Center for Materials, Devices and Integrated Systems
Fall Symposium 2017

http://cmdis.rpi.edu
INSIDE

WELCOME .............................................................................................................. 5

RESEARCH @ the CENTER ......................................................................................... 7

FACILITIES @ the CENTER ........................................................................................ 9

PROGRAM AT-A-GLANCE ......................................................................................... 11

ART-IN-SCIENCE SUBMISSIONS ............................................................................ 13

ORAL PRESENTATIONS .............................................................................................. 29

POSTER PRESENTATIONS ........................................................................................ 39

AUTHOR INDEX ............................................................................................................ 53
Welcome to the first annual cMDIS research symposium. We are delighted to have such a rich and full spectrum of presentations in the symposium, numbering 47 in total, and spanning the full spectrum of research activities within our center.

The cMDIS enables transformative research that spans the range from fundamental discovery to systems level assembly and manufacturing in the physical / chemical sciences and engineering at Rensselaer. It is responsible for the operation of two major experimental facilities on campus, the microscale and nanoscale fabrication cleanroom (MNCR) and the nanoscale characterization core (NCC). It has around 90 faculty members, 120 student and postdoc members, and five affiliated centers (SCOREC, CFES, CASE, LESA and CATS). Our student and postdoc program was initiated within the last year and is growing rapidly, with activities to date including establishing research focus groups (eight to date) and events such as career evenings and instrument tutorials. For more information see http://cmdis.rpi.edu and please let us know how you would like to participate.

During the day, please be sure to interact with your colleagues, ask them questions about their research, and tell them about your research. We hope that many new connections and collaborations are initiated today, and that you enjoy the event!

Finally, many thanks to Dr. Deniz Rende for her superb work in organizing this symposium.

With best wishes,

Robert Hull,
Director, Rensselaer Center for Materials, Devices and Integrated Systems

http://cmdis.rpi.edu
RESEARCH @ the CENTER

Research at the cMDIS spans the broad spectrum of the physical and chemical sciences and engineering, supporting advances in new materials, devices, and systems.

Advanced Computational Devices
New materials, devices and circuit designs for advancing the state-of-the art in computation, including studies of electronic transport at the nanoscale, THz-level circuit design, and materials for cognitive computing.

Advanced Polymeric Materials
Creation and discovery of new polymeric structures and properties with applications such as 3D-assembly, novel energy systems, and optical / electronic devices.

Energy Solutions
Research spanning new methods for energy storage, generation and transmission, including thermoelectric materials, advanced photovoltaic materials, and optimizing the energy grid.

Electrochemical Systems
Broad applications to fundamental mechanisms of corrosion, advanced battery systems, and nuclear waste storage.

Interfacial Engineering and 2D Systems
Creation of enhanced interfacial property combinations using molecular interlayers and synthesis, processing and characterization of new atomically thin layered systems with novel properties.

Materials Informatics and Data Analytics
Developing new methodologies for prediction of new materials with improved properties, and for maximizing extraction of information from data.

Modeling and Simulation
An extensive modeling and simulation eco-system, spanning first principles to atomistic to continuum methods, supported by one of the most powerful supercomputers on a US academic campus.

Nanostructured Systems
Fundamental research into creation of new structures at the nanoscale, with new property combinations, and novel opportunities for system assembly, particularly at the biological-abiotic interface.

Processing and Manufacturing Research
New methods for materials processing and assembly, spanning a broad range of materials, structures, robotics, control, and advanced manufacturing methods.
FACILITIES @ the CENTER

The cMDIS supports two major experimental facilities:

The Microscale and Nanoscale Cleanroom (MNCR) has 5,800 sqft, Class 100 space and contains a broad range of processing, measurement, and fabrication tools enabling researchers to create new structures, devices, and systems at the micro and nano-scale.

- Annealing
- Etching
- Lithography
- Deposition
- Sample Preparation
- Metrology

The Nanoscale Characterization Core (NCC) has 3,300 sqft space and provides a powerful suite of imaging, spectrometry, and diffraction instruments to interrogate structure, chemistry, and other properties from the atomic- to micro-scales.

- Diffraction
- Electrical Testing
- Mechanical Testing
- Microscopy
- Spectroscopy
- Thin Films

http://cmdis.rpi.edu
# PROGRAM AT-A-GLANCE

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:30 – 9:00</td>
<td>Registration and breakfast</td>
</tr>
</tbody>
</table>
| 9:00 – 9:15| Welcome<br>
**Robert Hull**<br>Director, Center for Materials, Devices and Integrated Systems |
<p>|            | <strong>OP.01 | Dustin Andersen</strong>&lt;br&gt;Distributions of Kinetic Pathways in Strain Relaxation of Heteroepitaxial Thin Films |
|            | <strong>OP.02 | Nathaniel Anderson</strong>&lt;br&gt;Synthesis and Characterization of Porphyrin-DNA Constructs for the Self-Assembly of Modular Energy Transfer Arrays |
| 9:15 – 10:30| <strong>OP.03 | Sagar Bhatt</strong>&lt;br&gt;Physical System modeling and simulation using HPC |
|            | <strong>OP.04 | Daniele Cheniak</strong>&lt;br&gt;H, d, and He Diffusion in Diamond - Experimental and Computational Studies |
|            | <strong>OP.05 | Michael Deagen</strong>&lt;br&gt;Residual-Layer-Free Transfer Molding of Mesoscale Periodic Structures |
| 10:30 – 10:50| <strong>Coffee Break and Networking</strong>                                       |
| 10:50 – 12:05| <strong>OP.06 | Debjit Ghoshal</strong>&lt;br&gt;Comprehending the Substrate-Independent Vertical Growth of ReS2 Nanosheets |
|            | <strong>OP.07 | Tushar Gupta</strong>&lt;br&gt;Phosphorus Nanoparticles Embedded in a Reduced Graphene Oxide Matrix for High-Performance Lithium-Ion Battery Anodes |
|            | <strong>OP.08 | Jennifer (John) Howell-Clark</strong>&lt;br&gt;Impurity Control for High Performance Gallium Nitride Device |
|            | <strong>OP.09 | Apostolos A. Karanastasis</strong>&lt;br&gt;Super-resolution nanoscopy study of crosslinking density variations in PNiPAm-based microgels |
|            | <strong>OP.10 | Lu Li</strong>&lt;br&gt;Development of Chemically Immobilized Sulfur Cathodes for Lithium Sulfur Batteries |
| 12:05 – 12:15| <strong>Center Group Photo (outside)</strong>                                        |
| 12:15 – 1:30| <strong>Poster Session and Lunch (Great Room)</strong>                              |
| 1:30 – 1:45| <strong>Art-in-Science Contest</strong>                                             |
| 1:45 – 3:00| <strong>OP.11 | Aaron Littlejohn</strong>&lt;br&gt;van der Waals Epitaxy of Large VS2 Nanoflakes on Muscovite Mica |
|            | <strong>OP.12 | Wei Peng</strong>&lt;br&gt;Molecular Dynamics Simulation on Rheological and Dynamic Properties of Polymer Nanocomposite System with Thermal Stiffening Behaviors |
|            | <strong>OP.13 | Ainsley Pinkowitz</strong>&lt;br&gt;Radiolysis-Influenced Localized Corrosion in the Liquid Cell Transmission Electron Microscope |
|            | <strong>OP.14 | Varun Sarbada</strong>&lt;br&gt;Crystallization of Ultra-Thin Li-V-O Cathode Films |
|            | <strong>OP.15 | Siddharth Sundaraman</strong>&lt;br&gt;New Optimization Scheme for Potential Development for Multi-component Oxide Glasses |
| 3:00 – 3:20| <strong>Coffee Break and Networking</strong> (program continues)                    |</p>
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
</tr>
</thead>
</table>
| 3:20 – 4:35 | **OP.16 | Yixuan Tan**  
Forward and Inverse Simulations of Heat Transfer and Grain Growth in Thin Films  
**OP.17 | Melih Turkseven**  
Magnetically Active Tactile Displays for Virtual Reality Applications  
**OP.18 | Hari Vijayamohanan**  
Spirothiopyran based photoreisists for large area sub-diffraction nanopatterning  
**OP.19 | Yiping Wang**  
Toward-Wafer Scale Ionic Epitaxy of Halide Perovskite Single Crystalline Thin Film Carrying Hidden Carrier Dynamics  
**OP.20 | Shuman Yu**  
Numerical Simulation of CO2 Injection Induced CH4 Production from Gas Hydrate-bearing Sediments |
| 4:35 – 5:30 | **Concluding Remarks and Awards**  
Happy Hour (IDs required)** |
AiS.01 | Dustin Andersen
Nebulas in a Starry Sky

