 10 nm.

When performing Auger analysis of some nanotechnology structures, it may also be advantageous to investigate the chemical environment under the probe beam. A new capability has been developed for the PHI Scanning Auger Nanoprobe to obtain high energy resolution spectral analysis. The Auger mapping analysis of a nanocone structure will be discussed to illustrate the combination of high spatial resolution Auger mapping and this new high energy resolution capability.

Complete Band Offset Characterization of the HfO_2/SiO_2/Si Stack using Charge Corrected X-ray Photoelectron Spectroscopy

*E. Bersch, *M. Di, **S. Consiglio, **R.D. Clark, **G.J. Leusink, and *A.C. Diebold
**College of Nanoscale Science and Engineering, University at Albany, 255 Fuller Rd., Albany, NY 12203*
***TEL Technology Center, America, LLC, 255 Fuller Rd., Albany, NY 12203*

The HfO_2-Si valence and conduction band offsets (VBO and CBO, respectively) of technologically relevant HfO_2/SiO_2/Si film stacks have been measured by several methods, with several groups reporting values within a range of 1 eV or more for both quantities. In this study we have used a combination of X-ray photoemission spectroscopy (XPS) and spectroscopic ellipsometry (SE) to measure the HfO_2-Si VBO and CBO of both as deposited and annealed stacks. Unlike previous XPS-based measurements of the HfO_2-Si VBO, we have corrected for the effect of charging in the XPS measurement. We find that after correction for charging, the HfO_2-Si VBOs are decreased from their typical XPS-measured values, and agree better with values measured by UV photoemission spectroscopy (UPS) and internal photoemission (IPE). We also report values for the rarely reported HfO_2-SiO_2 and SiO_2-Si VBOs and CBOs in HfO_2/SiO_2/Si stacks. In addition to the band offsets, XPS was used to measure the band bending in the Si substrate of HfO_2/SiO_2/Si film stacks. Unannealed HfO_2 stacks showed downward Si band bending of ~-0.4 – -0.5 eV, while annealed HfO_2 stacks showed negligible band bending. Finally, we investigated the composition of the SiO_2 layer in SiO_2/Si and HfO_2/SiO_2/Si. We observed that the growth of the HfO_2 films resulted in the growth of the SiO_2 underlayer and an increase in the level of sub-oxide species by decomposing the Si 2p spectra into the spin orbit partner lines of its 5 oxidation states. As we were able to decompose these spectra effectively using established relative binding energies for each oxidation state, we concluded that the SiO_2 films in HfO_2/SiO_2/Si stacks were composed primarily of stoichiometric SiO_2.

Programmable Nanoelectronics using Memristor Nanomaterials

J.E. Van Nostrand and B. Wysocki
Information Directorate, Air Force Research Lab, Rome, NY

R. Cortez
Department of Mechanical Engineering, Union College, Schenectady, NY

N. Cady and M. Bergkvist
Nanobioscience, Albany College of Nanoscale Science and Engineering, Albany, NY

Joseph.VanNostrand@rl.af.mil (315) 330-4920

This newly started research investigations is centered around three major research directions:
(1) *Metal oxide nanoshell memristors and nanowire synthesis including* TiO_2 *and ZnO.* The aim of this research is to develop practical techniques to synthesize metal oxide nanoshells and nanowires that exhibit memristance properties. A key requirement for synthesis techniques is to use processes that are compatible with CMOS electronics. This will allow for development of a synthesis process that can be used on finished CMOS wafers, and thus can take advantage of decades of advances in this technology. (2) *Nanofabrication technology that explores techniques such as functionalization and self-assembly for bottom up fabrication.* Fabrication of nanoshells and nanowires focuses on a bottom-up approach to computer architecture implementation. While it is essential to have techniques for the synthesis of nanoshells and nanowires with appropriate properties, these would be of no use without the ability to either place these electronic materials in their appropriate location or to synthesize the nanomaterials in place. Both of these techniques will be considered under this effort. (3) *Characterization of memristive nanoshells and nanowires, including electronic transport properties and morphology.* Probing the electronic properties of components at the nanometer scale poses significant challenges. The nanoshell memristors in this effort are often only a few hundred nanometers in diameter. Nanowires have lengths on the order of a few microns making them more amenable to measurement, but again have a diameter that is similar to nanoshells. Techniques such as SEM, TEM, and scanning conductance AFM will be used to characterize the microstructure, morphology and transport properties of these nanomaterials. The technical approach and current progress in this effort will be described.

