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2016 FALL MEETING

AVS HUDSON MOHAWK CHAPTER

Monday, Oct 24th, 2016
4-8pm

Amstuz Hall Room 104
Hudson Valley Community College
80 Vandenburgh Ave,
Troy, NY 12180

Meeting Agenda*

4:00 PM – 6:05 PM	**Oral Presentations**
6:05 PM – 6:30 PM	**Break – Pizza and beverages**
6:30 PM – 7:30 PM	**Poster presentations and networking**
7:30 PM – 7:45 PM	**Best presentation and poster announcement**
7:45 PM – 8:00 PM	**AVS Local Chapter Executive meeting**

*** The presentation schedule is attached in the next page.**

*Presentation Schedule:

(Oral presentations are of 15 minutes with 5 more minutes for Q&A.)

4:00 – 4:05 PM Welcome note by Prof. Harry Efstathiadis

Oral Presentations

4:05 – 4:25 PM GROWTH OF GRAPHENE ON Cu SINGLE CRYSTAL SUBSTRATES
Tyler Mowll,[1] Zachary Robinson,[2] and Carl Ventrice, Jr.[3]
[1] University at Albany-SUNY
[2] College at Brockport-SUNY
[3] SUNY Polytechnic Institute

4:25 – 4:45 PM REALIZATION OF SELF-ALIGNED ERBIUM-DOPED SILICON-CARBIDE NANOWIRES TOWARDS QUANTUM TECHNOLOGIES
Natasha Tabassum, Vasileios Nikas, Brian Ford, and Spyros Gallis
College of Nanoscale Sciences and Engineering, State University of New York Polytechnic Institute, Albany, New York 12203, USA

4:45 – 5:05 PM ELECTRON TRANSPORT IN NANOSCALE CONDUCTORS: FIRST-PRINCIPLES RESULTS
Tianji Zhou,[1] Pengyuan Zheng,[2] and Daniel Gall[1]
[1] Rensselaer Polytechnic Institute
[2] Micron Technology, Inc.

5:05 – 5:25 PM CURRENT INJECTION DEPENDENT MANGETORESISTANCE OF NICKEL NANOPARTICLES EMBEDDED IN SINGLE CRYSTAL Si
Girish Malladi, Mengbing Huang, and Hassaram Bakhru
SUNY Polytechnic Institute, Albany, NY 12203

5:25 – 5:45 PM APPLICATIONS OF THIN FILM MOLECULAR ASSEMBLIES AS ELECTROCHROMIC DEVICES
M. Jeremy Amdur and P. H. Dinolfo
Rensselaer Polytechnic Institute

5:45 – 6:05 PM DEVELOPMENT OF AN ETCH PROCESS TO IMPROVE RRAM PERFORMANCE METRICS
Karsten Beckmann,[1] Joseph Van Nostrand,[2] and Nathaniel C. Cady[1]
[1] SUNY Polytechnic Institute, CNSE, Albany, NY, United States
[2] Air Force Research Laboratory/RITB, Rome, NY, United States

6:30 – 7:30 PM Poster Presentations

Large grain Ge Heteroepitaxy Growth on Cube-Textured Ni(001) flexible Foils Through CaF_2 Buffer Layer*
L. Chen,[1] Z.-H. Lu,[1] T.-M. Lu,[1] I. Bhat,[2] S.B. Zhang,[1] A. Goyal,[3] L.H. Zhang,[4] K. Kisslinger,[4] and G.-C. Wang[1]
[1] Department of Physics, Applied Physics and Astronomy,
[2] Electrical, Computer and Systems Engineering Department, & cMDIS
Rensselaer Polytechnic Institute, 110, 8th Street, Troy, NY 12180, USA
[3] TapeSolar Inc. and U. at Buffalo, RENEW Institute, Buffalo, NY 14260
[4] Brookhaven National Lab, Center for Functional Nanomaterials, NY 11973, USA

ELECTRON SCATTERING AT Cu-Al AND Cu-Al_2O_3 INTERFACES

E. Milosevic and D. Gall
Department of Materials Science and Engineering, Rensselaer Polytechnic Institute

ANALYSIS of $CuIn_{1-x}Ga_xSe_2$ THIN FILM ABSORBER LAYERS USING SECONDARY ION MASS SPECTROSCOPY

Jesse Claypoole,[1] Bernadette Peace,[1] Neville Sun,[2] Dan Dwyer,[1] Matthew D. Eisaman,[3,4,5] Pradeep Haldar,[1] and Harry Efstathiadis[1]
[1] State University of New York Polytechnic Institute, Colleges of Nanoscale Science and Engineering, 257 Fuller Rd., Albany, NY 12203, USA
[2] Angstrom Sun Technologies Inc., 31 Nagog Park, Acton, MA 01720, USA
[3] Sustainable Energy Technologies Department, Brookhaven National Laboratory, Upton, NY 11973, USA
[4] Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY 11794, USA
[5] Department of Electrical and Computer Engineering, Stony Brook University, Stony Brook, NY 11794, USA

