Spring Meeting Hudson Mohawk Chapter of the AVS April 20, 2015

SUNY Polytechnic Institute
Nanoscale Science and Engineering (CNSE)
CESTM Rotunda and Auditorium
257 Fuller Rd
Albany, NY 12207

AGENDA

3:30 PM	Tour of CNSE Research Facilities
4:00 PM	Reception and Refreshments
4:20 PM	Welcome, Kim Michelle Lewis, Rensselaer Polytechnic Institute National AVS Update, Vincent Smentkowski, GE
4:30 PM	Oral Presentations
6:30 PM	Poster Presentations and Dinner
8:00 PM	Best Poster and Oral Presentation Awards and Brief Chapter Update
8:15 PM	Adjourn

ORAL PRESENTATIONS

SYNTHESIS AND PROPERTIES OF FERROMAGNETIC NANOSTRUCTURES EMBEDDED WITHIN A HIGH-QUALITY CRYSTALLINE SILICON MATRIX FOR SILICON BASED MAGNETICS

Girish Malladi, Mengbing Huang, Thomas Murray, Steven Novak, Akitomo Matsubayashi, Vincent LaBella, Hassaram Bakhru
SUNY College of Nanoscale Science and Engineering, Albany, NY 12203

DRAMATIC INCREASE OF RESISTIVITY DOMINATED BY SURFACE SCATTERING IN ULTRA-THIN EPITAXIAL COPPER FILMS

Y.P. Timalsina[1], A. Horning[1], K.M. Lewis[1], T.-S. Kuan[2], G.-C. Wang[1] and T.-M. Lu[1]
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CONTROLLING ELECTRICAL CONDUCTANCE ACROSS METAL-THERMOLECTRIC INTERFACES BY USING A MOLECULAR NANOLAYER

Thomas Cardinal[1], Devender[1], Theo Borca-Tasciuc[2], Ganpati Ramanath[1*]
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INVESTIGATION OF RESISTIVE MULTI-LEVEL SWITCHING ON CMOS-INTEGRATED RERAM IN DEPENDENCE OF PULSE-WIDTH

Karsten Beckmann[1], Joshua Holt[1], Tad Reese[1], Joseph Van Nostrand[2], Nathaniel Cady[1]
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CUBIC GaInN ON Si(001) FOR LONGER WAVELENGTH LEDs

Mark T. Durniak[1], Alexander Neumann[2], Anabil Chaudhuri[2], S.C. Lee[2], S. R.J. Brueck[2], and Christian Wetzel[1]
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HIGH RESOLUTION SIMS DEPTH PROFILING IN III-V COMPOUND SEMICONDUCTORS

M. J. P. Hopstaken, Y. Sun, A. Majumdar, C.-W. Cheng, B. A. Wacaser, D. K. Sadana, E. Leobandung
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ORAL PRESENTATION ABSTRACTS

SYNTHESIS AND PROPERTIES OF FERROMAGNETIC NANOSTRUCTURES EMBEDDED WITHIN A HIGH-QUALITY CRYSTALLINE SILICON MATRIX FOR SILICON BASED MAGNETICS

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Ferromagnetism in transition metal implanted Si has been reported earlier but unavoidably high density of structural defects in such materials render the realization of spintronic devices unviable. We report an ion implantation approach enabling the synthesis of a ferromagnetic layer within a relatively defect free Si environment using an additional implant of hydrogen (range: ~850 nm; dose: 1.5E16 cm^{-2}) in a region much below the metal implanted layer (range: ~60 nm; dose: 2.0E15 cm^{-2}). Upon annealing, nanocavities created within the H^+ implanted region act as gettering sites for the implanted metal, forming metal nanoparticles in a Si region of excellent crystal quality. Following annealing, the H implanted region is populated with Ni nanoparticles of size (~10-25 nm) and density (~$10^{11}/cm^2$) typical of those achievable via conventional deposition and other growth techniques. The magnetization properties for Si containing Ni nanoparticles were measured using a SQUID magnetometer and a transition from superparamagnetism to ferromagnetism-like was observed, with ferromagnetism persisting at 300K. With the aid of SIMS and high-resolution TEM, this transition is attributed to changes in both the amount of Ni in the nanoparticles and the inter-particle distances. RBS/channeling and high-resolution TEM show a fully recovered crystalline Si adjacent to these Ni nanoparticles. Furthermore, the magnetic switching energy barrier (~0.86 eV) increase by about one order of magnitude compared to their counterparts on Si surface or silica matrices. Preliminary electrical measurements on these devices show ~10% magnetoresistance at 300K. This is promising result towards implementing spintronic devices in Si for spin based computation as well as high-density and high-fidelity information storage technologies.

Malladi et al., J. Appl. Phys. 116, 054306 (2014)

DRAMATIC INCREASE OF RESISTIVITY DOMINATED BY SURFACE SCATTERING IN ULTRA-THIN EPITAXIAL COPPER FILMS

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The study of electron transport in ultra-thin metal films has been of great interest from both the fundamental and technological points of view. In bulk metals, resistivity arises mainly due to the scattering of electrons by phonons. However, in thin films, the primary source of electrical resistivity is the scattering of electrons from film surfaces as well as from boundaries between the discrete grains in the films. The surface scattering is increasingly important when the thickness of a film is reduced to less than the mean free path of the electrons which is tens nanometers in metals. Therefore, it is necessary to carry out in-depth investigations to understand the contributions of distinct scattering sources and their collective effect on the resistivity of ultra-thin metal films. Temperature dependent resistivity measurement at cryogenic temperatures is a viable approach to study the influence of various scattering mechanisms on the electrical resistivity of ultrathin metal films.

In this work, we report temperature dependent resistivity of ultrathin epitaxial copper films of thickness ranging from 500 nm to 5 nm grown on silicon (100) substrates in the temperature range 5-300 K. We quantify contributions from the surface scattering and the electron-phonon scattering. We demonstrate that the surface contribution to resistivity which is temperature independent component of resistivity can be described by root-mean-square-surface roughness and lateral correlation lengths with no adjustable parameter[1], using a recent quasi-classical model developed by Chatterjee and Meyerovich[2]. However, the electron-phonon contribution to resistivity which is temperature dependent can be described using the Bloch-Grüneisen formula with a thickness dependent electron-phonon coupling constant and a thickness dependent Debye temperature[1]. We show that the increase of the electron-phonon coupling constant with the decrease of film thickness gives rise to an enhancement of the temperature dependent component of the resistivity.