Characterization of Aluminum Oxide Tunnel Barrier for use in a Non-Local Spin Detection Device

J. Abel, J. Garramone, I. Sitnitsky, E. Bersch, A.C. Diebold, and V. LaBella

College of Nanoscale Science and Engineering, University at Albany, 253 Fuller Rd,
Albany, NY, 12203, USA

jabel@uamail.albany.edu

Aluminum oxide can be utilized as an interface layer between ferromagnetic metals and silicon to achieve spin injection into silicon. Utilizing the spin of the electron as well as its charge has the potential to be utilized for logic devices in the post CMOS era. The goal of our research is to inject and readout spins using a non-local measurement device that utilizes 1-3 nm aluminum oxide interface layers as tunnel barriers.

The first step of fabricating a non-local measurement device out of silicon is the growth of an aluminum oxide tunnel barrier[1]. Si (001) wafers were dipped in 49% HF solution for approximately 2 min to remove the native oxide layer. The wafers were then immediately loaded into an ultrahigh vacuum MBE machine, degassed at 400 C and cooled to room temperature. After cooling, a desired thickness of aluminum was deposited from a Knudsen cell. The sample was then transferred back into the load lock and exposed to approximately 130 mTorr of pure O_2 for 20 min. The process was repeated to create samples with a thickness of 1 nm, 2 nm, and 3 nm of aluminum oxide. Each thickness was grown in 0.5 nm and 1 nm steps. In addition, a 2 nm sample was grown, in one 2 nm step.

X-ray photoelectron spectroscopy was performed to characterize the film stoichiometry. It was observed that all the aluminum was bonded to the oxygen for the films grown in 0.5 nm and 1 nm steps. Whereas the 2 nm sample grown in one 2 nm step not all the aluminum bonded to oxygen, leaving a partially un-oxidized aluminum film. In addition XPS was used to measure the band gap of the fully oxidized films to be 6.61 eV in good agreement with films of similar thickness[2]. We will also report on current voltage measurements of these films after they have been capped with metal.

References:
[1] O. van’t Erve, A. Hanbicki, M. Holub, C. Li, C. Awo-Affouda, P. Thompson and B. Jonker, Appl. Phys. Lett. **91**, 212109 (2007).
[2] H.Y. Yu, et al., *Appl. Phys. Lett.*, 81:376, 2002

Hot Electron Transport Properties of Thin Copper Films Using Ballistic Electron Emission Microscopy

J.J.Garramone[1], J.R. Abel[1], I.L. Sitnitsky[1], L. Zhao[2], I. Appelbaum[2], V.P. LaBella[1]

[1]University at Albany,

[2]University of Maryland,

jgarramone@uamail.albany.edu (315) 527-4011

Copper is widely used material for electrical interconnects within integrated circuits. In addition it has been recently utilized as a base layer for hot electron spin injection and readout into silicon [1]. Integral to both their application is the knowledge of the electron scattering length. Surprisingly little work exists that directly measures the scattering length of electrons in copper. One method for studying hot electron transport on the nanometer length scale is ballistic electron emission microscopy (BEEM). BEEM is a three terminal scanning tunneling microscopy (STM) based technique, where electrons tunnel from a STM tip into the grounded metal base of a Schottky diode [2]. The electrons that transverse the metal overlayer and surmount the Schottky barrier are measured as the BEEM current by a backside contact to the semiconductor.

In this study we used BEEM to measure the hot electron attenuation length of copper on Si. The samples consists of Au/Cu/Si(001) Schottky diodes and the measurements were taken at 77K under UHV conditions. The Au capping layer is used to inhibit the growth of copper's native oxide. Analysis of BEEM current as a function of tip bias yield a Schottky barrier height of 0.64±0.02 eV. The barrier height is in good agreement with previous current-voltage measurements [3-5]. This, along with Rutherford backscattering spectrometry, indicates that we are measuring the Cu/Si Schottky height and have the ability to measure the attenuation length of copper by measuring the BEEM current as a function of Cu thickness. The measured hot electron attenuation length of Cu is 33.4±1.2 nm at a tip bias of 1.0 eV. The attenuation length decreases monotonically with increasing tip bias and is in good agreement with electron-electron scattering as derived from Fermi liquid theory with the addition of an elastic scattering term that is independent of tip bias. This provides insight into sources of both elastic and inelastic scattering of electrons in Cu.