VALENCE ELECTRON CONCENTRATION AS AN INDICATOR OF MECHANICAL PROPERTIES IN ROCKSALT STRUCTURES

Karthik Balasubramanian[1] and Daniel Gall[2]
[1] Department of Mechanical, Nuclear and Aerospace Engineering, Rensselaer Polytechnic Institute
[2] Department of Materials Science and Engineering, Rensselaer Polytechnic Institute

FIRST PRINCIPLES STUDY ON BAND ALIGNMENT OF TMDS BASED VDWS P-N JUNCTIONS

Baiwei Wang[1], Shenyuan Yang[2], Daniel Gall[1]
[1] Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180, USA
[2] Institute of Semiconductors, Chinese Academy of Science, Beijing, China, 100083

Investigation of Energy Transfer in Perylene Diimide Based Multilayer Light Harvesting Arrays

Louis Ayensu-Mensah,[1] Zhaorui Huang,[2] and Peter H. Dinolfo[1]
[1] Rensselaer Polytechnic Institute
[2] Stanford University

Development of an ionoluminescence measurement setup*

Subha Chakraborty and Mengbing Huang
SUNY Polytechnic Institute, Albany, NY 12203

Oral Presentation

GROWTH OF GRAPHENE ON Cu SINGLE CRYSTAL SUBSTRATES

Tyler Mowll,[1] Zachary Robinson,[2] and Carl Ventrice, Jr.[3]

[1] University at Albany-SUNY
[2] College at Brockport-SUNY
[3] SUNY Polytechnic Institute
Email: tmowll@albany.edu

Copper foils are frequently used to grow single-layer graphene by chemical vapor deposition (CVD). The primary reasons for this are the low costs of the Cu foils, the low solubility of carbon in Cu, and the relatively low cost of the equipment needed to grow the films. However, the polycrystalline nature of Cu foils can lead to numerous crystalline defects in the graphene, resulting in a reduction in the transport properties. To provide a systematic study of the CVD graphene growth process, a study of the growth of graphene on single crystal Cu substrates, with terminations along the (100), (110), and (111) planes, was performed. Synthesis was performed in an ultra-high vacuum (UHV) chamber using a modified setup to allow growth at pressures as high as 1 Torr. Ethylene was used as the precursor gas. To control Cu sublimation at the elevated growth temperatures, an Ar overpressure was used. This arrangement allowed for the preparation of clean Cu surfaces by sputtering and annealing the Cu crystals in UHV, followed by graphene growth at low pressure, and analysis with low energy electron diffraction in UHV without breaking vacuum. This avoided exposure of the crystal to atmospheric contaminants. It was found that surface termination plays a strong role in the rotational alignment of the nucleating graphene grains and the decomposition rate of the ethylene. It was observed that single-domain epitaxy is possible on Cu(111) when the ethylene pressure is 5 mTorr or less. However, growth on both Cu(100) and Cu(110) result in a minimum of two domains. In addition, ex-situ EELS is currently being performed on well-ordered epitaxial graphene films grown on Cu(111) and Cu(100) to determine the effect of the graphene-Cu interaction on the electronic properties of the graphene.

Oral Presentation

REALIZATION OF SELF-ALIGNED ERBIUM-DOPED SILICON-CARBIDE NANOWIRES TOWARDS QUANTUM TECHNOLOGIES

Natasha Tabassum, Vasileios Nikas, Brian Ford, and Spyros Gallis

Colleges of Nanoscale Sciences and Engineering, State University of New York
Polytechnic Institute, Albany, New York 12203, USA
Email: ntabassum@sunypoly.edu