AiS.02 | Tania Baltazar
3D printed blood vessels: a road map to organ survival
AiS.03 | Anirban Chandra
*CFD simulation of a Liquid droplet undergoing phase change*

AiS.04 | Michael Deagen
*Chaos from Order*
The propensity of ReS$_2$ to orient themselves perpendicular to substrate separates them from other TMDs which have a tendency to grow flat on the substrate. Densely grown ReS$_2$ forests with direct bandgap and an extremely large surface area are excellent candidates for studying light matter interaction and for solar energy harvesting.
This is an SEM image of graphene/Fe₃O₃ composite. Like the formation of stalactite, soluble materials could react and form various depositions under peculiar pressure and temperature. Through special pressure and temperature offered by hydrothermal reaction, graphene oxide and ferrous oxalate solution react, forming graphene nanosheet decorated by Fe₃O₃ nanoparticles.
The two images presented pertain to my current research interests of developing suitable Auto Place and Route techniques of an ARM architecture using RSFQ (Rapid Single Flux Quantum) Logic cells. The images describe the result of two separate trial runs of Auto Place and Route of a SCRAM2 computer using the Auto Place and Route Tool Innovus, where the device layout is composed of self built RSFQ Logic cells. For the Auto Place and Route simulation runs, the only user input was the structural verilog file (the netlist that describes how the logic cells are connected in a schematic) and the Library Exchange Format LEF file (the geometrical definition of the modular RSFQ cells that are to be used in the layout of the SCRAM2).

The output of these two trial runs generate the following layouts on the floorplan that resemble character profiles. It is to be noted that the particular routing scheme used by Innovus to create these expressions of abstract art are based on semi random algorithms. Thus the layout images obtained were once in a lifetime and could not be replicated again on separate trial runs for Auto Place and Route. The floorplan area for these two auto placed and routed designs were approx 8mm by 8 mm.

This SEM micrograph was taken of a vanadium disulfide sample grown by atmospheric pressure chemical vapor deposition onto a silicon dioxide substrate. It shows the defect-nucleated dendritic growth of two-dimensional material on a three-dimensional substrate. Scale bar is 250 nm.
The two images presented pertain to my current research interests of developing suitable Auto Place and Route techniques of an ARM architecture using RSFQ (Rapid Single Flux Quantum) Logic cells. The images describe the result of two separate trial runs of Auto Place and Route of a SCRAM2 computer using the Auto Place and Route Tool Innovus, where the device layout is composed of self built RSFQ Logic cells. For the Auto Place and Route simulation runs, the only user input was the structural verilog file (the netlist that describes how the logic cells are connected in a schematic) and the Library Exchange Format LEF file (the geometrical definition of the modular RSFQ cells that are to be used in the layout of the SCRAM2). The output of these two trial runs generate the following layouts on the floor plan that resemble character profiles. It is to be noted that the particular routing scheme used by Innovus to create these expressions of abstract art are based on semi random algorithms. Thus the layout images obtained were once in a lifetime and could not be replicated again on separate trial runs for Auto Place and Route. The floor plan area for these two auto placed and routed designs were approximately 8mm by 8 mm.

This AFM 3D image shows the phase separation in symmetric blends of PMMS (120k)/PS (88k) film. The ability to organize multicomponent polymer mixtures into mono-type microdomain structures plays an important role across a range of polymer nanocomposite material technologies. This topography inspired from Super Mario games will make your day while exploring in the science valley.
SEM-secondary electron image showing the 'cluster of LiV$_3$O$_8$ crystals' on a carbon tape which are synthesized by sol-gel process and sintered at 400°C (6hrs) in air for crystallization. LiV$_3$O$_8$ is a high specific capacity cathode material for Li-ion batteries.
SEM- secondary electron image showing a nanofabricated region in Si wafer using FIB milling, which is carried out to remove the insulative silicon nitride layer and make an electrical contact to the thin film battery on the other side.

SEM-secondary electron image showing the FIB sputtered regions with increasing ion doses (bottom to top) to approach different layers of the 50nm Si-N+200nm Ni+100nm Li-V-O+100nm LiPON (top to bottom). This nanofabrication experiment is carried out to calculate the dose required to remove Si-N and Ni to make an electron transparent Li-V-O + LiPON window for in-situ TEM crystallization studies.
Dustin Andersen
9:15 – 9:30
Distributions of Kinetic Pathways in Strain Relaxation of Heteroepitaxial Thin Films
Dustin Andersen¹ and Robert Hull²
¹ Center for Materials, Devices, and Integrated Systems; Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180
contact: anderd8@rpi.edu
² Center for Biotechnology and Interdisciplinary Studies
³ Center for Materials, Devices, and Integrated Systems, Rensselaer Polytechnic Institute, Troy, 12180
contact: andern3@rpi.edu

The deleterious nature of dislocations in heteroepitaxial semiconductor structures poses a unique challenge in process design and device manufacturing. In particular, variations in heterolayer composition, thickness, growth temperature, and growth rate can lead to drastically different outcomes in the final dislocation array. It is critical to understand and predict the impact of these variations on the kinetics of dislocation array evolution.

While techniques like discrete dislocation dynamics (DDD) yield insights into the microscopic forces upon dislocations and their interactions, continuum level simulations can yield insight into the evolution of the dislocation array as a whole over a broad range of growth parameters. When refined using experimental data, the continuum model can be used to provide predictive descriptions of layer relaxation. By further generating many individual simulation results for variations over multiple parameters, relaxation surfaces can be generated that highlight how the growth parameters interact with one another. Such relaxation surfaces can also illustrate what combinations of growth parameters lead to the highest sensitivity in the outcome of the dislocation array.

Additionally, the output of the dislocation simulator may be extracted to create a pseudo-randomly generated representation or “fingerprint” of the dislocation array as individual dislocations. While this does not have the microscopic predictive power of more local techniques (e.g., DDD), it can provide a useful visualization of how the path that an evolving dislocation array takes will affect its final state. For example, differences in dislocation nucleation may lead to very different dislocation arrays that have similar ensemble values. Furthermore, this representation has led to new insights into the stochastic nature of the dislocation array and the distributions of dislocation lengths and spacings.

The overarching goal is to establish a robust framework for predicting, interrogating, and optimizing strain relaxation pathways and underlying mechanisms, for misfit dislocations in strained heteroepitaxial films.

Acknowledgements: I would like to acknowledge the support of this work by the National Science Foundation under Grant Nos. DMR-9531696 (construction of original simulator) and DMR-1309535 (further simulator development and parametric, sensitivity, and fingerprinting analysis). Stochasticity work was supported by the NYSTAR Focus Center at RPI: C130117.