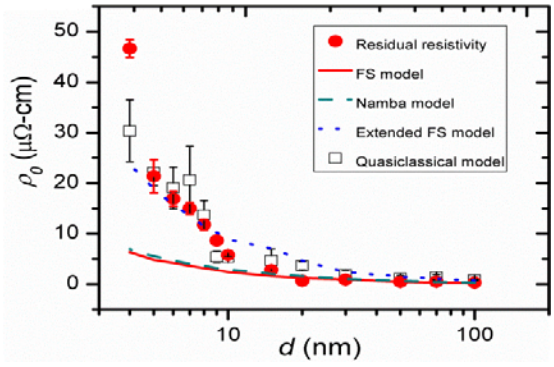

Fig. 1 Resistivity due to surface scattering

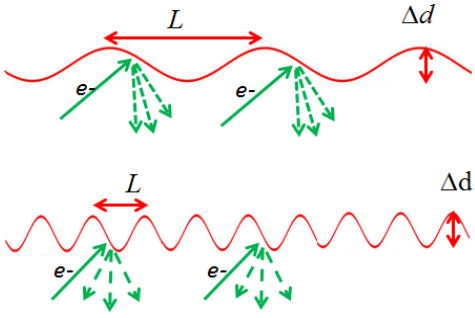

Fig. 2 Schematic showing electron scattering from two dissimilar rough surfaces

[1] Y.P. Timalsina, A. Horning, R.F. Spivey, K.M. Lewis, T.-S. Kuan, G.-C. Wang, and T.-M. Lu, Nanotechnology **26**, 075704 (2015).
[2] S. Chatterjee and A.E. Meyerovich, Phys. Rev. B **81**, 245409 (2010).

CONTROLLING ELECTRICAL CONDUCTANCE ACROSS METAL-THERMOLECTRIC INTERFACES BY USING A MOLECULAR NANOLAYER

Thomas Cardinal[1], Devender[1], Theo Borca-Tasciuc[2], Ganpati Ramanath[1*]

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Tailoring the electrical contact properties of metal-thermoelectric materials interfaces is important to realize high-efficiency solid-state refrigeration for many applications such as cooling hotspots in nanoelectronics devices and solar cells. This is because the energy conversion efficiency of thermoelectric devices fabricated from materials with high thermoelectric figures of merit is often limited by poor electrical transport across metal-thermoelectric interfaces. Here, we report a tenfold increase in electrical contact conductivity σ_c upon introducing a molecular monolayer of 1,8-octanedithiol (ODT) monolayer or 1,3-mercaptopropyltrimethoxysilane (MPTMS) at Cu-Bi_2Te_3 interfaces. For Ni-Bi_2Te_3 interfaces, introducing an ODT monolayer decreases σ_c by 20% while MPTMS results in a threefold σ_c increase. Our observations for ODT-modified interfaces are attributable to differences in interfacial bonding and phase formation at the two interfaces. Rutherford backscattering spectroscopy and X-ray diffraction reveal that ODT inhibits interfacial mixing and curtails interfacial Cu_2Te formation. X-ray photoelectron spectroscopy of ODT-modified interfaces show that the thiol termini of ODT bond to Cu more strongly than with Ni. Based upon similar correlations observed for MPTMS, we attribute the Σ_c enhancements at Ni-Bi_2Te_3 to silicide formation via reaction between the silane termini and Ni. Our findings show that nanomolecular monolayers could offer new possibilities for devising metallization schemes for efficient thermoelectric devices.

INVESTIGATION OF RESISTIVE MULTI-LEVEL SWITCHING ON CMOS-INTEGRATED RERAM IN DEPENDENCE OF PULSE-WIDTH

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Resistive Random Access Memory (ReRAM) is a form of non-volatile memory, typically based on a metal-insulator-metal (MIM) multilayer structure. A better understanding of the switching behavior dependence on switching parameters such as set/reset voltage and pulse-width could potentially lead to an improvement of the device properties. Another major challenge is the integration of ReRAM elements with standard CMOS-based integrated circuits. We have previously demonstrated ReRAM integration with CMOS using the IBM 65 nm 10LPe process flow. In addition to standard copper-based interconnects, we have also developed tungsten metal 1 (M1) and via 1 (V1) interconnects. This shift from copper-based interconnects enables us to use front-end-of-line (FEOL) as well as subsequent beck-end-of-line (BEOL) processing for deposition, cleaning and patterning of ReRAM elements, without risking copper poisoning of the underlying CMOS. For this work, the ReRAM material stack consisted of 6 nm HfO_2, 6 nm Ti and 150 nm TiN embedded between the tungsten M1 and copper M2. The Ti layer acts as an oxygen getter, resulting in a sub-stoichiometric HfO_x film. Tungsten and TiN serve as inert electrodes making our ReRAM function via oxygen anion movement, which creates a conductive path through oxygen vacancies within the HfO_x film. Several different ReRAM structures were implemented to perform discrete, pulse-based switching including, 1) individual ReRAM cells ranging in size from 100x100 nm^2 to 10x10 μm^2 and 2) 12 x 12 arrays of ReRAM in a crossbar configuration. We have shown that pulse operation is possible at relatively high reset current of approximately 200 µA with an external transistor. In this operational mode the ReRAM devices show excellent reliability with an endurance exceeding 10^4 switching events. We are able to change the low resistive state (LRS) by one order of magnitude by reducing the pulse-width from 10 ms down to 1 µs. The dependence of on/off ratio and high resistive state (HRS) will be shown and reliability as well as endurance data for each pulse-width will be investigated. The LRS, HRS and set/reset voltages for each pulse-width are accessible and will lead a better understanding of the relative filament dimensions that was formed within the device. The time dependence of the reset pulse in particular will be investigated to estimate the minimum pulse-width possible for which an acceptable on/off ratio can be achieved. This directly leads to the minimum power consumption necessary for one switching operation for this first generation CNSE tungsten ReRAM.

CUBIC GaInN ON Si(001) FOR LONGER WAVELENGTH LEDs

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III-V semiconductors are widely used today in lighting, lasers, and power devices. For lighting in particular, wurtzite GaInN has provided light emitting diodes (LEDs) from violet to red. Internal polarization fields in wurtzite, arising from material strain as a result of adding In to lower the bandgap, result in a quantum confined Stark effect. This directs the growth to narrow quantum wells with high carrier confinement and leading to high carrier concentrations and to non-radiative Auger recombination, widely thought of as the cause of LED efficiency droop. Cubic GaInN in the (001) orientation is a promising new material that offers all the benefits of wurtzite GaInN without polarization fields. Using microscale epitaxy large areas of cubic GaN are grown on commercially available Si(001) making it an ideal candidate for longer wavelength LEDs, laser diodes, and power devices. Without polarization fields, narrow quantum wells are no longer needed for confinement and carrier density can be lowered. Along with lower carrier concentrations, the cubic GaInN band structure also lends to mitigate Auger recombination. We study the growth and optoelectronic characteristics of cubic GaInN grown by metalorganic vapor phase epitaxy (MOVPE) on micropatterned Si(001) substrates. Si(001) is a substantially cheaper and larger substrate than traditional sapphire and offers the potential for Si CMOS/GaN integration. The opaque Si can be removed via mechanical and chemical means, freeing the cubic GaInN stripes allowing for a thin-film flip chip (TFFC) configuration. Simulations suggest a four-fold increase in light extraction efficiency for TFFC LEDs as compared to the planar configuration. Electroluminescence of TFFC a green cubic LED has been demonstrated. Additionally, cubic LEDs do not exhibit a blue-shift with varying current density confirming their lack of polarization fields. The stress and strain state of the cubic GaN is investigated using x-ray diffraction. Analysis of the cubic GaN 002 and 202 $\omega/2\theta$ curves indicates that the cubic GaN is under biaxial tensile stress. Further analysis of strain is performed in order to determine the impact on indium incorporation. Cathodoluminescence (CL) is employed to spatially map the spectrum of the GaInN samples to help understand the indium incorporation across the different phases.