Recent studies have shown that silicon carbide (SiC) is a promising host material for centers exhibiting single photon emission, which is an essential property for emerging quantum technologies. Furthermore, rare-earth ions are proposed to be good candidates as photo stable single emitters when doped in crystals. Erbium, in particular, attracts further interest due to its intra 4*f*-band transition at the technological wavelength for communications at ~1534 nm. Precise placement of single emitters in an ordered Si-based nano-architecture is essential for high functional practical applications. Herein we present a novel nanofabrication scheme for the synthesis of ultrathin (e.g. diameter, d < 20 nm) SiC nanowire (NW) arrays doped with erbium (Er^{+3}) ions with and without oxygen co-doping. The NWs were grown in a self-aligned manner through a catalyst-free chemical-vapor-deposition (CVD) synthesis route. Their structural and optical characteristics were studied by Fourier transform infrared spectroscopy (FTIR), ultraviolet-visible spectroscopic ellipsometry (UV-VIS-SE) and X-ray photoelectron spectroscopy (XPS). The evolution of the FTIR absorption spectra with forming-gas annealing temperature revealed a substantial narrowing of the FWHM at 1200 °C, which was accompanied by a change of the absorption spectrum lineshape from Gaussian to Lorentzian, comparable to values for high-quality crystalline SiC. Furthermore, the Er^{3+} emission from the doped nanostructured arrays was investigated by photoluminescence (PL) and PL excitation (PLE) spectroscopy. Specifically, the samples exhibit room-temperature Er^{+3} PL with a broad band excitation behavior over the UV-visible range (250-514 nm) and a ~two orders of magnitude PL increase in the case of SiC:O:Er NW compared to its thin-film counterpart. Furthermore, time-resolved and power-dependence PL suggest an efficient energy transfer mechanism from the SiC NW arrays to Er^{3+} ions.

Oral Presentation

ELECTRON TRANSPORT IN NANOSCALE CONDUCTORS: FIRST-PRINCIPLES RESULTS

Tianji Zhou,[1] Pengyuan Zheng,[2] and Daniel Gall[1]

[1] Rensselaer Polytechnic Institute, [2] Micron Technology, Inc.
Email: zhout2@rpi.edu

Non-equilibrium Green's function density functional calculations are used to simulate electron transport in 1-2 nm thick Cu films with atomic roughness, phonons, and surface steps. Predicting the resistivity of such nanoscale conductors is important because it is much larger than the bulk resistivity and therefore negatively affects sub-10-nm interconnects in integrated circuits. This size effect is traditionally described with the Fuchs-Sondheimer (FS) model for surface scattering which, however, underestimates the resistivity for films with thickness $d < 10$ nm, as it neglects quantum-mechanical and explicit surface-morphological effects.

Zero temperature calculations of atomically rough layers indicate that the resistivity is proportional to $1/d$, contradicting the classical FS prediction. The proportionality constant for this purely surface induced resistivity is determined by the ballistic conductance. Frozen phonon calculations at 870 K yield a bulk resistivity of (5.7±0.2) μΩ*cm, and a thin film resistivity increase of (4.7±0.2) μΩ*cm which is independent of d = 1-2 nm, suggesting additive surface+phonon scattering with, however, the phonon contribution being reduced by ~20% in comparison to bulk.

A Landauer formalism is applied to explicitly treat surface roughness effects, describing the morphology as discrete atomic height steps that cause electron reflection. The transmission probabilities at surface steps are calculated for Cu layers with d = 6 monolayers vs step height h. The resulting reflection probability is equal to h/d. Integration over a series of steps yields a resistivity due to roughness that is proportional to the surface slope and is additive to the total resistivity. The model predictions are quantitatively confirmed using electron transport on epitaxial W(001) layers which were deposited with variable roughness w and in-plane surface-mound correlation lengths ζ, as quantified by atomic force microscopy, yielding an additional resistivity that increases linearly from (0.5±0.2) to (8.7±0.5) μΩ*cm as $\zeta/(wd)$ increases from 0.001 to 0.037 nm^{-1} .

<u>Oral Presentation</u>

CURRENT INJECTION DEPENDENT MANGETORESISTANCE OF NICKEL NANOPARTICLES EMBEDDED IN SINGLE CRYSTAL Si

Girish Malladi, Mengbing Huang, and Hassaram Bakhru

SUNY Polytechnic Institute, Albany, NY 12203
Email: mmalladi@sunypoly.edu

Integrating magnetic functionalities with silicon based semiconductor devices offers a promise for novel devices with non-volatile storage combined with high speed processing at low powers. In this work, we demonstrate strong room temperature magnetoresistance (MR) in a ferromagnetic nanoparticle layer embedded within a relatively defect free Si environment.

A large moment of ~3000 uB to 8300 uB per nanoparticle was demonstrated for such nanoparticle ensembles using SQUID magnetometer and correlated to particle size and density using SIMS, TEM and RBS/Channeling results. Additionally, the high quality single crystal in the immediate vicinity of the nanoparticles resulted in enhancement of the magnetic switching barrier and resulted in room temperature ferromagnetism.