Nathaniel Anderson
9:30 – 9:45
Synthesis and Characterization of Porphyrin-DNA Constructs for the Self-Assembly of Modular Energy Transfer Arrays
Nathaniel Anderson¹,²,³, Xing Wang¹,²,³, Peter Dinolfo¹
¹ Department of Chemistry and Chemical Biology, Rensselaer Polytechnic Institute, Troy, 12180
² Center for Biotechnology and Interdisciplinary Studies, Rensselaer Polytechnic Institute, Troy, 12180
³ Center for Materials, Devices, and Integrated Systems, Rensselaer Polytechnic Institute, Troy, 12180
contact: andern3@rpi.edu

5’ azide-terminated single-stranded DNA (ssDNA) was covalently attached to a Zn-tetra(phenylethynyl)porphyrin (ZnTPEP) utilizing copper(I) catalyzed azide-alkyne cycloaddition (CuAAC) to form five DNA-porphyrin adducts containing one to four ssDNAs attached and rotated around a porphyrin core with 90° intervals. A central porphyrin molecule provides a convenient morphology for constructing a multivalent EnT system with the porphyrin acting as both a covalent attachment point as well as an energy acceptor known to allow for relatively simple tuning of the photophysical and redox properties. Furthermore, DNA-directed assembly has proven to be a viable method for the controlled spatial arrangements of external ligands with nanometer precision. Therefore, these newly synthesized DNA-porphyrin modular adducts allow us to assemble a new platform to build donor-acceptor energy transfer (EnT) arrays/constructs using complementary dye-labeled ssDNAs with different donor:acceptor ratios. The photophysical properties of the DNA-porphyrin constructs, along with the individual donor and acceptor fluorophores, were investigated by electronic absorption and steady-state emission spectroscopy. The data shows that A546 (donor) emission spectrum is significantly quenched in each of the constructs with EnT efficiencies increasing nearly linearly with the number of available donors. Comparing the spectroscopic data of the chromophore pairs to the predicted EnT determined through modeling the Förster resonance energy transfer (FRET) mechanism shows that increasing the donor:acceptor ratio increases the overall end-to-end EnT of the system and demonstrates the value of this modular construct.
Physical System modeling and simulation using HPC
Sagar Bhatt, Antoinette Maniatty
Department of Mechanical, Aerospace and Nuclear Engineering, Rensselaer Polytechnic Institute, Troy, 12180,
contact: bhatts8@rpi.edu

Computational Sciences has been at the forefront of Continuum Mechanics research for a long time. With
the advent of cheaper and faster compute capability, it is not only possible to study aspects of a physical
system where an experimental study might prove difficult, but also to numerically analyze problems with
very high granularity. We used High Performance Computing (HPC) techniques like MPI and OpenMP
to develop a Conjugate Gradient method based solver to solve systems of linear equations, which was used
to solve Laplace Equation in a 1000x1000 grid (996004 unknowns) within 10⁻⁶ units of the analytical
solution. A similar solver based on stabilized bi-conjugate gradient method was used to solve pressure
Poisson equation in a level-set based immersed boundary method code to investigate how pitching and
heaving affect the propulsion of a self-propelled oscillating airfoil. This study was used to shed some light
on the hydrodynamics and flow structures during the transient state of fish like locomotion (the first few
cycles during start of the motion). This task would have been especially difficult to simulate using an
experimental setup.

At the Computational Solid Mechanics Laboratory at RPI, we plan to model the material microstructure
evolution using codes that use HPC to do Monte Carlo simulations and Finite Element Method on
massively parallel systems. Simulations of microstructure evolutions under thermal and structural loading
will help us develop the exact methodology behind the control of these microstructure evolutions, and
regulate the material properties.

H, d, and He Diffusion in Diamond - Experimental and Computational Studies
D.J.Cherniak¹, V. Meunier², E.B.Watson¹
¹ Department of Earth & Environmental Sciences, Rensselaer Polytechnic Institute, Troy, NY, 12180-3590
² Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, NY, 12180-3590
contact: chernd@rpi.edu

Diamond grains can offer insight into conditions of the early history of Earth’s mantle, with trapped noble
gases in diamond having the potential to provide information about the early mantle’s isotopic
composition. The rate of He diffusion in diamond is key in assessing whether He isotopic ratios in
diamond are representative of early mantle conditions.

Natural diamond may also contain inclusions of hydrous minerals and H-bearing fluids; measurements of
hydrogen diffusion in diamond can establish constraints on conditions of diamond formation and
compositions of mantle fluids. Understanding hydrogen diffusion in diamond is also important in
technological applications, since chemical vapor deposition (CVD) is a primary technique to produce
diamond layers. As the carrier gas in these growth processes, hydrogen is incorporated into CVD-grown
diamond, and may affect electronic properties.

In this work, we have characterized diffusivities of helium, deuterium and hydrogen through both
experimental and computational studies. For experiments, polished slabs of diamond were implanted with
³He, d, or H, sealed in silica glass capsules and annealed in 1-atm furnaces. ³He, d and H distributions
were measured with Nuclear Reaction Analysis. We obtain the following Arrhenius relations:

\[
D_{\text{He}} = 4.00 \times 10^{-15} \exp(-138 \pm 14 \text{ kJ mol}^{-1}/\text{RT}) \text{ m}^2\text{sec}^{-1}.
\]

\[
D_{\text{d}} = 1.02 \times 10^{-4} \exp(-262 \pm 17 \text{ kJ mol}^{-1}/\text{RT}) \text{ m}^2\text{sec}^{-1}.
\]

\[
D_{\text{H}} = 2.60 \times 10^{-4} \exp(-267 \pm 15 \text{ kJ mol}^{-1}/\text{RT}) \text{ m}^2\text{sec}^{-1}.
\]

Diffusivities of H and d agree within experimental uncertainties, indicating little diffusive mass fractionation
of hydrogen isotopes. This finding is supported by quantum mechanical calculations based on density
functional theory, which shed light on the atomistic description of H and d diffusion.

These hydrogen diffusion parameters would result in a diffusion distance of 50 μm in 300,000 years at
500°C, and less than two weeks at 1000°C. H is considerably more mobile than He. For example, at
1000°C over 1000 years, diffusion distances for H and He would be ~1cm and ~20μm, respectively.
Unfortunately, this means that natural diamonds have not retained a memory of early-Earth conditions.
Residual-Layer-Free Transfer Molding of Mesoscale Periodic Structures

Michael Deagen\textsuperscript{1,2}, Linda Schadler\textsuperscript{1,2}, Chaitanya Ullal\textsuperscript{1,2}

1 Department of Materials Science & Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180,
2 Center for Lighting Enabled Systems & Applications, Rensselaer Polytechnic Institute, Troy, NY 12180
contact: deagenm@rpi.edu

Low-cost, large-area fabrication of submicron periodic structures is demonstrated through transfer molding, a layer-by-layer stamping technique predicated on the ability to fill the recesses of a mold (stamp) without a residual layer. Residual-layer-free filling of 1-D periodic stamps was achieved through a blade meniscus coating process, where the meniscus contact line remained below a critical velocity to avoid forming a residual film. The critical velocity of the coating meniscus was measured for different ink viscosities, stamp materials, and stamp feature periods. The framework of discontinuous dewetting for 2-D patterns is compared to 1-D patterns, whose anisotropy suggests a new picture for discontinuous dewetting when applied to 1-D patterns. A proposed map of wetting regimes for residual-layer-free transfer molding, combining macro- and micro-scale wetting considerations, provides a guide for achieving residual-layer-free filling at maximum throughput. Residual-layer-free transfer of isolated PDMS patterns is compared to 1-D patterns. When applied to 1-D patterns, whose anisotropy suggests a new picture for discontinuous dewetting, the proposed map of wetting regimes for residual-layer-free transfer molding, combining macro- and micro-scale wetting considerations, provides a guide for achieving residual-layer-free filling at maximum throughput.

Acknowledgements: This material is based upon work supported by the National Science Foundation under cooperative agreement EEC-0812056, the Graduate Research Fellowship Program under Grant No. DGE-12547271, and by New York State under NYSTAR contract C090145. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation. The authors would also like to thank Profs. Chulsung Bae, Chang Ryu, and Aram Chung for the use of equipment within their labs, Robert Zacharias for building the blade coating apparatus, and M. David Frey for assistance with SEM imaging.