This work was supported in part by the Engineering Research Centers Program of the National Science Foundation under NSF Cooperative Agreement No. ***EEC-0812056,*** *by New York State under NYSTAR contract C090145, and in part by the Sandia National Laboratories Campus Executive Fellowship for Laboratory Directed Research and Development.*

HIGH RESOLUTION SIMS DEPTH PROFILING IN III-V COMPOUND SEMICONDUCTORS

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Recently, there has been renewed technological interest for application of InGaAs and related III-V high-mobility materials as a potential replacement for the MOSFET Si-channel [1]. Successful integration of novel materials and processes requires accurate physical characterization of in-depth chemical distribution with nm-scale resolution. Here, we will address some of the challenges regarding Secondary Ion Mass Spectrometry (SIMS) depth profiling of III-V compound thin-film materials and propose analytical solutions for the accurate characterization of more complex III-V based multilayered substrates, impurities therein, and Ultra-Shallow Junction (USJ) doping profiles.

Ion beam based sputtering of III-V compounds is intrinsically more complex and less well documented than in mainstream Si substrates. One of the major issues with sputter depth profiling of III-V materials is their higher sensitivity to formation of ion-beam induced topography, which has a detrimental impact on depth resolution [2]. We have previously reported anomalous sputtering behavior of (In)GaAs under low energy O2+ ion beam irradiation, causing severe degradation of depth resolution [3].

In case of low energy Cs+ ion beam irradiation at oblique incidence, we have achieved uniform sputtering conditions on a wide variety of III-V compounds (e.g. InxGayAl1-x-yAs, InP) with no significant topography formation, as evidenced from crater bottom AFM. We have demonstrated constant depth resolution in III-V multilayer structures with decay lengths as low as 2 nm/decade on abrupt chemical transitions in different III-V compounds at low Cs+ impact energies (down to 250 eV).

We will address some of the analytical challenges regarding the quantification of depth and concentration scales in multi-layer structures, comprised of different III-V compounds grown by heteroepitaxy. We typically employ explicit corrections for yield variations using appropriate (multiple) standards in their respective matrixes. A special case occurs for depth profiling of group IV n-type dopants (i.e. M= Si, Ge), which are typically monitored as negative cluster ion attached to the group V element (e.g. MAs-, MP-) for reasons of sensitivity. We have developed a quantification scheme to determine [Si] doping profiles in hetero-epitaxial (e.g. InxGayAl1-x-yAs / InP) structures, composed from the negative cluster ions (e.g. SiAs-, SiP-) in the respective matrices.

In summary, this work has improved our fundamental understanding of low-energy ion beam interactions in III-V materials, which is essential for achieving sub-nm depth resolution in thin-film structures. In addition, this work has provided with an optimum window of analytical conditions for quantitative analysis of a wide variety of impurities and dopants with high sensitivity in different III-V materials.

References:

1. Y. Sun et al., IEDM 2013 Conf. Proc., p. 48-51.
2. E.-H. Cirlin, J. J. Vajo, R. E. Doty, and T. C. Hasenberg, J. Vac. Sci. Technol. A 9, 1395 (1991).
3. M. J. P. Hopstaken et al., J. Vac. Sci. Technol. B 28, 1287, (2012).

POSTER PRESENTATIONS

WORK FUNCTION TUNING AT THE GOLD-HAFNIA INTERFACE USING AN ORGANOPHOSPHONATE NANOLAYER

Matthew Kwan[1], Hubert Mutin[2], Ganpati Ramanath[1]
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EPITAXIAL NbN(001) LAYERS: LATTICE CONSTANTS, POINT DEFECTS AND MECHANICAL PROPERTIES

K. Balasubramanian,[a] K. Zhang,[a,b] B.D. Ozsdolay,[a] C.P. Mulligan,[a,c] W.T. Zheng,[b] and D. Gall[a]
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EXAMINATION OF CHARGE-TRANSFER PROCESSES AND AND ELECTROCHEMICAL RECTIFICATION OF MOLECULAR MULTILAYERED FILMS FOR USE IN DYE-SENSITIZED SOLAR CELLS

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TUNING THE PHASE AND OPTICAL PROPERTY OF SnS_x SEMICONDUCTOR FILMS

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SILICON NANOWIRES FOR PHOTOVOLTAIC APPLICATIONS

Caitlin Rouse, Zhouying Zhao, Harry Efstathiadis, Pradeep Haldar
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LOW LER TIN CARBOXYLATE PHOTORESISTS USING EUV

Ryan Del Re,[a] Miriam Sortland,[a] James Passarelli,[a] Mark Neissar,[c] Daniel A. Freedman,[b] and Robert L. Brainard[a]*
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FATIGUE BEHAVIOR AT COPPER-SILICA INTERFACES

M. Braccini[1,2*], M. Kwan[1], M. Lane[3], G. Ramanath[1]
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FIRST-PRINCIPLES INVESTIGATION OF ELECTRON TRANSPORT IN Cu LAYERS

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METROTROLOGY FOR CIGS USING SPECTROSCOPIC ELLIPSOMETRY

Sravan Sunkoju, Sandra Schujman,* Dhairya Dixit, Pradeep Haldar
SUNY College of Nanoscale Science and Engineering, Albany, New York 12203, USA

MODELING THE THERMOELECTRIC FIGURE OF MERIT OF NANOBULK Bi_2Te_3 AS A FUNCTION OF DOPING, POROSITY, AND GRAIN STRUCTURE

Andrew Gaul, Devender, Ganpati Ramanath, and Theodorian Borca-Tasciuc
Rensselaer Polytechnic Institute, Troy, NY 12180

STRUCTURAL STUDY OF TOPOLOGICAL INSULATOR MATERIALS USING X-RAY DIFFRACTION, TRANSMISSION ELECTRON MICROSCOPY, AND SECOND HARMONIC GENERATION

Avery J. Green, Yong Q. An, Robin Jacobs-Gedrim, Samuel O'Mullane, and Alain C. Diebold
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EPITAXIAL AND POLYCRYSTALLINE WN_x FILMS DEPOSITED BY REACTIVE DC MAGNETRON SPUTTERING ON MgO(001), MgO(111), AND Al_2O_3(0001)

Brian Ozsdolay,[1] Karthik Balasubramanian,[1] Christopher P. Mulligan,[1,2] Michael J. Guerette[1], Liping Huang,[1] and Daniel Gall[1]
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THE FEASIBILITY OF ACHIEVING THE RESOLUTION LIMIT OF BILAYER PMMA / MMA WITH LIFT – OFF

Michael J. Ostrelich
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ROLE OF SURFACE TERMINATION ON THE GROWTH OF GRAPHENE ON CU

Tyler R. Mowll[1], Eng Wen Ong[1], Parul Tyagi[2], Zachary R. Robinson[3], Carl A. Ventrice, Jr.[4]
[1]University at Albany-SUNY, [2]Global Foundries, [3]U.S. Naval Research Laboratory, [4]SUNY Polytechnic Institute

STUDYING SECONDARY ELECTRON BEHAVIOR IN EUV RESISTS USING EXPERIMENTATION AND MODELING

Amrit Narasimhan,[1] Bharath Srivats,[1] Henry Herbol,[1] Liam Wisehart,[1] Steven Grzeskowiak,[1] Chris Kelly,[1] William Earley,[1] Leonidas E. Ocola,[2] Mark Neisser,[3] Greg Denbeaux,[1] and Robert L. Brainard[1]
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THERMOELECTRIC POWER FACTOR ENAHNCEMENT BY DILUTE SULFUR DOPING IN Bi_2Te_2Se NANOCRYSTS