Magnetotransport measurements with applied fields up to 9T fields were performed on the Schottky devices with embedded Ni nanoparticles fabricated on p- and n-type Si samples and a large magnetoresistance of ~155% was observed. This was more an order of magnitude increase in MR compared to Schottky devices fabricated on control Si samples. The MR vs field data was fitted with a spin-split band model based on different mobilities and conduction channels for majority and minority spin carriers and the exchange splitting (Δ_{ex}) and the *g*-factor for holes and electrons was estimated for different samples. An estimate of the spin polarization (>50%) achieved in such samples was made. The MR vs applied current/bias was also investigated at different temperatures and we observed a decrease in the MR with increasing applied current. The data was correlated to the different current injection regimes for the Schottky device. A plausible explanation of decreasing MR with temperature was made based on spin-dependent scattering of carriers under higher injection conditions.

This work shows a promising approach to implementing viable room temperature spintronic devices in Si for developing spin based computation as well as high-density and high-fidelity information storage technologies.

Oral Presentation

APPLICATIONS OF THIN FILM MOLECULAR ASSEMBLIES AS ELECTROCHROMIC DEVICES

M. Jeremy Amdur and P. H. Dinolfo

Rensselaer Polytechnic Institute
Email: amdurj@rpi.edu

Electrochromism is the property of a material to exhibit different colors in its different oxidation states. Electrochromic (EC) materials often find commercial uses in smart windows, antiglare mirrors, and in certain batteries as state-of-charge indicators. Most research into solid state EC systems has focused on EC polymers due to the ease of growing large chains growth and simple implementation into modern devices. Often overlooked, however, are the applications of a thin film molecular assembly as a potential EC device. Applying the layer by layer approach used in synthesizing many molecular assemblies to an EC system would allow for much greater control over the properties of the device. We have made preliminary steps in designing a bifunctional molecular assembly with one constituent that is EC during oxidation, and another that is EC during reduction. By applying Copper (I) Catalyzed Azide-Alkyne Cycloaddition (CuCAAC), films composed of alternating chromophores were grown and analyzed with common spectroelectrochemical techniques. By applying our method to a variety of systems, we believe that we can lay the foundation for the production of novel EC devices made using thin film molecular assemblies

Oral Presentation

DEVELOPMENT OF AN ETCH PROCESS TO IMPROVE RRAM PERFORMANCE METRICS

Karsten Beckmann,[1] Joseph Van Nostrand,[2] and Nathaniel C. Cady[1]

[1] SUNY Polytechnic Institute, CNSE, Albany, NY, United States
[2] Air Force Research Laboratory/RITB, Rome, NY, United States
Email: kbeckmann@sunypoly.edu

Resistive Random Access Memory (RRAM) is a new class of electronic device whose resistance level can be modulated by feeding a current through the device. The resistance level (memory state) of RRAM devices is non-volatile, making them a viable replacement for flash memory. In addition, this characteristic can be utilized for various circuit level designs including neuro-inspired hardware. In this contribution we integrated a RRAM device with CMOS fabricated on a 300mm wafer platform. The IBM 65nm 10LPe process technology was used as a base for this customized integration effort, with modifications to accommodate the RRAM devices between metal 1 (M1) and metal 2 (M2). By changing the M1 interconnect to tungsten it is possible to utilize front-end-of-the-line (FEOL) tools for the hafnium dioxide atomic layer deposition. Above the custom tungsten M1 layer, a dual tungsten/copper via structure was developed to accommodate RRAM device fabrication. The hafnium dioxide RRAM switching layer was capped with a titanium oxygen getter layer and an inert titanium nitride electrode. The capping layers were etched with reactive ion etch (RIE) whereas two approaches were tested for the hafnium dioxide removal: 1) a wet etch with diluted hydrofluoric acid (dHF) and 2) a BCl_3 based reactive ion etch (RIE) process. The test platform for the vertically-integrated RRAM devices included: 1) 12x12 crossbar arrays with 100x100 nm^2 size devices 2) single RRAM (1R) devices with sizes ranging from 100x100 nm^2 to 10x10 μm^2 and 3) 1 transistor 1 RRAM (1T1R) structures with 100x100 nm^2 size devices. The impact on the RRAM devices for both etch processes was investigated with respect to the physical structure, the electrical characteristics and the yield. The electrical characteristics include simple I-V DC sweeps and pulse-based endurance measurements. The functional principle of these RRAM devices is consistent with a valence change mechanism (VCM), which is filament-based, and therefore area independent. RRAM devices fabricated using the dHF wet etch with layer thicknesses of 5.8 nm of hafnium dioxide and 6 nm of titanium exhibited endurance values exceeding 10^8 cycles with an average on/off resistance ratio of 5 and set/reset voltages below 1/-1.5 V. The dHF etch negatively impacted the physical device structure of the RRAM devices, which was reflected by the resulting electrical performance. By moving to a dry etching (RIE) process, an improvement in yield, reliability, endurance and retention is expected. In particular, yield is expected to increase due to reduced undercut of the titanium oxygen getter layer, which is characteristic of the dHF etch. In summary, we will show the progress towards a complete dry etch definition of the RRAM device stack and compare the current results to achieved switching performance with the previous etch recipe utilizing RIE and dHF for structuring the RRAM device stack.