References:

[1] Biqin Huang, et al., Phys. Rev. Lett. 99 177209 (2007)
[2] L. D. Bell and W. J. Kaiser, Phys. Rev. Lett. 61 2368 (1988)
[3]R. W. Soshea, et al., Phys. Rev. 138 A1182 (1965)
[4] J. M. Seiller, et al., Solid State Commun. 15 973 (1974)
[5]C. R. Crowell, et al., Phys. Rev. 127 2006 (1962)

Sputter Deposition of Highly Flexible ITO on Polymeric Substrates

Brian Scherer, Min (Martin) Yan, Ahmet Gün Erlat, Paul McConnelee, Anil Duggal,
Thomas Feist

GE Global Research

scherer@research.ge.com (518) 387 7693

High quality Indium Tin Oxide (ITO) coated polymeric films serve as the ideal substrate for flexible optoelectronic devices such as organic light emitting diodes (OLEDs) and photovoltaics. However, achieving ITO coatings that are substantially uniform and flexible while maintaining low sheet resistance is not trivial. In this contribution we describe a novel modification to a conventional DC magnetron sputtering setup that allowed us to make highly transparent, flexible, and uniform coatings of ITO with low sheet resistance. This was achieved by blocking the deposition from certain areas of the ITO sputtering target with the insertion of a shadow mask in-between the substrate and target.

Formation of $CuInAlSe_2$ Films Using Co-sputtered Precursors and Selenization

Daniel Dwyer[1], Ingrid Repins[2], Harry Efstathiadis[1], Pradeep Haldar[1]

[1]College of Nanoscale Science and Engineering, University at Albany, State University of New York, Albany, NY 12203
[2]National Renewable Energy Laboratory, Golden, CO 80401
DDwyer@uamail.albany.edu 518-796-6768

Much of the work on Cu-chalcopyrite absorber materials has been focused on $CuInGaSe_2$ (CIGS). In these films Ga is substituted for In in the $CuInSe_2$ lattice to increase the band gap (E_g) from ~1 eV ($CuInSe_2$) to as high as ~1.7 eV ($CuGaSe_2$). Theoretically an absorber layer with an E_g ~ 1.4 – 1.45 eV would give the highest efficiency for a single junction device, however high efficiency CIGS are limited to an E_g ~ 1.15 eV. This equates to a Ga/(Ga+In) ratio of ~ 0.3. As more Ga is introduced beyond this point device efficiencies decrease, presumably as a result of defects which degrade the electronic properties of the films.

Aluminum can be used as an alternative to gallium to increase the absorber band gap. $CuInAlSe_2$ (CIAS) films have a band gap range of ~1 eV ($CuInSe_2$) to ~2.7 eV ($CuAlSe_2$). A CIAS film would require less than half the Al substitution for In as Ga would be needed in CIGS to produce the same band gap film. This means reduced lattice deformation in CIAS, which may result in fewer defects associated with higher band gap films.

CuInAl precursor films with increasing Al/(In+Al) concentrations were co-sputtered onto Mo coated soda-lime glass substrates. Precursor film morphology was investigated with scanning electron microscopy (SEM), crystalline phases were determined with x-ray diffraction (XRD), chemical composition was measured with electron probe microanalysis (EPMA), and compositional depth profiles were obtained with Auger electron spectroscopy (AES). Films were then selenized under high vacuum using thermally evaporated elemental selenium using a single-step high temperature heating profile. Surface and cross-sectional morphology of selenized films was observed with SEM, XRD was used to determine crystalline phases and amount of Al incorporation in the film, chemical composition was measured with EPMA, and depth profiles were obtained with AES. Analysis of the properties of co-sputtered precursors and selenized films will be presented, as well as the effect of selenization annealing parameters on co-sputtered CuInAl precursors.

Si/SiC Quantum Wells for Thermoelectric Applications

Sean Teehan, Harry Efstathiadis, Pradeep Haldar
College of Nanoscale Science and Engineering,
University at Albany, State University of New York, Albany, NY.

Dan Krommenhoek and Norbert Elsner
Hi-Z Technology, Inc., San Diego, CA.

The recovery of waste heat from internal combustion engines, truck and car exhausts, furnaces, etc., requires high performance power-generating thermoelectric materials to meet challenging cost goals. One third of the fuel that goes into a vehicle goes to the exhaust. This kind of inefficiency leads to greater consumption of nonrenewable resources, with greater pollution in the form of exhaust gases and waste heat The field of thermoelectrics is on the verge of a revolution, based on the use of multilayer film structures. The use of structures with quantum well (QW) confinement and decreased thermal conductivity leads to striking increase in the efficiency of thermoelectric power generating devices, which in turn reduce the cost/watt.

Recent advances in thermoelectric conversion, in the area of QW thin film (thickness of each layer is ~10 nm) materials, have demonstrated the potential for achieving the desired high-efficiencies and power densities that can be used for fabricating future power supplies, self powered appliances, and space power supplies.

The performance of a thermoelectric device is quantified by the dimensionless figure of merit ZT=S2σT/K, where S is the Seebeck coefficient, σ is the electrical conductivity, T is the absolute temperature and K is the thermal conductivity. Currently the best known bulk material can only achieve a ZT of around 1 at room temperature.