Devender[†], Pascal Gehring[‡], Marko Burghard[‡], Theodorian Borca-Tasciuc[#], Klaus Kern[‡], and Ganpati Ramanath[†]
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INTERGRATION OF A DC MAGNETRON SPUTTERING SYSTEM INTO AN ULTRA-HIGH VACUUM CHAMBER FOR FABRICATION OF SCHOTTKY DIODES

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SUNY Polytechnic Institute, The Colleges of Nanoscale Science and Engineering

NEGATIVE MAGNETORESISTANCE AND ELECTRICALLY DETECTED ZERO FIELD SPLITTING IN A LOW-K DIELECTRIC

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POSTER PRESENTATION ABSTRACTS

WORK FUNCTION TUNING AT THE GOLD-HAFNIA INTERFACE USING AN ORGANOPHOSPHONATE NANOLAYER

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Tuning the effective work function Φ of metal contacts to high-dielectric permittivity gate oxides such as hafnia is important to align the metal Fermi level with n- and p-doped Si in metal/gate/Si stacks. Here, we demonstrate that the effective work function of Au at Au-HfO_2 interfaces can be tuned in the $0 \leq \Phi_{Au} \leq 0.5$ eV range by introducing a mercaptan-terminated organophosphate molecular nanolayer (MNL). Variable angle photoelectron spectroscopy indicates that all the organophosphonates studied form monolayers via phosphonic acid termini tethering onto HfO_2 and mercaptan moieties anchoring onto Au surfaces. Ultraviolet photoelectron spectroscopy measurements of the change in vacuum level of MNL-functionalized Au and HfO_2 surfaces, and Au/MNL/HfO_2 structures, allow us to deduce the contributions of each interface to the overall work function shift $\Delta\Phi_{Au}$. We find that the S-Au bonds at the MNL-Au interface have a greater influence than the combined effects of MNL-HfO_2 interface bonding and the intrinsic dipole moments of the molecules. Additionally, altering the organophosphonate molecular length results in a lower $\Delta\Phi_{Au}$ on the Au/MNL/HfO_2 interfaces than that seen on MNL-modified free Au and HfO_2 surfaces. Based upon these results, we describe an empirical model to describe the contributions of molecular bonding, orientation and MNL morphology on $\Delta\Phi_{Au}$ at the Au-HfO_2 interface.

EPITAXIAL NbN(001) LAYERS: LATTICE CONSTANTS, POINT DEFECTS AND MECHANICAL PROPERTIES

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NbN_x layers were deposited by reactive magnetron sputtering on MgO(001) substrates in 5 mTorr pure N_2 at T_s = 600-1000 °C. $T_s \geq$ 800 °C leads to epitaxial layers with a cube-on-cube relationship to the substrate: $(001)_{NbN}||(001)_{MgO}$ and $[100]_{NbN}||[100]_{MgO}$. The layers are nearly stoichiometric with x = 0.95-0.98 for $T_s \leq$ 800 °C, but become nitrogen deficient with x = 0.81 and 0.91 for T_s = 900 and 1000 °C. X-ray diffraction indicates a relaxed lattice constant that decreases from 4.372 Å for x = 0.81 to 4.363 Å for x = 0.98. First principles calculations were performed to explain this unexpected trend. In particular, the predicted lattice constants indicate that both niobium and nitrogen vacancies are present in NbN_x layers and that their concentrations increase and decrease with increasing x, respectively. This is consistent with the relatively small calculated formation energies for nitrogen and niobium vacancies of 1.00 and -0.67 eV at 0 K and -0.53 and 0.86 eV at 1073 K, respectively. Nitrogen interstitials and antisite defects (Niobium and nitrogen) are found to be thermodynamically unfavorable with defect energies of 2.17, 5.72 and 11.95 eV at 0 K and 3.70 , 8.78 and 8.89 eV at 1073 K, respectively. The predicted isotropic elastic modulus of 335 GPa and the indentation modulus of 361 GPa along [100], obtained from the calculated elastic constants c_{11} = 641 GPa, c_{12} = 140 GPa, and c_{44} = 78 GPa, are slightly larger than the experimental value of 315 GPa measured by nanoindentation on $NbN_{0.98}$.

EXAMINATION OF CHARGE-TRANSFER PROCESSES AND ELECTROCHEMICAL RECTIFICATION OF MOLECULAR MULTILAYERED FILMS FOR USE IN DYE-SENSITIZED SOLAR CELLS

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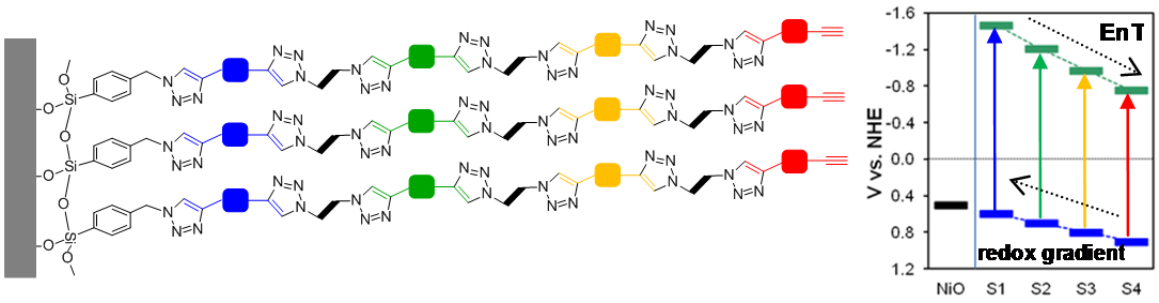
We have designed a method utilizing Copper(I)-catalyzed Azide-Alkyne Cycloaddition (CuAAC) chemistry to assemble light-harvesting arrays for use in Dye-sensitized Solar Cells (DSCs).[1–3] This rapid method produces uniform, multilayer films with highly controllable photophysical and electrochemical characteristics. Improvement of these properties is critical in order to pursue replacement of the most commonly used iodide/triiodide redox mediator, which limits the maximum achievable efficiency for DSCs, with alternatives that utilize an outer-sphere redox mechanism. Tailoring DSC design to allow for these mediators is of great interest in order to improve device function. We have found our films possess an electrochemical rectifying property allowing charge transfer to the redox mediator while blocking recombination with the electrode surface. Herein we study the effectiveness of the rectification capabilities of our films, as well as examine factors such as rates of charge transfer and mediator-dye interactions. Our focus is highly relevant, as it offers an interesting method to possibly improve DSC efficiencies by further utilizing the dye component already present in current designs.