Poster Presentation

LARGE GRAIN Ge HETEROEPITAXY GROWTH ON CUBE-TEXTURED Ni(001) FLEXIBLE FOILS THROUGH CaF_2 BUFFER LAYER*

L. Chen,[1] Z.-H. Lu,[1] T.-M. Lu,[1] I. Bhat,[2] S.B. Zhang,[1] A. Goyal,[3] L.H. Zhang,[4] K. Kisslinger,[4] and G.-C. Wang[1]

[1] Department of Physics, Applied Physics and Astronomy,
[2] Electrical, Computer and Systems Engineering Department, & cMDIS
Rensselaer Polytechnic Institute, 110, 8th Street, Troy, NY 12180, USA
[3] TapeSolar Inc. and U. at Buffalo, RENEW Institute, Buffalo, NY 14260
[4] Brookhaven National Lab, Center for Functional Nanomaterials, NY 11973, USA
Email: luz@rpi.edu

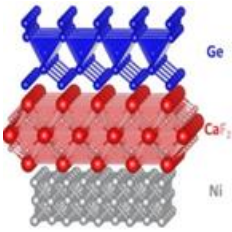
Single crystal Ge wafers are extremely useful for optoelectronic applications. GaInP/GaInAs/Ge multijunction solar cells with efficiencies of over 40% have been achieved using Ge wafers as the substrates. However, single crystal Ge substrates are expensive due to material and processing costs which prevent its prevalence in commercial applications. In this work we report the growth of epitaxial $CaF_2(001)/Ni(001)$ by thermal evaporation despite the large lattice mismatch between $CaF_2(001)$ (a = 0.546 nm) and Ni(001) (a = 0.352 nm). Epitaxial $CaF_2(001)$/ Ni(001) is then used as the substrate to grow thick epitaxial Ge(001) film by thermal evaporation at ~400 ^oC. The epitaxial growth temperature is much lower than the bulk Ge crystallization temperature.

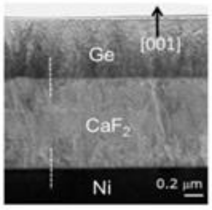
X-ray pole figure results indicate that the $CaF_2(001)$ lattice is rotated 45^o in-plane relative to the Ni(001) substrate to allow a better coincident lattice match. The in-plane epitaxy relationships are $CaF_2[110]//Ni[100]$ and $CaF_2[\bar{1}10]//Ni[010]$. The epitaxial $CaF_2(001)$ film contains no rotation domains. When the Ge film is grown on $CaF_2(001)/Ni(001)$, the Ge film (lattice constant a = 0.566 nm) forms a parallel epitaxial relationship with $CaF_2(001)$ (a = 0.546 nm) due to the small mismatch between Ge(001) and $CaF_2(001)$ [1]. Transmission electron microscopy cross-section images and diffraction patterns support these results. Electron back scatter diffraction mapping shows that the Ge grain size in the epitaxial Ge film is comparable to the Ni grain size in the Ni foil substrate in the range of 50 microns. TEM energy dispersive spectroscopy across the Ge and CaF_2 interface indicates limited inter-diffusion of Ge and CaF_2 [2]. The epitaxial Ge film with large grain size could be used as the substrate to grow semiconductor films such as CdTe and GaAs for roll-to-roll fabrication of optoelectronic applications.

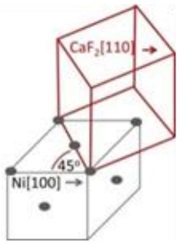
*****This work is supported by the NSF DMR-1305293 and the NYSTAR Focus Center at RPI, C130117. TEM studies were carried out in whole at the Center for Functional Nanomaterials, BNL, which is operated by the DOE, Office of Basic Sciences, DE-AC02-98CH10886.

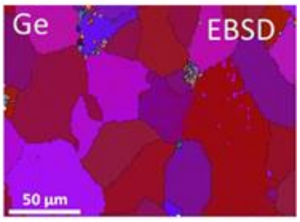
[1] L. Chen, W. Xie, G.-C. Wang, I. Bhat, S. Zhang, A. Goyal, and T.-M. Lu, Thin Solid Films, V. 603, 2016, 428–434, http://dx.doi.org/10.1016/j.tsf.2016.03.007.