Comprehending the Substrate-Independent Vertical Growth of ReS\textsubscript{2} Nanosheets

Debjit Ghoshal\textsuperscript{1}, Anthony Yoshimura\textsuperscript{2}, Yanwen Chen\textsuperscript{1}, Tianmeng Wang\textsuperscript{2}, Tushar Gupta\textsuperscript{3}, Swastik Basu\textsuperscript{3}, Vincent Meunier\textsuperscript{1}, Suifei Shi\textsuperscript{1,2}, Nikhil Koratkar\textsuperscript{1,3,4}

1 Department of Chemical and Biological Engineering, Rensselaer Polytechnic Institute, Troy, 12180.
2 Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, 12180.
3 Department of Mechanical, Aerospace and Nuclear Engineering, Rensselaer Polytechnic Institute, Troy, 12180.
4 Department of Material Science and Engineering, Rensselaer Polytechnic Institute, Troy, NY, 12180.
5 Department of Electrical, Computer, and Systems Engineering, Rensselaer Polytechnic Institute, Troy, NY, 12180.
contact: ghoshd2@rpi.edu

Rhenium Disulphide (ReS\textsubscript{2}) differs fundamentally from other group-VI transition metal dichalcogenides (TMDs) due to its low structural symmetry, which results in its optical and electrical anisotropy. While the optoelectronic properties of ReS\textsubscript{2} have been the subject of extensive study, little attention has been placed on the vertical and anisotropic growth of ReS\textsubscript{2} during chemical vapor deposition. Although vertical growth has been observed in some TMDs under special conditions, vertical growth in ReS\textsubscript{2} is very different in that it is highly spontaneous and substrate-independent. In this study, we discovered that the governing mechanism for ReS\textsubscript{2} growth involves two distinct stages. In the first stage, ReS\textsubscript{2} grows parallel to the growth substrate, consistent with conventional TMD growth. However, subsequently vertical growth is nucleated at points on the lattice where Re atoms are “pinched” together. At such sites, an additional Re atom binds with the two pinched Re atoms, leaving an under-coordinated S atom protruding out of the ReS\textsubscript{2} plane. This under-coordinated S is “reactive” and binds to free Re and S atoms, initiating growth in a direction perpendicular to the ReS\textsubscript{2} surface. We demonstrate the utility of such vertical ReS\textsubscript{2} arrays in applications where high surface-to-volume ratio and electric-field enhancement are essential, such as surface enhanced Raman spectroscopy, field-emission and solar-based bacterial disinfection.
Phosphorus Nanoparticles Embedded in a Reduced Graphene Oxide Matrix for High-Performance Lithium-Ion Battery Anodes

Tushar Gupta
Department of Mechanical, Aerospace, and Nuclear Engineering, Rensselaer Polytechnic Institute, Troy, 12180
contact: guptat@rpi.edu

Red phosphorus (P) shows huge potential as a high-performance and cost-effective anode material in Lithium (Li)-ion batteries. This is because it alloys with Li forming Li3P, which translates to a theoretical capacity of ~2595 mAh/g (~7 times better than conventional graphite). Further, the cost of bulk P is ~$25/kg which is comparable to battery-grade graphite. However, there are two basic problems that prevent successful deployment of P in Li-ion battery anodes, viz. its low electrical conductivity and its high volume change on cycling that leads to pulverization and loss of electrical contact. To address these problems, electro-spraying and far-infrared reduction were used to fabricate composites of P and reduced graphene oxide (rGO). The electro-spraying process enables ultra-small P particle size (5-10 nm), which suppresses stress-induced pulverization and drastically reduces Li-ion diffusion distances. The low electrical conductivity of P is also not a limitation at such small particle sizes. The far-infrared reduction establishes carbon-phosphorous bonds enabling efficient electron transfer between the rGO matrix and the P nanoparticles. The C-P bonding also prevents surface migration and agglomeration of P. The P/rGO anode delivers outstanding performance for all major metrics including specific capacity (~1763 mAh/g at current density of ~0.1 A/g), extraordinary high-rate capability (up to ~40 A/g) and long cycle-life (> 1000 cycles with ~99% coulombic efficiency).

Impurity Control for High Performance Gallium Nitride Device

Jennifer (John) Howell-Clark
Department of Mechanical, Aerospace, and Nuclear Engineering, Rensselaer Polytechnic Institute, Troy, 12180
contact: howelj2@rpi.edu

Gallium Nitride (GaN) is an attractive choice for high-voltage power devices due to its high breakdown field (> 3 MV/cm). This property, stemming from its wide band gap of 3.4 eV, allows for large voltages to be supported on thinner, more heavily doped layers than would be possible for more conventional materials like silicon, which have smaller critical fields. As a result, the specific on-state resistances (R_on,sp) of GaN devices can be much smaller than equivalent silicon devices. Smaller R_on,sp increases the efficiency of power electronic applications, and can also reduce the necessary die size, enabling more compact power systems. However, the material properties of GaN present several practical challenges which are not encountered in silicon. Many of these challenges center on doping and impurities. Magnesium is the only impurity that has been shown to reliably result in p-type conductivity in GaN, but Mg performs poorly in comparison to p-type doping in silicon. Our approach to these issues is twofold. First, by using first-principles understanding and material characterization, we can improve the performance of Mg-doped GaN layers, and predict the quality of samples prior to fabrication. We have recently demonstrated that the performance of GaN p-i-n rectifiers is substantially improved when a uniformly doped p-layer is replaced with a layer of nonuniform doping. This improvement is obtained even when the surface Mg concentration is 2 x 10^{20} cm^{-3}, much higher than what is typically understood to be the self-compensation limit of Mg-doped GaN. We also develop alternative doping – with carbon - to replace Mg in device structures where p-type conduction is not necessary. The acceptor level of carbon in GaN is too deep to create p-type conductivity, but can still be used to block high voltages in a unipolar device.

Acknowledgements: The authors wish to acknowledge the support of the Rensselaer Presidential Graduate Fellowship, which currently funds the first author of this work. We also wish to acknowledge use of the MNCR, which was used for device fabrication.
Poly(N-isopropylacrylamide) microgels (PNiPAm µgels) have drawn substantial scientific interest mainly due to the combination of their unique thermal behavior in aqueous media and their colloidal nature. The structure and morphology of this materials class has been primarily elucidated via scattering. Despite their unequivocal strength and applicability, scattering techniques predicate the use of models for the interpretation of reciprocal space data or involve the use of intricate numerical inverse transforms in order to decipher real space information. On the other hand, the advent of super-resolution nanoscopy allowed the investigation of soft matter in the native state with nanoscale precision and directly into real space. Our present work focuses on resolving crosslinking density variations in PNiPAm µgels with different degrees of structural heterogeneity utilizing state-of-the-art 4pi-SMS and STED super-resolution nanoscopy. To this end, we have synthesized a novel functional methacrylamide crosslinker monomer with pendant free amine groups, as a versatile molecular platform for the anchoring of photostable chromophores. Dye-functionalized crosslinker monomers were employed in the preparation of PNiPAm µgels with i) batch free-radical precipitation polymerization, which lead to the formation of heterogeneously crosslinked particles and ii) an analogous monomer starve-feed method, which lead to particles with homogeneous crosslinking density. We report on the direct 3D reconstruction of crosslinking density variations with 4pi-SMS. Extraction of equivalent information was achieved by image analysis of 2D projections acquired with STED. Additionally, insight on the mechanical properties of µgels was provided by characterization with SEM and AFM, while their thermal response was monitored with DLS. Our results reveal distinctive structural and morphological features between homogeneous and heterogeneous particles. Surprisingly, the derived radial crosslinking density distributions via 4pi-SMS deviate from the traditional “fuzzy-sphere” model, which is established through scattering experiments. We tentatively ascribe the observed discrepancy to the absence of the “free-radical self-crosslinking” mechanism in our system.

Acknowledgements: AAK would like to thank Dr. Deniz Rende and Dr. Sungmin Park for assistance in the operation of the cMDIS core facility FEI Versa Electron Microscope. AAK would like to thank Prof. Ravishankar Sundaranan for helpful discussions on numerical inverse transforms.