It has been shown that using 30+ periods of alternating Si/SiGe multilayers of 8-10nm thickness per layer we can achieve ZT values closer to 4, which is necessary for commercialization. This is due to QW confinement of phonon transmission due to Bragg reflection at lattice interfaces. Recently Germanium is becoming more popular in the IC industry and its cost has risen, so for this reason we are investigating the use of SiC as an alternate material to replace the SiGe.

We are using RF sputtering to deposit doped Si/SiC superlattices while varying the number of periods, and quantum well thicknesses. These depositions have been performed at various substrate deposition temperatures. From these depositions we have obtained uniformly smooth and dense multilayer films. With further annealing (>1000˚C) it has been shown using XRD that we have induced some crystallinity. The thermoelectric measurements on these samples at ~600K have achieved electrical resistivites on the order of mOhms, Seebeck coefficients greater than 500µV/K, and have shown thermal conductivity a magnitude lower than amorphous bulk material.

To proceed further with this work, we are trying to understand the development of crystallinity within the layers, and how this will affect our interfaces, defect density and disorder. For this we will use x-ray reflectivity measurements to measure periodicity and roughness, rocking scans for long-range lateral roughness, x-ray diffraction for crystallinity, and cross section transmission electron microscopy to view the superlattice.

Mass Spectrometer Calibration for Measurement of Photoresist Outgassing Species Identification and Quantification

Alin O. Antohe[1], Gregory Denbeaux[1], Chimaobi Mbanaso[1], Leonid Yankulin[1], Yu Jen Fan[1], Warren Montgomery[2]
[1]College of Nanoscale Science and Engineering, University at Albany, NY
[2]SEMATECH, Albany, NY

alinantohe@gmail.com 518-258-9992

Reduced Extreme Ultra Violet (EUV) optics lifetime, due to contamination caused by EUV irradiation of lithographic imaging materials, continues to impact the timing of EUV exposure tool introduction. The Resist Outgassing and eXposure system (ROX) at the College of NanoScale Science and Engineering (CNSE) in collaboration with the vertically integrated Resist and Materials Development Center (RMDC) which is the newly formed Resist Center of Excellence within SEMATECH's lithography division, has been one of the key tools used to test resist outgassing.

One of most difficult tasks, when characterizing outgassing, continues to be the accurate calibration of the mass spectrometer in order to obtain the desired sensitivity of the measurements. In order to carefully characterize the molecular fragments, evolved during exposure, a quadrupole mass spectrometer is used. The Resist outgassing team is always looking for ways to refine and improve testing accuracy.

As part of a continuous improvement activity, the team has implemented a linear algebra-based deconvolution algorithm which will further refine the isolation of the signal produced by each outgas species.

Relationship of Aluminum Grain Size to the Grain Size of Polycrystalline Silicon Produced by the Aluminum Induced Crystallization of Amorphous Silicon

Emilio Stinzianni, Kathleen Dunn, Zhao Zhouying, Manisha Rane-Fondacaro,
Harry Efstathiadis, and Pradeep Haldar

Energy and Environmental Applications Center (E2TAC)
College of Nanoscale Science and Engineering
University at Albany, State University of New York

estinzianni@uamail.albany.edu (518)894-6354

The aluminum-induced crystallization and layer exchange process shows great promise for converting amorphous silicon into large-grained polycrystalline silicon for solar cell applications. To investigate the relationship between the grain size of the aluminum and the final grain size of polycrystalline silicon, a series of samples were deposited by RF magnetron sputtering 165 nm of aluminum onto SiN/SiO_2 coated (100) silicon substrates. The aluminum grain size was varied by vacuum annealing prior to the deposition of 195 nm of amorphous silicon. Figure 1 presents the TEM cross section of the film stack upon completion of the layer exchange process. The process resulted in poly-Si films forming adjacent to the substrate, which were then characterized with plan view TEM. The average grain size in the poly-Si was found to increase by 2.7µm with increasing aluminum grain size, consistent with the grain-boundary nucleation model for this process. The microstructure of the poly-Si film can therefore be manipulated by altering the properties of the as-deposited aluminum layer with an isothermal anneal.

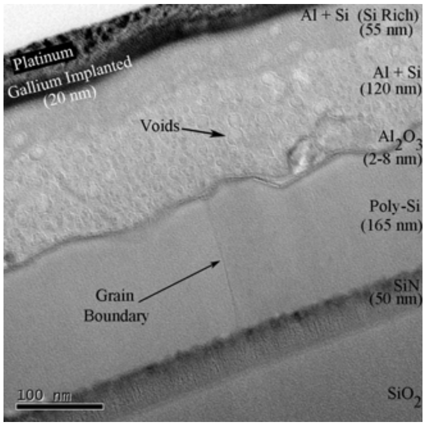


Figure 1. Cross-sectional TEM image of the completed sample that used an as-deposited aluminum film prior to the AIC anneal at 450°C. The aluminum and silicon layers have exchanged positions and the silicon is now adjacent to the SiN substrate. The a-Si has also been crystallized into poly-Si.