[2] L. Chen, Z.-H. Lu, T.-M. Lu, I. Bhat, S.B. Zhang, A. Goyal, L.H. Zhang, K. Kisslinger, and G.-C. Wang, MRS Advances, Published online. DOI: http://dx.doi.org/10.1557/adv.2016.517









Poster Presentation

ELECTRON SCATTERING AT Cu-Al AND Cu-Al_2O_3 INTERFACES

E. Milosevic and D. Gall

Department of Materials Science and Engineering, Rensselaer Polytechnic Institute
Email: milose@rpi.edu

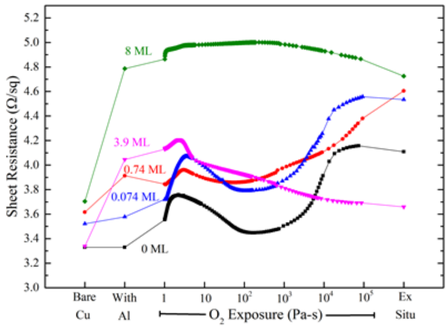


Figure 1. Sheet resistance vs. oxygen exposure of five 10.1±0.1 nm thick epitaxial Cu(001) layers that were coated with 0, 0.074, 0.74, 3.9, and 8 monolayers of Al.

Electron scattering at surfaces is a major contributor to the resistivity of narrow conductors and limits the downscaling of integrated circuits. Epitaxial 10-nm-thick Cu(001) layers were grown and their resistivity ρ studied as a function of surface modification using *in situ* transport measurements. The resistivity increases from ρ = 3.36±0.09 to 3.61±0.05, 3.95±0.05, 4.08±0.05, and 4.83±0.05 μΩ-cm as the Cu layer is capped with d_{Al} = 0.074, 0.74, 3.8 and 8 monolayers (ML) of Al, respectively. This is attributed to an increasingly diffuse electron-surface scattering associated with localized electron states in the Al cap, and is well described by an exponential decay in the scattering specularity with increasing Al thickness. *In situ* oxygen exposure causes time-dependent variations in the resistivity. In particular, oxygen monolayer adsorption results in a peak in the ρ vs exposure curves at 2 Pa-s, while subsequent chemical oxidation of Al and Cu yields a continuous increase for exposures >10^3 Pa-s and d_{Al} = 0-0.74 ML (Fig 1), leading to a 17% resistivity increase for the bare Cu layer, from 3.36±0.09 to 3.94±0.05 μΩ-cm. In contrast, layers capped with 3.9 and 8.0 ML show a resistivity reduction during oxygen exposure, ultimately resulting in a lower overall ρ. More specifically, the oxygen-exposed layer with d_{Al} = 3.9 ML has a ρ = 3.70±0.05 μΩ-cm, which is 6% lower than the corresponding value for the pure Cu layer. This beneficial effect of the Al capping layer is attributed to a decrease in diffuse electron surface scattering as the local electron density of states in the Al cap is reduced during oxidation, while simultaneously suppressing Cu oxidation.

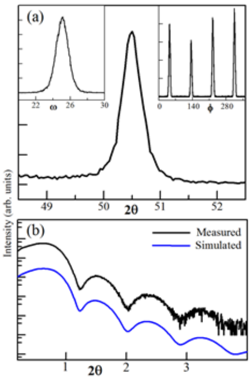


Figure 2. (a) X-ray diffraction Cu(002) 2θ scan. Left inset: ω rocking curve of Cu(002) reflection. Right inset: φ scan of Cu(311) reflection. (b) X-ray reflectivity scan.

Poster presentation

ANALYSIS of $CuIn_{1-x}Ga_xSe_2$ THIN FILM ABSORBER LAYERS USING SECONDARY ION MASS SPECTROSCOPY

Jesse Claypoole,[1] Bernadette Peace,[1] Neville Sun,[2] Dan Dwyer,[1] Matthew D. Eisaman,[3,4,5] Pradeep Haldar,[1] and Harry Efstathiadis[1]

[1] State University of New York Polytechnic Institute, Colleges of Nanoscale Science and Engineering, 257 Fuller Rd., Albany, NY 12203, USA
[2] Angstrom Sun Technologies Inc., 31 Nagog Park, Acton, MA 01720, USA
[3] Sustainable Energy Technologies Department, Brookhaven National Laboratory, Upton, NY 11973, USA
[4] Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY 11794, USA
[5] Department of Electrical and Computer Engineering, Stony Brook University, Stony Brook, NY 11794, USA
Email: JClaypoole@sunypoly.edu

$CuIn_{1-x}Ga_xSe_2$ (CIGS) is a promising candidate as an absorber material for low cost and high efficiency photovoltaic devices with a reported record efficiency of 22.3% approaching that of silicon photovoltaic devices. Secondary Ion Mass Spectroscopy (SIMS) depth profiles were performed on CIGS samples deposited using one stage CIGS samples in order to see what affects of changing the Ga/(Ga+In) ratio had on depth profile parameters. Three stage CIGS absorber layers with graded Ga/(Ga+In). were then deposited using SIMS. We found that the actual and measured SIMS depth profiles in CIGS absorber layers were shifted by 100 nm in samples that had a large Ga/(Ga+In) grading dip.