Development of Chemically Immobilized Sulfur Cathodes for Lithium Sulfur Batteries
Lu Li1, Jian Gao2, Feng Li2, Wencai Ren2, Chandra Veer Singh2, Hui-Ming Cheng2, Nikhil Koratkar2
1 Rensselaer Polytechnic Institute, Troy, NY, United States. 2 Institute of Metal Research, CAS, Shenyang, China. 3 University of Toronto, Toronto, ON, Canada.

Lithium sulfur (Li-S) batteries, with specific energy several times higher than that of state-of-the-art Li-ion batteries, have generated great interest as next-generation energy storage systems for portable electronics as well as automotive applications. However, the insulating nature of sulfur/Li2S and the dissolution of lithium polysulfides (LiPSs) in the electrolyte with subsequent parasitic reactions lead to low sulfur utilization and poor cycle life. The integration of nanostructured carbon materials with sulfur is one of the primary strategies for improving the electrical conductivity of the composites and for suppression of the LiPSs shuttle effect through physical confinement. However the weak interaction between non-polar carbon-based materials and polar LiPSs/Li2S species leads to poor confinement and easy detachment of LiPSs from the carbon surface. The resulting diffusion of LiPSs into the electrolyte is responsible for rapid capacity decay and poor rate performance. Here we rationally design and develop chemical immobilizers as sulfur hosts towards building high-performance Li-S batteries. Nitrogen-doped graphene, poly ReS2 nanosheets grown perpendicular to a carbon substrate and few-layer phosphorene nanosheets deposited on a carbon scaffold are employed as highly efficient polysulfide immobilizers and catalysts to significantly accelerate the redox reaction of sulfur species and to greatly improve the cycle life of Li-S batteries. A fundamental understanding of the binding of LiPSs to chemical adsorbents and the relevant reaction mechanisms in Li-S batteries, can pave the way towards the realization of sustainable and high-performance energy storage technologies.
Two dimensional (2D) materials such as transition metal dichalcogenides (TMDs) have attracted great attention due to the various interesting properties associated with reduced dimensionality. As predicted by theoretical calculations and confirmed by experimental measurements, when the synthesized or exfoliated film thickness approaches the monolayer limit, new material properties emerge that differ from those of the bulk material. Furthermore, growth of a film on a 2D material, known as van der Waals epitaxy (vdWE), creates a film/substrate interface devoid of chemical bonds. This relaxes the constraint of lattice matching as is required for traditional heteroepitaxy and aids in the growth of a strain-free film despite severe mismatches with the substrate’s atomic spacing and symmetry.

I will discuss the atmospheric pressure chemical vapor deposition synthesis of 2D TMD vanadium disulfide (VS\textsubscript{2}) on the van der Waals mica(001) surface. By tuning several key growth parameters, VS\textsubscript{2} flakes with diameters over 100 \textmu m and thicknesses below 10 nm have been achieved, making them attractive for electronic and optoelectronic applications. X-ray diffraction and high-resolution transmission electron microscopy confirm the flakes’ monocrystalline quality. Remarkably, a superlattice area mismatch model [A. S. Yapsir et al. J. Appl. Phys. 67, 796, 1990] is able to predict the preferred epitaxial alignment exhibited by the VS\textsubscript{2}/mica samples and is consistent with TEM, EBSD, and optical images. This demonstrates that despite the weak interface established via vdWE, the substrate’s atomic periodicity influences the arrangement of the atoms in the epitaxial layer as in conventional heteroepitaxy.

Acknowledgements: This work is supported by the NYSTAR Focus Center at RPI, C130117, and makes extensive use of cleanroom and characterization facilities in the Center for Materials, Devices and Integrated Systems (cMDIS) at RPI.
Though pitting corrosion is common on passivating metals such as aluminum and stainless steel, the mechanism of pit initiation is still not well understood. We image such nucleation events in a Liquid Cell in the Transmission Electron Microscopy (TEM). However, Liquid Cell TEM introduces an additional variable in the corrosion cell environment; energetic primary electrons which generate radiolytic products in the liquid through generation of secondary electrons, which can thereby influence the microstructural evolution of the passivating film.

In this study, we observe that the polycrystalline aluminum film locally corrodes in the area irradiated by the electron beam, depending upon the irradiating electron current density. Different potential radiolysis mechanisms are investigated: radiolysis of the liquid leading to pH change, interaction of the secondary electrons at the liquid-passive film interface, and break-down of bonds in the passive oxy-hydroxide.

We observe that aluminum samples do not undergo this preferential corrosion in the absence of the chloride-containing electrolyte, however, the beam-irradiated area will preferentially corrode even if the electrolyte is introduced after the irradiation has ceased. We have also observed samples with a thicker alumina film that the amorphous alumina film would crystalize for sufficient dose of electrons; it is expected that this crystallization accompanies voiding of the film. Finally, a square trench was milled out of the deposited aluminum by focused ion beam we observed that the edge of the square, covered in passive oxide, was not attacked randomly but along the whole perimeter upon irradiation. These experiments suggest that the electron beam interacts primarily with the oxide film, where structural changes may permit intrusion of the aggressive chloride, leading to corrosion.

In summary, this work seeks to explain an observed pitting initiation mechanism developed under electron irradiation, and thereby allow enhanced understanding of localized corrosion mechanisms.

Acknowledgements: The authors would like to acknowledge NSF for funding this research (DMR-1309509) and use of the Micro and Nanoscale Fabrication Clean Room and the Nanoscale Characterization Core within the Center for Materials, Devices, and Integrated Systems at RPI. In particular we thank Ray Dove, and Deniz Rende for technical assistance on the instruments used in this study, and Brent Engler for assistance with sample preparation.

Electrode microstructure plays a vital role in the electrochemical performance of Li ion batteries. Understanding the crystallization process during annealing of electrode thin films can provide potential new avenues to control of electrode microstructure in thin film battery systems. Thermal annealing experiments both in the vacuum of a transmission electron microscope (TEM) and in an Ar environment are performed to understand the crystallization of amorphous Li-V-O thin films (50-100 nm) sputter deposited from a LiV2O8 target. It is observed that the annealing atmosphere (vacuum vs Ar) has a profound effect on the Li-V-O phase crystallized. Depending on annealing atmosphere and temperature, either completely delithiated phases (V2O5, V2O3 and VO2) or partially delithiated uncatalogued Li-V-O phases are generated, but not the desired LiV2O8 stoichiometry. This is due to low Li concentration in the as-deposited thin films determined by nuclear reaction analysis (NRA). Approaches to contain the Li during annealing of the 50-100 nm films, using nickel diffusion barrier coatings and/or Li-rich coatings (LIPON) are unsuccessful in maintaining the desired LiV2O8 stoichiometry. We overcome the challenge of maintaining the Li stoichiometry by using thicker films (~1 μm), where the Li concentration at the middle of these films is close to LiV2O8 phase and formed LiV2O8 electron transparent films (~100nm) by controlled FIB nanofabrication.

In this work, combined nano- and micro-scale diffraction, spectroscopic and imaging analysis provide the necessary understanding regarding the Li concentration depth profile and phase distributions in such films, for future development of thin film battery systems.

Acknowledgements: This work is supported as part of the Center for Mesoscale Transport Properties, an Energy Frontier Research Center supported by the U.S. Dept. of Energy, Office of Science, Basic Energy Sciences (award #DE-SC0012673). Work at RPI made extensive use of the cleanroom and characterization facilities in the Center for Materials, Devices and Integrated Systems (cMDIS).

http://cmdis.rpi.edu
New Optimization Scheme for Potential Development for Multi-component Oxide Glasses

Siddharth Sundararaman\textsuperscript{1,2}, Simona Ispas\textsuperscript{2}, Walter Kob\textsuperscript{2} and Liping Huang\textsuperscript{1}

1 Rensselaer Polytechnic Institute, USA
2 Universite Montpellier, France

A dearth of satisfactory interaction potentials for multi-component oxide glasses that can reasonably describe a variety of properties is a major stumbling block facing the glass community. In this work, a new optimization scheme was developed to parameterize effective pairwise potentials for molecular dynamic (MD) simulations of multi-component oxide glasses. Our approach was to fit to results from accurate first principles calculations and explicitly incorporate the radial distribution function (RDF) of the equilibrium liquid at multiple temperatures, the vibration density of states (VDOS) and the density of glass at different pressures into the cost function of the fitting scheme. This new optimization scheme has successfully improved potentials for silica glass and alkali silicate glasses, which can not only predict the elastic moduli at ambient conditions, but also their response to external stimuli like high pressure and temperature. This new optimization scheme is being extended to multi-component oxide glasses.