Aberration-Corrected HRTEM and HAADF-STEM Simulation Study of Few-Layer Graphene

F. Nelson[1], A.C. Diebold[1], R. Hull[2]

[1]College of Nanoscale Science and Engineering, University at Albany, Albany, N.Y. 12203

[2]Rensselaer Polytechnic Institute (RPI), 110 8th St., Troy, NY 12180

FNelson@uamail.albany.edu

Graphene's high mobility and mechanical integrity make it an attractive material for the “beyond CMOS” technology that will replace today’s transistor. Acceleration of process and device technology requires considerable advances in the imaging and characterization of graphene. The physical dimensions of available single and multi-layer samples are not large enough for many metrology methods. Electron microscopy of graphene is also challenging due to carbon's low atomic number. The high mobility of single layer and misoriented two and three layer graphene make it attractive for nanoelectronic devices. The current investigation explores HRTEM and HAADF-STEM simulations of graphene stacking configurations AAA/ABA/ABC as well as bilayers with misorientations between the individual layers. Images calculated using the multislice algorithm show discernable differences between the stacking sequences when simulated in the presence of random noise. A collaboration with the National Center for Electron Microscopy (NCEM) is currently being pursued in order to experimentally image suspended FLG samples with the aberration-corrected TEAM instrument at 80kV. To that end, we present Raman data used to identify layer number, and subsequently transfer few-layer regions to Si_3N_4 TEM grids.

The Relative Classification of Carbon Containing Molecules Related to the Contamination of Extreme Ultraviolet Lithography (EUVL)

Leonid Yankulin, Rashi Garg, Alin Antohe, Petros Thomas, Yu Jen Fan, Chimaobi
Mbanaso, Gregory Denbeaux, - College of Nanoscale Science and Engineering,
University at Albany, NY
Vibhu Jindal, Andrea Wuest, SEMATECH, Albany, NY 12203
lyankulin@uamail.albany.edu 518-366-3426

Extreme Ultra Violet Lithography (EUVL) is likely the next photon-based image transfer method to be used in high volume semiconductor manufacturing. Before that can be a reality, contamination of the optics needs to be understood and mitigated, to enable sufficient throughput. To gather enough data to understand and model the effects, a rapid contamination agent was needed. Several species were tested including Benzene, Tert-Butanol, Diphenyl Sulfide, and Methyl Methacrylate. It was discovered that outgassing from carbon tape designed for scanning electron microscope (SEM) sample mounting produced the highest rate of contamination from the chemical species tested. The analysis included the tape at room temperature, as well as heating the tape to high temperatures under vacuum/inert atmospheres, and exposing optics in the said atmosphere to extreme ultra-violet radiation.

Wavelength Dependence of Carbon Contamination on Mirrors with Different Capping Layers

Petros Thomas, Leo Yankulin, Rashi Garg, Chimaobi Mbanaso, Alin Antohe, Yujen Fan,
Gregory Denbeaux, CNSE, University at Albany, NY 12203

Vibhu Jindal and Andrea Wuest, SEMATECH, Albany, NY 12203
pthomas@uamail.albany.edu 434-249-7211

Optics contamination is one of the challenges of Extreme ultraviolet (EUV) lithography. In addition to the desired wavelength near 13.5 nm (EUV), sources used in EUV exposure tools emit a wide range of out of band (OOB) wavelengths extending out to the visible region. In the past, studies have shown that the contamination rate due to OOB is significantly more than that of EUV. To that effect, we built a flat field spectrometer to study in detail the wavelength dependence of carbon contamination. We present preliminary experimental results of contamination rates for EUV and OOB using the custom-built spectrometer and a Xe plasma source. Heated carbon tape is used as a source of hydrocarbons in the vacuum chamber.

Low Relaxation Rate in Epitaxial Vanadium Doped Iron Ultrathin Films

Lili Cheng*, Christian Scheck, and William Bailey

Materials Science and Engineering Program, Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY 10027

Chengl3@rpi.edu, 518-276-8670 (*now postdoc at RPI)

As data rates in magnetic information storage approach 1GHz and above, strategies to control the magnetization dynamics in films become a more pressing need. Materials-based techniques to control relaxation can offer a straightforward implementation for this purpose. The longest relaxation time and sharpest frequency content in ferromagnetic precession is determined by the intrinsic relaxation rate G. For many years, pure iron has had the lowest known value of G for all pure ferromagnetic metals or binary alloys. We show that an epitaxial iron alloy with vanadium possesses values of G which are significantly further reduced. High quality MgO(100)/$Fe_{1-x}V_x$ epitaxial thin films are deposited by UHV deposition, with the 35 GHz FMR linewidth (42 Oe) of MgO(100)/Fe film even smaller than the narrowest linewidth of Fe ever reported. As V is doped in, intrinsic relaxation rate decreases. The minimum G value observed is only 14% of that of undoped Fe film, and is even only 34% of the lowest G value ever reported on metallic ferromagnets. The decrease in the Gilbert damping G is closely related to the reduced magnetic anisotropy in the system.