Poster Presentation

VALENCE ELECTRON CONCENTRATION AS AN INDICATOR OF MECHANICAL PROPERTIES IN ROCKSALT STRUCTURES

Karthik Balasubramanian[1] and Daniel Gall[2]

[1] Department of Mechanical, Nuclear and Aerospace Engineering, Rensselaer Polytechnic Institute
[2] Department of Materials Science and Engineering, Rensselaer Polytechnic Institute
Email: balask2@rpi.edu

Transition metal nitrides and carbides, which generally crystallize in rocksalt structures, have been of considerable interest due to widespread use as coatings for cutting tools, decorative coatings, diffusion barrier coatings, corrosion resistance and their excellent mechanical properties. One of the key challenges of using transition metal nitrides and carbides is the brittleness of these films. Advances in computational materials science have enabled the design of alloys by calculating mechanical stability and energetics of defects to acquire the desired mechanical properties and toughness.

First principle calculations are employed to determine the mechanical stability and the formation energies E_f of point defects in rock-salt phase group III B – VI B transition metal nitrides and carbonitrides. The vacancy formation energy decreases when moving towards the right in the periodic table, from $E_f = 5.1$ to -7.1 eV for anion vacancies in ScN and WN, respectively, and from $E_f = 3.2$ to -12.0 eV for the corresponding cation vacancies.

This decrease is accompanied by a decrease in the single crystal shear modulus, from $c_{44} = 161$ for ScN to 164, 126, and -120 GPa, for TiN, VN, and CrN. Calculations of c_{44} as a function of valence electron concentration, for carbo nitrides from group IIIB to VI B, indicates a c_{44} maximum of 150 ± 15 corresponding to a valence electron concentration of 4.5 and a transition to mechanical instability at a valence concentration of 5.3. Hardness estimations using Tian's model yield values of 22 ± 4 GPa for a valence electron concentration of 4.5 and reduces subsequently to 14 ± 5 GPa for a valence electron concentration. This analysis enables the prediction of hardness and shear modulus of potential ternary and quarternary transition metal alloys solely based on valence electron concentration.

Poster Presentation

FIRST PRINCIPLES STUDY ON BAND ALIGNMENT OF TMDS BASED VDWS P-N JUNCTIONS

Baiwei Wang[1], Shenyuan Yang[2], Daniel Gall[1]

[1] Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180, USA
[2] Institute of Semiconductors, Chinese Academy of Science, Beijing, China, 100083
E-mail: wangb12@rpi.edu

Two-dimensional (2D) materials are attracting considerable attention due to their desirable properties for semiconductor devices, making them promising building blocks for energy conversion, catalysis and optelectronic applications. Here, a first principles study of the electronic properties of 2D transitional metal dichalcogenides (TMDs) van der Waals (vdWs) heterostructures is presented, suggesting strain and alloying are two effective methods to engineer their band structures. Different stacks of heterostructures are investigated, including WSe_2/MoS_2, WS_2/MoS_2, $MoSe_2/MoS_2$ and $MoTe_2/MoS_2$, where the TX_2 (T = Mo, W; X = S, Se, Te) layers in the heterostructures interact with each other through vdWs forces. Strain and alloying allows to tune the band edge positions and the bandgaps by 0.0 -1.5 eV and 0.3 -1.6 eV, respectively. While WSe_2/MoS_2 has a direct band gap, the gaps for WS_2/MoS_2 and $MoSe_2/MoS_2$ are indirect and $MoTe_2/MoS_2$ is metallic, in agreement with previous studies. Increasing biaxial strain from -14% to 8%, WSe_2/MoS_2, WS_2/MoS_2 and $MoSe_2/MoS_2$ systems exhibit metal-semiconductor-metal transitions. For the WS_2/MoS_2 and $MoSe_2/MoS_2$ systems, the band gap remains direct between -3.5% and 0.0% and between -3.0% and -1.0% strain, respectively. Single layers of $MoS_{2(1-x)}Te_{2x}$ and single layers of MoS_2 have been used to form alloy heterostructures. Increasing x leads to a linear increase in the lattice parameter of the p-n junction and a decrease in the bandgap, indicating the potential for bandgap engineering by Te-doping of MoS_2.