Forward and Inverse Simulations of Heat Transfer and Grain Growth in Thin Films

Yixuan Tan\textsuperscript{1}, Arun Baskaran\textsuperscript{2}, Genevieve Kane\textsuperscript{2}, Chengjian Zheng\textsuperscript{2}
Daniel Lewis\textsuperscript{2}, Antoinette Maniatty\textsuperscript{1}, John Wen\textsuperscript{1,3} and Robert Hull\textsuperscript{1,2}

1 Department of Mechanical, Aerospace, and Nuclear Engineering, Rensselaer Polytechnic Institute
2 Department of Materials Science and Engineering, Rensselaer Polytechnic Institute
3 Department of Industrial and Systems Engineering, Rensselaer Polytechnic Institute
contact: tany3@rpi.edu

In this work we solve the inverse problem for current input to generate desired grain size distribution in a copper thin film during thermal processing using a micro-heater array. The entire problem is solved based on successful development of two simulation modules: inverse finite element heat transfer simulation and inverse Monte Carlo grain growth simulation.

In the first simulation module, a finite element model of the micro-heater system is used to define a discrete set of non-linear equations used as a basis for the inverse problem solution. A direct minimization method with Tikhonov regularization is used to iteratively find the local optimal solution. A uniform and a linear temperature distribution could be attained in the central region above the micro-heater array. The regularization method allows for a smoother solution compared with solution without regularization.

In the second simulation module, we develop a Monte Carlo (MC) algorithm to model material microstructure evolution in the presence of a non-uniform temperature field that may vary with time and space. We propose a novel parallel MC algorithm for accurately scaling to physical time and space. We first scale the MC model to physical observation by fitting experimental data. Based on the scaling relationship, we derive a grid site selection probability (SSP) function to consider the effect of a spatially varying temperature field. The SSP function is based on the differential MC step, which allows it to naturally consider time varying temperature fields too. We verify the model and compare the predictions to other existing formulations in two-dimensional cases.

A complete inverse problem is formulated by coupling the inverse finite element heat transfer simulation module with an inverse MC grain growth simulation module. Given the target grain size distribution in the film, the historical current in the heater lines of the micro-heater array is solved by driving the two modules. Specifically, the grain size distribution is measured in the MC simulation and used as the feedback for updating current input in the heater lines.
Magnetic Active Tactile Displays for Virtual Reality Applications

Melih Turkseven¹, Charlotte Teunisse¹, Deniz Rende²,³, Suvranu De¹

¹ Mechanical, Aerospace, and Nuclear Engineering, Rensselaer Polytechnic Institute, Troy, 12180
² Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, 12180
³ Center for Materials, Devices and Integrated Systems, Rensselaer Polytechnic Institute, Troy, NY 12180

When excited by an external magnetic field, magnetically active materials present rapid changes in their mechanical properties. This research aims to utilize this phenomenon to modify the hardness of a magnetically active surface for displaying tactile cues to human fingertips upon contact. The purpose of this work is to present the fabrication process of magnetorheological (MR) elastomers as active surfaces and recent progress on investigating their suitability for high-resolution tactile displays. Samples of MR surface are fabricated by infusing carbonyl iron particles into a PDMS elastomer matrix in varying ratios. In order to achieve a soft elastomer matrix, a polymerization process outlined in the literature is performed for each sample. An array of miniature solenoids was prototyped to investigate the behavior of the prepared samples under the limited magnetic field created by the solenoids. Through our investigation, we expect to obtain a thin layer of active surface capable of displaying hard shapes when palpated by fingertip. Rendering millimeter-scale tactile cues to fingertips is an ongoing challenge with a huge potential impact on virtual reality oriented applications.

Spirothiopyran based photoresists for large area sub-diffraction nanopatterning

Hari Vijayamohan¹, Edmund Palermo¹, Chaitanya Ullal¹

¹ Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180

Optical interference lithography is an attractive technique to cheaply and rapidly pattern three dimensional features in polymer photoresists. However, both resolution and feature size obtained are limited by the diffraction limit. In the past few years, Stimulated Emission Depletion Microscopy (STED) inspired lithography schemes using reversibly saturable switching systems have shown the ability to direct-write features well below the diffraction limit using light. However, the high laser intensity required for saturation limits their use to point by point writing. The Menon group has pioneered the use of photochromic molecules for sub-diffraction patterning, utilizing the difference in solubility and transmission between two diarylethene photo-isomers. However, the high extinction coefficients of these molecules restrict these patterning strategies to 2D.

Here, we propose combining the reversibly saturable photoisomerization of Spirothiopyran with the Michael addition ‘click’ chemistry to formulate a low intensity threshold photoresist suitable for sub-diffraction resolutions over large areas. Proton NMR studies confirm an exponential decrease in the ‘writing’ reaction yield with low depletion intensity required for saturation. Photokinetic simulations demonstrate the potential to fabricate patterns with feature sizes less than 50 nm over range spanning hundreds of microns using a simple 2W 532 nm laser. Furthermore, spatial control of crosslinking is demonstrated using a Spirothiopyran-PEG Methacrylate copolymer. Absorption within the photoresist can be mitigated by controlling the concentration of the photoswitch covalently attached to the polymer comprising the photoresist. These experiments demonstrate the viability of a Spirothiopyran based photoresist to become a prime candidate for large area 3D direct writing with sub-diffraction resolutions.
**OP.19** | Yiping Wang  
4:05 – 4:20  
*Toward-Wafer Scale Ionic Epitaxy of Halide Perovskite Single Crystalline Thin Film Carrying Hidden Carrier Dynamics*

Yiping Wang1, Xin Sun2, Zhizhong Chen1, Toh-Ming Lu2, Jian Shi1  
1 Department of Material Science & Engineering, Rensselaer Polytechnic Institute, Troy, 12180  
2 Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, 12180  
contact: wangy33@rpi.edu

High-temperature vapor phase epitaxy (VPE) has been proved ubiquitously powerful in enabling high-performance electro-optic devices in III-V semiconductor research and industrial community. A typical example is the successful growth of p-type GaN by VPE for blue light emitting diodes. VPE excels as it well controls the film defects such as point defects, grain boundary and interphase defects, thanks to its high-temperature processing condition and controllable deposition rate.  

In this report, for the first time, we have demonstrated single crystalline high-temperature VPE halide perovskite thin film – a unique platform on unveiling previously uncovered hidden carrier dynamics in inorganic halide perovskite materials. Towards wafer scale epitaxial and grain boundary-free film is grown with alkaline halides as substrates. We show the metal alkali halides could be used as a universal substrate for the VPE growth of perovskite due to their similar material chemistry and close crystal symmetry and lattice constant. With VPE, hot photoluminescence and nanoseconds photo Dember effect were revealed in inorganic halide perovskite. These two phenomena suggest that inorganic halide perovskite could be as compelling as its organic-inorganic counterpart in terms of optoelectronic properties and help explain the long carrier lifetime in halide perovskite. Our findings suggest a new avenue on developing high quality large scale single crystalline halide perovskite films requiring precise control of defects and morphology.

**Acknowledgements:** The author acknowledges the support from CMDIS for morphology and characterizations by the Scanning Electron Microscope FEI VERSA.