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TUNING THE PHASE AND OPTICAL PROPERTY OF SnS_x SEMICONDUCTOR FILMS*

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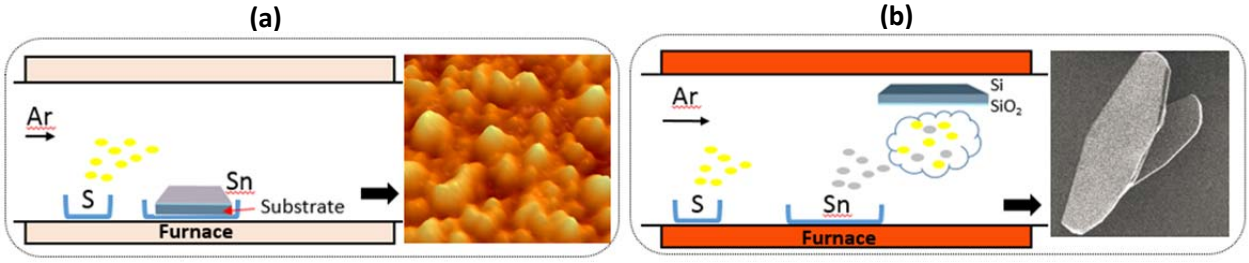
The layered metal dichalcogenides films with intrinsic optical band gaps in the range of 1 to 3 eV have attracted considerable interest for the potential applications in optoelectronics and electronics. SnS_x is one of these promising materials that possess the advantages of non-toxic to environment and earth-abundant. Tin sulfides can be formed in several phases such as SnS, SnS_2, and Sn_2S_3 depending on the relative amount of sulfur to tin and the temperature during film growth. The SnS film has an optical bandgap of 1.0 to 1.5 eV and can be used as an absorber in solar cells. The SnS_2 film has an optical bandgap from 2.0 to 2.5 eV and has been demonstrated to have fast photocurrent response time in a few micro sec.

The dominant SnS, dominant SnS_2 and pure SnS_2 films were prepared by evaporating ultrathin Sn (~20 nm thick) film on amorphous substrates (quartz or 300 nm thick Si oxide on Si wafer) and subsequently sulfurized in the temperature range from 200 to 500 °C under Ar flow in a quartz tube (Fig. a). The synthesized films were characterized using grazing incident X-ray diffraction (GIXRD), atomic force microscopy (AFM), scanning electron microscopy (SEM), UV-Vis spectroscopy, Raman spectroscopy and photoluminescence spectroscopy (PL). The GIXRD reveals that the film synthesized at 200 °C has a mixture of dominant SnS orthorhombic phase and a minor hexagonal SnS_2 phase whereas the film synthesized at 225 °C has a dominant SnS_2 phase. The SnS_2 film synthesized at 500 °C has a single phase of hexagonal structure. The UV-Vis spectrum of low temperature synthesized film shows a high absorption coefficient larger than 10^5 cm^{-1} above the optical band gap of 1.34 ± 0.02 eV. The high temperature synthesized film shows an optical band gap of 2.29 ± 0.02 eV. Raman spectra from the low temperature synthesized film with mixed phases has four SnS vibrational modes and one SnS_2 vibrational mode whereas the Raman spectra from high temperature synthesized film shows a single SnS_2 vibrational mode at 314 cm^{-1}. The PL spectra shows a single peak around 551 nm for all synthesized films that is attributed to SnS_2. The flake-shape, single phase SnS_2 of about ten micron size can also be grown using co-evaporation of Sn at 600 °C and S at 150 °C in the quartz tube inside the furnace (Fig. b). This growth method provides an alternative cost effective way to grow inexpensive semiconductor films on amorphous substrates for a wide range of applications.

*Work supported by NSF DMR-1305293, NSF CHE-1255100, NY State Foundation of Science, Technology and Innovation (NYSTAR) through Focus Center-New York, and Rensselaer.



SILICON NANOWIRES FOR PHOTOVOLTAIC APPLICATIONS

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In an effort to decrease the cost of manufacturing photovoltaics, new technologies, such as thin film silicon solar cells are being utilized. However, due to high recombination of minority carriers at grain boundaries, these technologies do not have a high efficiency compared to traditional silicon wafer solar cells. Incorporating nanostructures, such as silicon nanowires (SiNWs), into thin film technology offers a solution to the recombination problem. SiNWs are a good choice because they are less sensitive to impurities and exhibit low reflective losses compared to planar silicon. We grew SiNWs on p-type silicon substrates and used characterization methods such as Scanning Electron Microscope (SEM), X-Ray Diffraction (XRD), UV-vis reflectance measurements and Raman spectroscopy. The nanowires are crystalline with an average diameter ranging from forty to fifty nanometers. We then fabricated and measured devices.

LOW LER TIN CARBOXYLATE PHOTORESISTS USING EUV

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Organic chemically amplified photoresists have dominated the microelectronics industry for two generations of manufacturing technologies (λ= 248 nm and 193 nm). These systems have shown to be quite capable of achieving the necessary photolithographic performance to allow the industry to follow Moore's law. However, we are rapidly approaching a barrier in which the cost and complexity of achieving smaller feature sizes faces diminishing returns. Extreme ultraviolet (EUV, λ= 13.5 nm) is one promising next generation printing technique, but there exists many challenges that must be resolved before it can be implemented. One major challenge in successful EUV implementation is photoresist design.

EUV photons are much higher energy than 193 nm photons, so traditional photoresist design may be inadequate to continue resolving increasingly smaller patterns. As we decrease film thickness to compensate for smaller patterning without line collapse, organic films may be unable to absorb the photons efficiently which may lead to poor sensitivity and line edge roughness (LER). Etch resistance may also be inadequate in these thinner, organic films. We have previously reported on a new resist system, MORE (Molecular Organic Resists for EUV), that seeks to rectify the potential obstacles that face EUV resist design. By using elements that have a high EUV optical density, we propose that we can create a molecular film that is capable of absorbing more precious EUV photons which may result in higher resolution patterns with better sensitivity and LER.

Here, we present recent lithographic results of several MORE mononuclear tin compounds that have been spin coated into a thin film and exposed to EUV light. We have synthesized a series of tin compounds of the general type $(Benzyl)_2Sn(COOR)_2$ = $(C_6H_5CH_2)_2Sn(OOCR)_2$ in an attempt to study the effects of increasing ligand bulk and decarboxylative activity on photosensitivity and lithographic performance. While we found that the sensitivity of these compounds is overall poor, one compound, $(C_6H_5CH_2)_2Sn(OOC(CH_3))_2$, obtained high resolution patterning (16 nm) with low LER (2.1 nm) and moderate resolution patterning (22 nm) with excellent LER (1.4 nm), Figure 2. We also see a linear trend when we compare molecular weight with E_{max}.

FATIGUE BEHAVIOR AT COPPER-SILICA INTERFACES

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Metal-ceramic heterointerfaces are widely used in diverse applications such as nanoelectronics, renewable energy and biomedicine. In such applications, subcritical debonding of interfaces under cyclic loading (fatigue), are likely to significantly affect the performance and reliability of materials and device structures. Fatigue crack growth driven by sub-critical loading is an insidious failure mode that can be exacerbated in aggressive chemical environments. While fatigue has been widely investigated in bulk materials, very little is known about fatigue at heterointerfaces. This lacuna is significant given that interfaces are well known failure sites.