Poster Presentation

INVESTIGATION OF ENERGY TRANSFER IN PERYLENE DIIMIDE BASED MULTILAYER LIGHT HARVESTING ARRAYS

Louis Ayensu-Mensah,[1] Zhaorui Huang,[2] and Peter H. Dinolfo[1]

[1] Rensselaer Polytechnic Institute
[2] Stanford University
Email: ayensl@rpi.edu

We have used copper(I)-catalyzed azide-alkyne cycloaddition (CuAAC) chemistry to assemble multilayered light harvesting arrays from molecular components. Three new PDIs were synthesized with phenoxy (PhO-PDI), dodecylthiol (Thiol-PDI), and pyrrolidine (Pyrr-PDI) substituents in the bay positions. These have optical absorption and emission spectra that span a large portion of the visible region. The fluorescence properties of multilayer films grown from these PDIs are highly dependent on the alkyne linking group, with ethynyl-analine groups providing films with the highest fluorescence quantum yield. The Förster resonance energy transfer efficiency between multilayers was examined, with Pyrr-PDI as a terminal acceptor, using steady-state fluorescence spectroscopy. FRET efficiency was found to be quite high over several layers. This rapid and versatile multilayer fabrication method allows for the creation of ordered and uniform thin films with highly controllable photophysical and electrochemical characteristics. This tunability offers the possibility of incorporating multiple different dyes, leading to specifically designed panchromatic arrays with unidirectional energy transfer for increasing the limits of maximum achievable efficiencies for dye-sensitized semiconductor solar cells or organic photovoltaics.

Poster Presentation

DEVELOPMENT OF AN IONOLUMINESCENCE MEASUREMENT SETUP*

Subha Chakraborty and Mengbing Huang

SUNY Polytechnic Institute, Albany, NY 12203
Email: SChakraborty@sunypoly.edu

Growing need of miniaturization of semiconductor devices have motivated interest in sensing and controlling the impact location of energetic ions over nano-devices during doping and lithography processes. For this purpose, we have developed an ionoluminescence measurement instrument and installed it on the beamline of an ion implanter to investigate the properties of ion induced luminescence from thin film organic scintillators. The scintillator thin films are fabricated on silicon wafer by spin-coating a solution of polystyrene and different types of fluors in specific mass-ratios in Toluene. Four types of fluors, 1) para-Terphenyl (pTP), 2) 2,5-Diphenyloxazole (PPO), 3) 1,4-Bis(5-phenyl-2-oxazolyl)benzene (POPOP) and 4) Coumarin 6, each in two different mass-ratios to PS, have been used. In Figure 1, typical ionoluminescence spectra from four types of samples are shown when He ions are used. Kinetic energy of the ions is varied from 50 keV to 350 keV. The integration time of the spectrometer is set to 10 sec for recording the spectrum. pTP and PPO emits in the ultra-violet wavelengths whereas POPOP emits in the violet ranges and Coumarin 6 in the green ranges. From the ion-luminescence spectra, the photon yields are calculated. In Figure 3, the photon yields as a function of kinetic energy of the ions are shown for He ions. It can be seen that the photon yield increases with increasing kinetic energy and decreases with the mass of ion species. A model involving a set of rate equations for describing energy transfer and quenching of molecular excitations is used to understand the effects of ion flux and dose on ionoluminescence from organic scintillator thin films. Such basic understanding will be useful for developing novel radiation sensors.

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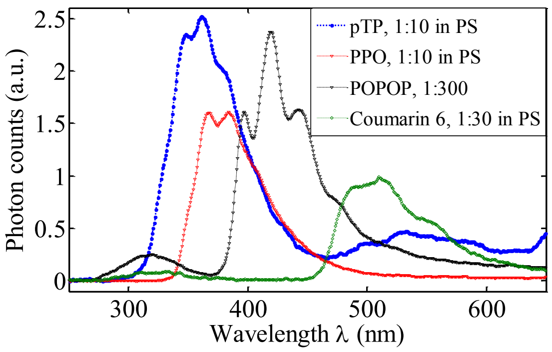

Figure 1: Emission spectra of the fluors with He ion irradiation. Kinetic energy of ions is 350 keV.

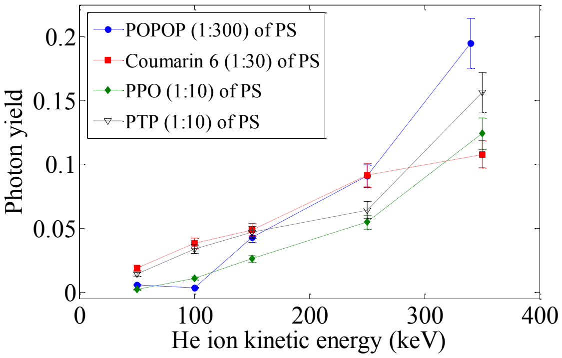

Figure 2: Photon yield (No. of photons per unit ion) measurement from the He ions at different kinetic energies.