Two-Dimensional Computer Modeling of Single Junction a-Si:H Solar Cells

Changwoo Lee, Harry Efstathiadis, James E. Raynolds, Pradeep Haldar

Energy and Environmental Applications Center (E2TAC)
College of Nanoscale Science and Engineering
University at Albany, State University of New York
CLee@uamail.albany.edu 518-944-1497

A two dimensional physically-based computer simulation of single junction pin amorphous silicon solar cells is presented using Sentaurus, TCAD by Synopsys Inc. The simulation program solves the Poisson, the continuity, and the current density equations by using a standard procedure for amorphous materials, including the continuous density of state model, Shockley-Read-Hall and Auger recombination mechanisms, and computes the generation function of electron-hole pairs from the optical parameters of each layer. The simulator is applied to the analysis of a *pin* single junction a-SiC:H/a-Si:H/a-Si:H solar cell, obtaining results comparable to one dimensional simulation results using AMPS-1D. The electrical properties inside the solar cells such as the distribution of generation and recombination rates, electric fields and electron and hole concentrations are obtained taking into account the doping level, thickness of each layer and their effect on cell efficiency. More advanced simulation models for novel solar cell devices such as tandem cell are in progress, with the aim of achieving an optimal design of solar cells based on amorphous materials in advance.

Results of the first version of a two dimensional computer simulation designed to optimize amorphous silicon solar cells are presented using the standard density of state model for modeling of dangling bond in amorphous material. A single junction a-SiC:H/a-Si:H/a-Si:H cell has been chosen as an example case to compare with AMPS-1D in one dimensional simulation.

Impact of Carbon Contamination on Patterned Extreme Ultraviolet (EUV) Masks

Yu-Jen Fan[1,2], Leonid Yankulin[1], Alin Antohe[1], Rashi Garg[1], Petros Thomas[1], Chimaobi Mbanaso[1], Andrea Wüest[2], Frank Goodwin[2], Sungmin Huh[2]
Patrick Naulleau[3], Kenneth Goldberg[3], Iacopo Mochi[3]
Gregory Denbeaux[1]

[1]College of Nanoscale Science and Engineering, University at Albany
[2]SEMATECH
[3]CXRO, Lawrence Berkeley National Lab
yfan@uamail.albany.edu 518-956-7012

Carbon contamination of extreme ultraviolet (EUV) masks is an issue of significant concern, due to the potential degradation of imaging performance and throughput. In this work, a series of carbon contamination experiments was performed on a patterned EUV mask. Carbon contamination was accumulated by exposing selected fields of the mask to EUV radiation in a controlled environment. Contaminated features were then inspected with a reticle SEM, and images of these features were printed with the SEMATECH Berkeley micro-field exposure tool (MET). In addition, the mask was analyzed using the SEMATECH Berkeley actinic-inspection tool (AIT), and atomic force microscope (AFM) measurements were performed to determine the effect of the contamination on the absorbing features and printing performance.

To estimate the actual contamination topography, aerial image simulations were performed and compared to the experimental data. Best overall agreement was reached for a topography in between purely conformal and direct contamination. With the knowledge of the topography, modeling was then used to predict the effect of other thicknesses of the contamination layer, as well as how an optical correction on the clean mask can be employed to reduce the enhanced shadowing effect due to contamination.

Platinum Monolayer Electrocatalysts for O2 Reduction: Pt Monolayer on Carbon-Supported PdIr Nanoparticles

Seth L. Knupp[1], Miomir Vukmirovic[2], Radoslav Adzic[2] and Pradeep Haldar[1]

Sknupp@uamail.albany.edu 518-275-9216

[1]College of Nanoscale Science and Engineering, University at Albany, State University of New York, Albany, New York 12203, USA
[2]Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973-5000

The kinetics of oxygen reduction was investigated in acid solutions on Pt monolayers deposited on modified carbon supported PdIr nanoparticles using rotating disk-electride technique. The electrocatylst were prepared via depositing Pt monolayers involving the galvanic displacement by Pt of an underpotentially deposited Cu monolayer on a PdIr/C substrate and characterized by induced coupled plasma, scanning electron microscopy and transmission electron microscopy. Pd/C was first treated with 2/3 monolayer coverage of Ir. With subsequent annealing, Pd will segregate to the surface while Ir moves to the subsurface creating a tensile strain on a pseudomorphic Pd skin. A Pt monolayer was then deposited on to the PdIr/C. The kinectics of O_2 reduction shows a significant enhancement at Pt monolayers PdIr nanoparticle surfaces in comparison with the reaction on Pt nanopartilcles. The results demonstrate that modifying the substrate (Pd/C) via Ir with subsequent Pt monolayer deposition is an attractive method of improving O_2 reduction electrocatalysts. Also, by using this method, the Pt content is reduced significantly. The Pt mass and specific activities of the PtPdIr/C are both ~10 times higher than that of commercial Pt/C electrocatalyst. The noble mass-specific are two times higher than that of Pt/C.