Here, we present the results of an investigation that captures the fatigue behavior of copper-silica interfaces. All our experiments were carried out in a four-point bending test system equipped with a piezo-actuator to generate sinusoidal waveforms at preset loading amplitudes and frequencies. For a constant loading frequency f = 10 Hz the crack growth rate was measured for different loading amplitudes and a constant load ratio R = 0.1. For intermediate crack growth rates in the $10^{-7} \leq da/dN \leq 10^{-4}$ m.cycle^{-1}, we observe a power-law dependence on the maximal energy release rate G_{max}. Additionally, the behavior conforms to Paris law $\frac{da}{dN} = CG_{\max}^{m}$ where da/dN is the crack growth rate per cycle, and C and m are empirical parameters. The frequency-dependence was investigated at a constant G_{max} = 2.15 Jm^{-2} corresponding to intermediate crack growth rates. Crack growth rates obtained across four frequency decades of $0.1 \leq f \leq 100$ Hz indicate an increase in crack growth rate when the frequency is decreased. This time-dependent behavior is attributed here to water activity.

The dynamic fatigue results will be discussed in terms of the stress-corrosion behavior (static fatigue) of Cu-silica interfaces. Based on our results, we will present an empirical description of the observed changes in properties.

FIRST-PRINCIPLES INVESTIGATION OF ELECTRON TRANSPORT IN Cu LAYERS

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First-principles calculations are used to investigate the increase in the resistivity of Cu interconnect wires with decreasing size, which becomes a major challenge for the downscaling of integrated devices. The calculated density of states (DOS) at the Fermi level at a Cu(001) surface is 3.7 $eV^{-1}nm^{-2}$. The addition of a Ti cap layer with a thickness of 0.25, 0.5, and 1.0 monolayers (ML) causes a 4 to 7-fold increase to 15.0-27.4 $eV^{-1}nm^{-2}$. However, oxidation with an increasing oxygen-to-titanium ratio from 0 to 2 leads to a decrease of the DOS to 2.4-6.5 $eV^{-1}nm^{-2}$. This calculated increase and decrease in the DOS is attributed to localized surface states and explains the experimentally observed transition from specular to diffuse to specular electron surface scattering.

The calculated two-dimensional Fermi surface of Cu layers is approximately cylindrical, with a nearly constant Fermi velocity of $5.7\text{-}6.0*10^5$ m/s which is also nearly independent of the thickness of 0.3 to 3 nm, close to the predicted bulk value of $8*10^5$ m/s from the free electron model. A qualitative analysis of the band structure of a system with a periodic surface roughness indicates a reduced Fermi velocity which is due to the larger lattice period which, in turn, leads to a reduced conductance.

To investigate the effect of the Cu surface roughness on the layer resistivity, first-principles calculations are combined with a non-equilibrium Green's function approach to directly calculate the resistance of a scattering region between two semi-infinite electrodes. The ballistic conductance in a 1 nm thick (6 ML) Cu layer with atomically smooth surfaces is $0.50*10^{15}\ \Omega^{-1}m^{-2}$, close to the reported bulk value of $0.55*10^{15}\ \Omega^{-1}m^{-2}$. However, one single atom adsorbed on the surface causes an additional resistance of 35 Ω. This effect is reduced to 10 Ω as the film thickness increases to 2 nm. This single atom roughness leads to a partial reflection that reduces the transmission coefficient to 97%. Two separated surface adatoms lead to a reduced transmission probability of 94%. Atomic height surface steps, as simulated with a transition from a 6 to 8 to 6 ML thickness causes a 20% resistance increase in the limit of a large scattering region length L > 20 ML. One atomic height surface steps simulated by layer displacements can also increase the resistance by 30%, and the reflection coefficient is proportional to the step height.

Initial results for a random atomic level surface roughness suggest a linear increase in the resistance with increasing length of the scattering region, from $9.7*10^2$ Ω for L = 2 ML to $1.2*10^3$ Ω for L = 16 ML, indicating a resistivity of 8.3 μΩ*cm, which is purely due to surface scattering.

METROLOGY FOR CIGS USING SPECTROSCOPIC ELLIPSOMETRY

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Deposition of copper indium-gallium diselenide thin film photovoltaic absorbers ($CuIn_{1-x}Ga_xSe_2$; CIGS) is done through thermal 3-stage Co-evaporation process as it yields highest efficiency devices. This deposition process requires optical models to be used in the inline metrology tools for accurate process control. Spectroscopic Ellipsometry is powerful non-destructive method to develop the optical models which can be used to characterize and control thickness and optical properties during the deposition process. In this study, Spectroscopic Ellipsometry (SE) has been applied for all three processing stages of CIGS ($Cu(In,Ga)Se_2$) based solar cells in the energy range of 0.7eV to 5.1eV. Dielectric functions have been determined for samples stopped after each deposition stage of the three stage Co-Evaporation process. As the samples are thick (>1.5um), thickness non-uniformity along with surface roughness have been included in the SE analysis. Critical-point line-shape analysis has been used in this study to determine the critical point energies of the CIGS based layers.

MODELING THE THERMOELECTRIC FIGURE OF MERIT OF NANOBULK Bi_2Te_3 AS A FUNCTION OF DOPING, POROSITY, AND GRAIN STRUCTURE

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Designing thermoelectric materials with a high figure of merit ZT is a challenge because it requires retaining a high Seebeck coefficient α and electrical conductivity while minimizing the thermal conductivity σ. Recent advances in microwave-stimulated wet-chemical synthesis techniques have allowed the production of a new class of sulfur doped, nanostructured bulk n-type Bi_2Te_3. We used Boltzmann transport equation and Debye-Callaway theory to understand and optimize both the electronic and thermal transport properties of bulk nanostructured materials to obtain insights into strategies for maximizing ZT. By modeling scattering due to nanostructuring and doping we are able to explain the transport properties in p- and n-type Bi_2Te_3 nanocrystals and their bulk assemblies. Our results show that bulk polycrystalline Bi_2Te_3 pellets with ≳95% mass density comprised of ~100 nm grains doped with ~3000 ppm sulfur can yield a 15% higher ZT of ~1 than bulk Bi_2Te_3 single-crystal. We will present preliminary density functional theory results on the effect of sulfur on defect formation energies, band structure, and density-of-states in Bi_2Te_3, with the goal of enhancing our understanding of how sulfur affects a sharper increase in $\alpha^2\sigma$ than predicted by extant Boltzman transport models. These results provide a basis to realize high ZT nanomaterials through a combination of suppression through nanostructuring and $\alpha^2\sigma$ enhancement through band structure engineering via doping.