---

**OP.20** | Shuman Yu  
4:20 – 4:35  
*Numerical Simulation of CO₂ Injection Induced CH₄ Production from Gas Hydrate-bearing Sediments*

Shuman Yu1 and Shun Uchida1  
1 Civil and Environmental Engineering Department, Rensselaer Polytechnic Institute, Troy, 12180,  
contact: yus5@rpi.edu

Gas hydrates are ice-like clathrates enclosing small guest molecules in solid lattices of water molecules. In nature, gas hydrates predominantly have methane (CH₄) as guest molecules and constitute a vast natural gas resource with worldwide quantity of 3000 to 30000 trillion cubic meters. CH₄ hydrates are stable under conditions of high pressures and low temperatures found in sediments below the seafloor and permafrost. To exploit this potential energy resource, CH₄ gas needs to be released from gas hydrate-bearing sediments in situ. Three common dissociation-based approaches of depressurization, thermal stimulation, and inhibitor injection have been examined in theoretical studies, experiments and field trials, where depressurization method has demonstrated better recovery efficiency over the other two methods. However, geomechanical instability problems such as sand production were observed in depressurization-induced production trials and reservoir cooling from the endothermic process of hydrate dissociation would impede gas production in the long-run.

A new recovery approach – carbon dioxide (CO₂) injection – provides an emission-neutral favored energy production strategy from CH₄ hydrate-bearing sediments. Difference of phase equilibrium between CH₄ hydrate and CO₂ hydrate provides the basis for recovery of CH₄ gas and sequestration of CO₂ gas into the sediments. This CO₂-CH₄ hydrate exchange has been confirmed by laboratory experiments and 2012 Ignik Sikumi field trial in Alaska North Slope, which enhances geomechanical stability of hydrate-bearing sediments compared with dissociation methods. However, low rate of CH₄ production still remain as problem before potential commercialization of CO₂ injection method, which urges the elucidation of complex mechanism in CO₂-CH₄ hydrate exchange process. It necessitates sound numerical simulation to advance the understanding of such complex behavior and investigate the optimal CO₂ injection conditions. Here a coupled thermo-hydro-chemo-mechanical (THCM) formulation is presented for analyzing CO₂-CH₄ hydrate exchange processes based on hydrate formation and dissociation equation for each hydrate.

**Acknowledgements:** This research is ongoing under the support of Uchida Research Group in Civil and Environmental Engineering Department at RPI.
Skin microvasculature not only promotes graft survival by supplying skin cells with oxygen and nutrients but is also known to modulate inflammation and immune cell migration to the wound site. Vascularization of skin grafts is crucial for successful skin engraftment. Here, using a 3D bioprinting platform, we show successful integration of a vascularized bed in a 3D printed human skin model. In addition, we show the influence of different human cell sources (fibroblasts, endothelial cells and pericytes) in controlling the formation of vasculature in vitro. 3D printed vascularized skin substitutes formulated with human endothelial progenitor cells (EPC) were implanted on the backs of immunodeficient mice, showing human vascular structures that were perfused. Such structures were absent in the samples lacking human EPC. These data illustrate the feasibility of studying 3D printed skin composed of human primary cells in immunodeficient mice, and also the ability of EPC to produce perfusable vasculature in the grafted 3D printed skin. Moreover, we hypothesize that the pre-vascularized skin construct will enable faster integration with the host skin, and accelerated recovery of blood perfusion to the wound site to promote healing and permanent graft integration. These advances will allow the fabrication of human skin tissues suitable for clinical translation.

Deviation from Randomness in Material Microstructures and Atomic Arrangements
Grace Rabinowitz¹, Arun Baskaran¹, Daniel J Lewis¹
1 Department of Material Science, Rensselaer Polytechnic Institute, Troy, 12180
contact: rabing@rpi.edu

A random microstructure is one in which the structural properties such as grain size are not a function of spatial coordinates. However, a microstructure graded in structure or composition can consequently provide a gradation in material properties. Surface Evolver was used to study the kinetics of different graded microstructures, differing in the extent of gradation. The study was conducted for different microstructures that begin evolving with an identical mean grain area but different statistical variance of grain sizes. The incorporation of variance mimics the generation of a hypothetical microstructure that could be generated by spatial thermal gradients. The simulations allowed to test a possible correlation between a microstructure's initial variance, a geometric property of the polycrystalline network, and its growth rate. It was observed that the microstructures evolved at different growth rates, and the microstructures with the largest and smallest variances evolved with highest and lowest growth rates. The analysis was performed in the normal grain growth regime. Research is also being conducted to theoretically study the atom packing in amorphous materials like glass. Random closed packed (RCP) model is the typical model used to characterize the packing fractions of solid objects in a random fashion. This model can be used to describe the structure of ionic and metallic glasses in addition to some liquids. A key property of a RCP lattice is the average number of neighbors, which has been found to be 13.397 in a perfect RCP structure. Currently, research is being undertaken to study how factors such as interatomic interactions and atomic size distribution can cause a deviation from the average by using a computational approach to test existing algorithms.

Acknowledgements: This material is based upon work supported by the National Science Foundation under Grant No. CMMI-1334283, and sponsored URP supported by Corning Inc.
Slip Avoidance in Dual-Arm Manipulation

David S. Carabis1, John T. Wen1,2
1 MANE, Rensselaer Polytechnic Institute, Troy, NY, 12182,
2 ISE, Rensselaer Polytechnic Institute, Troy, NY, 12182
contact: carabid2@rpi.edu

Maintaining force closure during motion and interaction with the environment is critical in multi-finger or multi-arm grasps with friction contacts. Violation of this condition leads to contact slippage and potential loss of grasp. This issue is particularly important in space robotics, where catastrophic consequences could result from the loss of grasp. There is ample literature on grasp stability and force closure under static conditions. Our work investigates multi-arm grasping during motion and while the grasped object interacts with the environment. Under these conditions, the inertial force from the load could or external forces due to contacts with the environment may adversely affect grasp stability. Our approach dynamically adjusts the applied squeeze force in both situations to maintain a safe force closure condition. For the object motion and environment interaction cases, we also dynamically adjust the object/robot motion and desired external contact force, respectively, if dynamic squeeze force adjustment does not maintain a safe force closure condition alone. The application scenario we investigate is based on transporting and berthing an object in a micro-gravity environment using a dual-arm manipulator. We use a planar air bearing table to approximate space dynamics on earth. Grasping, transporting, and berthing of an air bearing object is performed by a fixed-base dual-arm robot integrated with the air bearing table. Our experimental results show that the proposed methods are effective at avoiding contact slippage during object motion and when the object is in contact with the environment. Sample results for object transportation are shown for one end effector in the accompanying figure. These results show the reduction in the ratio of tangent to normal forces at the contact point when the slip avoidance compensation is turned on. If this force ratio exceeds the coefficient of friction, slip will occur.

Acknowledgements: The authors gratefully acknowledge the support of this project by NASA Goddard. The authors would also like to thank Brian Park, Glenn Saunders, and Kenneth Myer for their help in designing and constructing the test fixture, Daniel Kruse for his valuable input, and cMDIS for the use of their facilities.

Determining Spatially Resolved Temperature Gradients for In-Situ TEM Electromigration Experiments

Brent Engler1, Robert Hull1
1 Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, 12180
contact: engleb2@rpi.edu

Electromigration and its effects are widely studied due to their relevance to the semiconductor device industry. In-situ TEM allows investigation into failure mechanisms with high temporal and spatial resolution, as well as control over key parameters including temperature and current density. However, these experiments are complicated by the thermal gradients which result from Joule heating of the metal lines; high current densities in the test samples and ultra-low thermal conduction through the electron transparent silicon nitride support films contribute to relatively large increases in temperature. We have performed finite element modeling to calculate the resulting temperature distributions due to resistive heating of electromigration test structures so that observations can be accurately related to the local temperature. The very low thermal conductance of free standing electron transparent silicon nitride films results in temperature gradients which are highly dependent on the magnitude of thermal conductivity in the film. We have measured the thermal conductivity of these films in-situ by Joule heating an aluminum resistor/sensor strip in the center of the electron transparent window, which has been calibrated to relate resistance to temperature. A very high aspect ratio for the window, large heat sink, and small heating current allow for good approximation of 1D heat flow through the nitride to the surrounding silicon, and calculation of thermal conductivity.