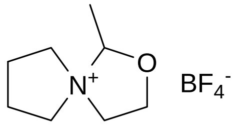
Eutectic Mixtures of Room Temperature Ionic Liquids Electrolytes for Electric Double Layer Capacitors

Seiichiro Higashiya[1], Thamarai selvi Devarajan[1], Manisha V. Rane-Fondacaro[1], Pradeep Haldar[1]

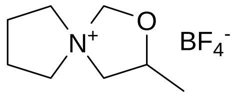
[1]Energy and Environmental Applications Centre (E2TAC), Collage of Nanoscale Science and Technology, University at Albany, 257 Fuller Road, Albany, New York 12203, USA
sei@albany.edu 518-533-8481

Improvement of energy density of electric double layer capacitors (EDLC) while maintaining the high power density, cycle life, and safety is one of the most awaited technological developments for sustainable society. Electrolytes with wide operational (potential and temperature) window, high ion conductivity and concentration are important for further improvement. Aliphatic room temperature ionic liquids (RTIL) are expected to meet these requirements while the characteristics such as melting points, conductivity, and viscosity are not sufficient. Especially, extending the operating potential V drastically increases in the energy density E of EDLC by the relationship $E=1/2CV^2$ where C is the capacitance.

Earlier we had reported oxygen-containing spirobipyrrolidinium RTIL for EDLC application though the melting points were relatively high. Here, we demonstrate an application of eutectic mixtures of two oxygen-containing spirobipyrrolidinium RTIL, 2MOP BF_4 and 5MOP BF_4 as electrolytes for EDLC.



2MOP BF_4



5MOP BF_4

The Ionic liquid mixtures (in various proportions) exhibit lower melting points with comparable conductivity and viscosity. The potential window of mixed RTIL was about 5.5 V (50 $\mu A/cm^2$ threshold, glassy carbon-working electrode). The potential window was also investigated in EDLC configuration, using electrodes that comprised of activated carbon material attached to aluminum current collector. The EDLC test cells with RTIL mixtures exhibit higher breakdown potential (> 4.6 V) as compared to conventional molecular solvent (acetonitrile)-based cells (~4.0 V). These RTIL mixtures lead to higher equivalent series resistance (ESR) and lower capacitance. Increase in ESR was found to initiate at 3.9 V, resulting in increase in the time constant (RC). Cycling of negative electrode at 4.6 V led to delamination of carbon from the current collector. This might be the reason for increase in the ESR, while the positive electrode kept the integrity as carbon sheets.

The results show high energy density EDLC based on RTIL with the higher operational potentials are feasible with further improvements in RTIL conductivity, current collector-electrode interface integrity, and electrode materials especially the negative electrodes.

Porous Silicon Based Electric Double Layer Capacitors

Thamarai selvi Devarajan[1], Seiichiro Higashiya[1], Manisha V. Rane-Fondacaro[1] and Pradeep Haldar[1]

[1]College of Nanoscale Science and Engineering, University at Albany, SUNY,
Albany NY, 12203
tdevarajan@uamail.albany.edu 518-253-1894

Electrical double layer capacitor (EDLC) is promising energy storage technology. It has high power density and long cycle life compared to batteries. However, its energy density is very low as compared with battery technology. Since the energy density is proportional to the square of the maximum voltage before electrolyte breakdown, organic electrolytes and especially ionic liquids are preferred over aqueous electrolytes.

Novel oxygen containing spiro ammonium salt, oxazolidine-3-spiro-1'-pyrrolidinium tetrafluoroborate ($OPBF_4$) has been synthesized in-house. Comparison of $OPBF_4$ with the traditional EDLC electrolyte $TEABF_4$ (tetraethyl ammonium tetra fluoroborate) shows comparable voltage window (in EDLC bag cell) and higher capacitance in the $OPBF_4$ compound. Moreover, higher dissolution of $OPBF_4$ salts in acetonitrile yield much higher molarity of 3 M, as compared with only 1.5 M for $TEABF_4$ salts, which is especially important for high energy density electrochemical capacitors. Thus, $OPBF_4$ proves to be a reasonable alternative to $TEABF_4$.