STRUCTURAL STUDY OF TOPOLOGICAL INSULATOR MATERIALS USING X-RAY DIFFRACTION, TRANSMISSION ELECTRON MICROSCOPY, AND SECOND HARMONIC GENERATION

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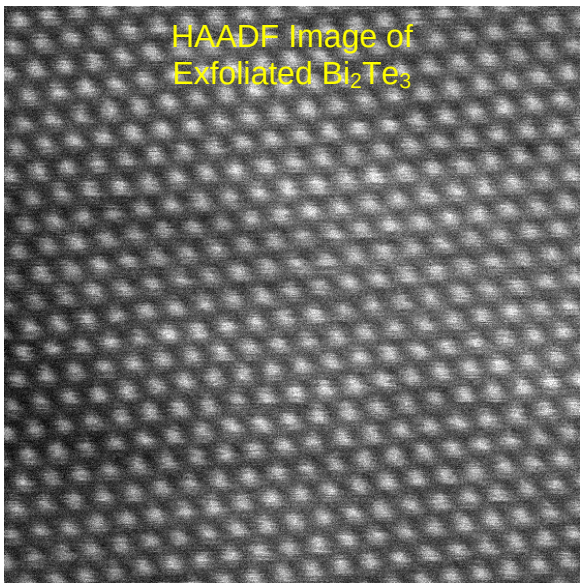
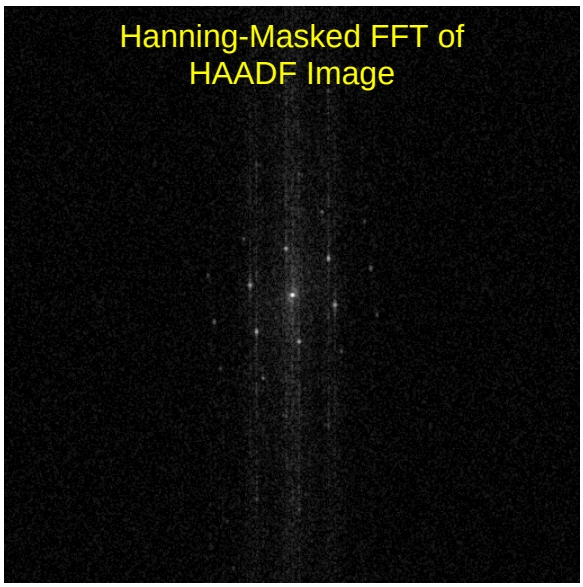
Topological Insulator (TI) materials have increasingly been the subjects of intense scientific interest in the last decade. In the 2D regime, these materials have band gaps and spin-polarized surface Dirac cones. Though these materials have been thoroughly described in theory (Kane 2005, Kane 2007, Qi 2008, Zhang 2009), the experimental realization and measurement of these surface states has been rare. Theory predicts that TI surface states are protected against various defects, but in order to understand the difficulty in these surface state measurements, it is essential to study the perturbations in defective TI crystals. XRD, TEM, and SHG are all means of probing the periodicities and symmetries of crystal lattices. Further, with HAADF STEM, it is possible to view the locations and types of microscopic defects, down to the atomic level. These data constitute a necessary first step and precursor to experimentally correlating structural defects with discrepancies seen between theory and energetic measurement.





EPITAXIAL AND POLYCRYSTALLINE WN_x FILMS DEPOSITED BY REACTIVE DC MAGNETRON SPUTTERING ON MgO(001), MgO(111), AND Al_2O_3(0001)

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WN_x layers, 1.45-µm-thick, were deposited by reactive magnetron sputtering on MgO(001), MgO(111), and Al_2O_3(0001) in 20 mTorr N_2 at T_s = 500-800 °C. X-ray diffraction ω-2ϑ scans, ω-rocking curves, φ scans, and reciprocal space maps show that all layers deposited from 500-700 °C exhibit the cubic rock-salt structure. Energy dispersive and photoelectron spectroscopies yield a N-to-W ratio x which decreases with increasing T_s = 500-700 °C from x = 1.20 to 0.83. T_s = 500 and 600 °C yields polycrystalline predominantly 111 oriented WN on all substrates. In contrast, deposition at 700 °C results in epitaxial growth of WN(111) and WN(001) on MgO(111) and MgO(001), respectively, while deposition on Al_2O_3(0001) yields a 111-preferred orientation, misoriented cubic WN grains as well as N-deficient bcc W. T_s = 800 °C causes nitrogen loss and WN_x layers with primarily BCC W grains and x = 0.04. The decreasing nitrogen content with increasing deposition temperature results in a relaxed lattice constant which decreases from 4.299-4.171Å. The measured elastic modulus ranges from 110-260 GPa for 500-700 °C and decreases with increasing N-content, and increases to 350 GPa for T_s = 800 °C. The resistivity decreases with increasing T_s from 4500-1100 µΩ-cm at 290 K and increases 25% for epitaxial $WN_{0.92}$/MgO(001), 16% for epitaxial $WN_{0.83}$/MgO(111), and 7% for $WN_{0.93}$/Al_2O_3(0001) at 77 K, indicating weak carrier localization as well as a resistivity decrease with increasing crystalline quality and phase purity. For samples deposited at T_s = 700 °C, nanoindentation on WN on MgO(001), MgO(111), and Al_2O_3(0001) provides hardness values of 9.8 ± 2.0, 12.5 ± 1.0, and 10.3 ± 0.4 GPa, and elastic moduli of 240±40, 257±13, and 242±10 GPa, respectively. Brillouin spectroscopy measurements show shear modulus values of 52±2 GPa and 123±3 GPa for WN on MgO(111) and Al_2O_3(0001) respectively, while measurements of WN on MgO(001) showed an upper bound of 43±4 GPa for the shear modulus.

THE FEASIBILITY OF ACHIEVING THE RESOLUTION LIMIT OF BILAYER PMMA / MMA WITH LIFT – OFF

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A well established process for creating microstructures on the surface of a substrate using a sacrificial layer of photoresist is called Lift – Off. However before this process can be applied several lithography steps must occur before Lift – Off. The preceding steps of applying the bilayer resist of PMMA / MMA, the electron beam exposure of the resist, the resist development and the application of metal coatings will all affect the resolution performance. Each process parameter provides exceptional capability as individual contributor but as an assemblage of technology, the elusive goal of determining the best combination or magic formula is a challenge. The contribution of each process is investigated for strengths and weaknesses to provide a determination that would be beneficial for nanofabrication.

ROLE OF SURFACE TERMINATION ON THE GROWTH OF GRAPHENE ON CU

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Graphene growth on on-axis Cu(100) and Cu(111) substrates and a Cu(111) substrate intentionally miscut by 5° was performed to determine the effect that the substrate termination has on both the rate of carbon deposition and the crystal quality of the graphene. A CVD process using C_2H_4 was used to grow the graphene. All experiments were performed in a UHV chamber, and the surfaces were cleaned using multiple Ar sputtering and annealing cycles until the LEED demonstrated a clean surface. By heating the substrates to 900°C in UHV and then backfilling with 5 mTorr of C_2H_4, graphene could only be grown on the off-axis Cu(111) surface. This is attributed to the high vapor pressure of Cu and the low reactivity of the on-axis surfaces. By first backfilling with 5 mTorr of C_2H_4 and heating the substrate to 900°C, graphene could be grown on both the on-axis Cu(100) and off-axis Cu(111) substrates. To achieve growth on the on-axis Cu(111) substrate, an argon overpressure was used to suppress Cu sublimation. Growth of graphene at 900°C using a mixture of 5 mTorr C_2H_4 and 45 mTorr of argon produced single domain epitaxial films on the Cu(111) substrates and two domain epitaxial films on the Cu(100) substrate.