The voltage window of $OPBF_4$ as measured in a half cell yields a value of 5.1 V, while measurement in a bag cell yields a value of 3.7 V. The half-cell test uses glassy carbon material, which is inherently devoid of any functionality; the activated carbon has much functionality, which in-turn leads to chemical degradation at lower voltage. It is extremely difficult to rid activated carbon material of its functionalities; hence, we are developing inert material electrodes made of porous silicon for ultracapacitor application.

We are developing porous silicon with optimized pores for high-energy density ultracapacitor application. This requires optimization of pore parameters such as pore diameter, length and volume, to improve the surface area. The conductivity of porous Si will then be improved by metallization or doping. Finally, the ultracapacitor will be assembled and the performance evaluated using galvanostatic charge discharge experiments or cyclic voltammetry. Our initial results indicate better performance by 2X as compared with literature.

Angle Resolved XPS and its Application in Advanced High-K Gate Dielectric Research

S. Consiglio, R. D. Clark, C. S. Wajda, and G.J. Leusink

TEL Technology Center, America, LLC, 255 Fuller Road, Albany, NY, 12203, USA
steve.consiglio@us.tel.com 518-320-1976

With the advent of high-k dielectrics in the manufacturing of MOSFET devices comes the need to further scale the electrical properties of the dielectric material and to also tune the threshold voltage to meet device specifications. In this regard, research targeted towards further improvement and modification of the currently adopted Hf-based gate dielectrics (HfO_2, Hf silicate, and nitrided Hf silicate) is ongoing in order to extend the usage of high-k dielectrics to future technology nodes. These stacks typically contain a thin SiO_2-based bottom interfacial layer which preserves some of the properties of the near ideal SiO_2/Si system[1] and, more recently, high-k capping layers which are introduced to tune the threshold voltage of the completed device by means of a proposed interfacial dipole effect.[2]

For chemical and physical analysis of thin (<50Å) Hf-based dielectric stacks, X-ray photoemission spectroscopy (XPS) is a powerful technique for probing the entire stack since the attenuation length of photoelectrons is on the order of the total stack thickness. A variant of conventional XPS, angle resolved XPS (ARXPS), relies on the angular dependence of the emitted photoelectron attenuation and enables non-destructive measurements of key parameters of thin high-k stacks such as thickness, relative ordering of chemical species, and depth distribution of the species in a multilayer stack.

In this presentation we will show examples of the utility of angle resolved XPS in the research of advanced high-k dielectrics and explain how the key parameters mentioned earlier are readily obtained by manipulation of angle dependent data. In particular, relative layer positioning is obtained from straightforward intensity ratios while film thickness of these layers is extracted from manipulation of the Beer Lambert law for photoelectron attenuation combined with the predictive equation for attenuation length proposed by Tanuma, Powell, and Penn (TPP-2M equation)[3]. In order to overcome the ill-conditioned nature of transforming angular dependent data into depth dependent data a maximum entropy algorithm[4] is utilized to obtain depth profile reconstructions. This method relies on maximizing the joint probability function and tends to strike a balance between the information content (entropy) and the raw data fit (chi-squared error) resulting in a smooth profile, and thus avoids overfitting.

References:
[1] K. Maitra et al., *J. Appl. Phys.,* **102,** 114507 (2007)
[2] K. Kita et al., *Appl. Phys. Lett.,* **94,** 132902 (2009)
[3] R. P. Champaneria et al., *Surf. Interface Anal.,* **35,** 1028 (2003)
[4] R. L. Opila et al., *Prog. Surf. Sci.,* **69,** 125 (2002)

Chromatic White Light Profilometer

Rosalyn L. Neander and Sara G. Ostrowski,
General Electric Research and Development

Surface roughness plays an important role in determining how a real object interacts with its environment and is a good predictor of the performance of a mechanical component. Surface roughness can help us to understand the super hydrophobicity of a material, it can be correlated with poor electron mobility in semi-conductors, it can aid in understanding adhesion strength of materials, and it can even be correlated with haze in plastics.

There are a number of instruments that can provide researchers with pictures to understand what is happening at the surface, but there are few instruments that can actually capture surfaces topography and calculate the surface roughness. Some of these instruments are the Atomic Force Microscope (AFM), Optical Profilometer (OP), and the Chromatic White Light Sensor (CWLS).

The CWLS is an instrument that utilizes chromatic aberration to measure surface roughness. White light passes through a lens; the chromatic aberration of the lens is calibrated to break the white light up into a spectrum of individual wavelengths each with a distinct focal point and therefore height. As the sample is scanned, only one wavelength of light from the vertical stack is in focus on the sample surface at one time. This wavelength is reflected back to the spectrometer and output as the corresponding z height at that x-y position.