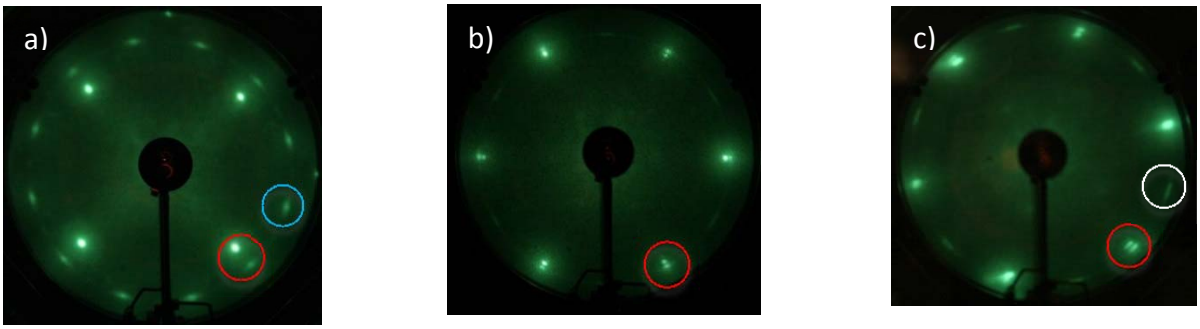

Figure 1: LEED images for growth of graphene by backfilling the UHV chamber with 5 mTorr of C_2H_4 and 45 mTorr of Ar then heating to 900 °C. Growth was done on a) an on-axis Cu(100) substrate where a two-domain epitaxy is observed (red and blue circles), b) an on-axis Cu(111) substrate with a predominantly single-domain epitaxy (red circle), and c) an off-axis Cu(111) substrate with a predominantly single-domain epitaxy (red circle) with some second domain growth (white circle).

STUDYING SECONDARY ELECTRON BEHAVIOR IN EUV RESISTS USING EXPERIMENTATION AND MODELING

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ABSTRACT

EUV photons expose photoresists by complex interactions starting with photoionization that create primary electrons (~80 eV), followed by ionization steps that create secondary electrons (10-60 eV). Ultimately, these lower energy electrons interact with specific molecules in the resist that cause the chemical reactions which are responsible for changes in solubility. The mechanisms by which these electrons interact with resist components are key to optimizing the performance of EUV resists.

An electron exposure chamber was built to probe the behavior of electrons within photoresists. Upon exposure and development of a photoresist to an electron gun, ellipsometry was used to identify the dependence of electron penetration depth and number of reactions on dose and energy. We will present the results of this experiment.

In parallel, our group developed LESiS, a robust software that uses first-principles based Monte Carlo simulations to track secondary electron production, penetration depth, and reaction mechanisms within materials-defined environments. LESiS was used to model the thickness loss experiments (Figure 1) to validate its performance with respect to simulated electron penetration depths to inform future modeling work.

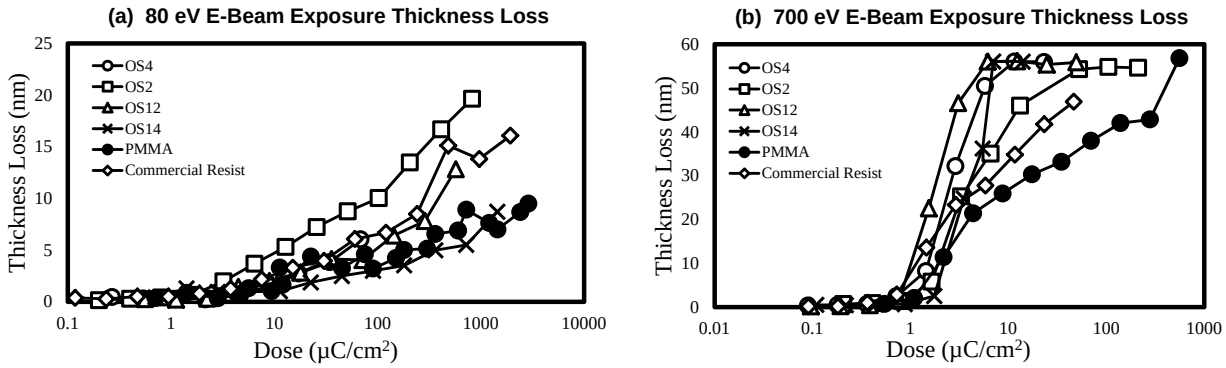

Figure 8. (a) Experimental thickness loss for all resists with 80 eV electrons. **(b)** Experimental thickness loss for all resists with 700 eV electrons.

THERMOELECTRIC POWER FACTOR ENAHNCEMENT BY DILUTE SULFUR DOPING IN Bi_2Te_2Se NANOCRYSTS

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Realizing materials with high thermoelectric power factor is an exacting challenge because it entails simultaneously obtaining a high Seebeck coefficient α and a high electrical conductivity σ, while these properties are usually unfavorably coupled. Here, we show that 0.1 to 2 at.% sulfur doping can result in multifold increases in the power factor $\alpha^2\sigma$ in ternary Bi_2Te_2Se nanocrystals grown by chemical vapor deposition. Hall measurements of the nanocrystals at 50 K ≤ T ≤ 300 K show that the electron concentration *n* monotonically increases with sulfur doping, but saturates at $n \sim 2\times10^{20}$ cm^{-3} for sulfur doping levels above 2 at.%. The maximum values of α = -180 μVK^{-1} and $\sigma = 1.8\times10^5$ $\Omega^{-1}m^{-1}$ for $BiTe_2Se$ for 2 at.% sulfur doping. The observed increases in $\alpha^2\sigma$ are attributed to sulfur-doping-induced increase in density of states effective mass m_{DOS}^*- obtained by fitting seebeck coefficient with Mott's relation. For instance m_{DOS}^* for Bi_2Te_2Se nanocrystals doped with 2 at.% sulfur is threefold higher than that of undoped Bi_2Te_2Se. The resultant increase in the electron density of states near the Fermi level E_F lead to increases in α without decreasing σ. Exploiting these effects should be attractive for realizing high figure of merit thermoelectric nanomaterials.

INTERGRATION OF A DC MAGNETRON SPUTTERING SYSTEM INTO AN ULTRA-HIGH VACUUM CHAMBER FOR FABRICATION OF SCHOTTKY DIODES

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A DC magnetron sputtering system was installed into a UHV chamber for sputtering of metal thin films with little contamination. Control of the DC power, chamber pressure and deposition time is crucial to deposit metal films with reproducible thicknesses and topographies. A graphical user interface was created to efficiently control all potential process variations.

Thin films of tungsten were deposited on both n-Si and p-Si using Argon as the ionizing gas. Scanning tunneling microscopy was used *in situ* to analyze the surface roughness. Ballistic electron emission microscopy was utilized to provide nanometer scale insight into the homogeneity of the tungsten-silicon Schottky barrier.

NEGATIVE MAGNETORESISTANCE AND ELECTRICALLY DETECTED ZERO FIELD SPLITTING IN A LOW-K DIELECTRIC

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We observed negative magnetoresistance in amorphous SiCOH, a low-k dielectric, applying modest magnetic fields (< 150 Gauss) at room temperature. The change in conductivity due to the applied magnetic field increases with the electric field applied to the sample and has little or no temperature dependence over the range studied. The magnitude of the effect is independent of the orientation of magnetic field relative to the direction of current flow. The effect is attributed to spin constraints associated with double occupancy of a trap site under the assumption that trap sites which have double occupancy have lower hopping frequencies than traps that have single occupancy. Furthermore, when the carrier concentration in the material is relatively high the conductivity as a function of magnetic field exhibits two minima which are split on the order of ten Gauss right around zero magnetic field. This zero field splitting is attributed to electron-electron interactions amongst charge carriers which causes two electron spin states, singlets and triplets, to have different energies at zero magnetic field.