With this approach, we have calculated a value of 2.02±0.17 Wm⁻¹K⁻¹ as the thermal conductivity of the film. Using Finite Element Modelling we have examined a range of potential electromigration structures for testing high resistivity films. Ti in this study, based upon the calculated thermal conductivity. The optimal structure tested shows a temperature increase of less than 10°C at a current density of 1x10⁶ Acm⁻² and an accessible range of up to 7x10⁶ Acm⁻². This work establishes a platform for truly quantitative in-situ electromigration analysis.

Acknowledgements: This work was supported by the NYSTAR Focus Center at RPI, C130117, and made extensive use of cleanroom and characterization facilities in the Center for Materials, Devices and Integrated Systems (cMDIS) at RPI.
In order to achieve nanoscale electronic devices beyond the 10 nm limit predicted by Moore’s Law, molecular electronic devices are being studied as alternatives to circuit elements such as diodes, switches, and transistors. Porphyrin molecules are of interest because they have been shown to exhibit switching and diode behavior. In addition, shorter porphyrins (3-5 nm) can be used as interconnects because their low attenuation constants $\beta < 0.1$ 1/A allow for long range electron conduction. Our work investigates three types of short porphyrins: a free base porphyrin (FBP), and porphyrins with either a zinc (Zn-P) or an iron (Fe-P) atom ligated to the porphyrin ring. Nanostructures are formed by depositing porphyrins into a 3-5 nm gap created by electromigration of a 30x50 nm gold nanowire to create a molecular junction (MJ). In order to determine the mechanism for electron conduction through these porphyrin MJs, temperature dependent current/voltage (I/V) studies have been performed and compared to existing models of electron transport, and are shown to be direct tunneling. Since the electron transport mechanism is direct tunneling, the calculation of the electron attenuation coefficient, $\beta$ is possible, even for samples only measured at 4.3 K. The average $\beta$ for FBP is 0.231 1/A, for Zn-P <0.188 1/A, and for Fe-P 0.177 1/A. Inelastic electron tunneling spectroscopy (IETS), which is the second derivative of I/V, is measured simultaneously at temperatures from 4.3 to 300 K. IETS is used to verify the presence of a molecule in the gap. Peaks in the spectra indicate the excitation of a vibrational mode, which are compared to Fourier transform infrared spectroscopy.
Reservoir computing is a promising computing architecture born out of artificial neural network theory. As opposed to the typical Turing-Von Neumann architecture, reservoir computing is better suited for computation of abstract tasks not easily solved by algorithmic instructions. Hardware implementation of the architecture using photonics is driven by the low power, high bandwidth characteristics offered by photonic platforms.

In the past, computations done using photonic reservoir computing have typically been done serially, with no ability of the system to compute two or more separate tasks at a single time. Parallel implementations have been explored, but have been physically limited to only supporting up to two cores. This presentation seeks to answer whether a photonic parallel computing system can be created that is highly scalable, supporting up to n cores. Such a system could be used to increase the bandwidth and decrease computation time for a single task, or it could be used to compute multiple tasks simultaneously.

A system demonstrating such scalability is shown using simulation. The key device not used in previous reservoir computing schemes is the arrayed waveguide grating which implements frequency division multiplexing of the carrier signals to create the separate cores. Simulations show a negligible decreased performance when using the parallel architecture to compute both single tasks at an increased bandwidth and multiple tasks simultaneously. Lastly, this presentation will discuss current attempts at experimental verification of the system described above.

In this presentation, we demonstrate the viability of our team’s approach to forensic data curation with examples of visualizations and machine learning analyses performed on two manufacturing archives. Currently, large archives of manufacturing-process data are collected during government research programs and stored in in government repositories. Such archives could provide valuable insights and even directions for future productive research thrusts, if only the technical content could be consumed and processed in an automated manner. The challenge to automated processing and thus to re-use of the archival information is primarily two-fold: understanding (and storing) the unknown structure of the manufacturing archives due to the large variety of file structures potentially possible and lack of informative metadata; and establishing the meaning and significance of both the archival structure and file content in the face of incomplete or absent documentation of both the file structure and technical content. As a solution to this challenge, our team has: developed and applied examples of manufacturing/processing ontologies to two manufacturing archives (DMO, AMPO); developed a browser interface (Magellan); and performed visualizations and analyses enabled by the ontological curation, leading to new insights and models of the data. Machine learning analyses and visualizations were performed on subsets of two archives – one archive concerned composites toughness processing and testing, the second archive concerned additive manufacturing of a high temperature alloy by a wire deposition process.

Selected examples are shown for the analyses and visualizations we developed for the two available archives, leading to new insights and models of the data. The processing and testing information of the composites archive was ideal for machine learning, so we developed a classification model for predicting the parameters (composition, surface preparation, etc.) advisable to produce a composite having toughness above a desired threshold of 6in-lb; as well we developed a step-wise linear regression algorithm to predict the composite toughness as a function of the processing parameters yielding a correlation coefficient of 0.97 over the test conditions and materials system for which we had data. Since the additive manufacturing archive contained process parameters for each printed point in the build, we combined various data-files to create interesting visualization of the process parameters such as bead width, beam current and chamber vacuum level, which are useful to understand and control the sources of process variability important in meeting the reproducibility challenges of additive manufacturing.

Acknowledgements: The authors gratefully acknowledge support from DARPA under contract number HR0011-16-2-0030.
Integrated Cascaded Bragg Gratings for On-Chip Optical Delay Lines

Lingjun Jiang1, Zhaoran Rena Huang1

1 Department of Electrical, Computer and Systems Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180

contact: jiangl2@rpi.edu

We have demonstrated on-chip optical delay lines that consist of slow-light cascaded Bragg grating segments. Integrated optical true delay line is one of the key elements in many optical systems for time alignment or control of optical path length. Single on-chip grating segment delay line cannot meet the need due to finite chip dimension. To increase total delay time, multi-stage cascade Bragg grating is explored in this work.

Fig. 1(a) shows the schematic of the fabricated delay lines. Each segment is a side-wall Bragg grating that uses Super Gaussian apodization to reduce spectrum ripples. The device that consist of 1, 2 and 4 grating segments are fabricated on a SOI, and the device parameters are determined by 3-dimensional finite-different time domain (FDTD) simulations to ensure single mode propagation at telecommunication wavelengths.

The transmission spectrums for the delay lines are measured and it is found that the optical band edges are aligned at ~λ = 1548 nm. The primary loss mechanism is the coupling loss at chip facets (~10 dB/facet). The group index ng of delay line is measured at and extracted with an interference method. In Fig. 1(b) the maximum ng is 12.2 for a 2-segment cascaded grating with each segment of 3.6 mm long. Total delay is 292 ps, corresponding to 41 ps/mm.

Our results show that the band gap and the group index of cascaded gratings are very similar to that of a single grating segment, which means longer time delay can be achieved by cascading more grating segments, likely at the cost of bandwidth. This work poses a potential for densely integrated on-chip delay lines for time delay on the order of nanoseconds or even microseconds.
Control of Polycrystalline Copper through In-Situ FIB-SEM Observation of Microstructural Evolution using Resistive Heating Techniques

Genevieve A. Kane1, Chengjian Zheng2, Yixuan Tan2, Dr. Antoinette Maniatty2, Dr. John Wen2, 3, Dr. Robert Hull1
1 Department of Materials Science and Engineering,
2 Department of Mechanical, Aerospace, and Nuclear Engineering,
3 Department of Industrial and Systems Engineering, Rensselaer Polytechnic Institute, Troy, NY, 12180,
contact: kaneg@rpi.edu, Genevieve.kane24@gmail.com

In this presentation, we describe the methods we are developing for real-time control of grain growth in metals. We are integrating control and simulation methods with in-situ FIB-SEM observations of thermal grain growth in polycrystalline copper films, with the goal of achieving active control of microstructural evolution.

Ten-channel micro-heater arrays were designed using finite element analysis (FEA) and fabricated using microfabrication techniques to allow for controlled heating profiles across one square mm of surface films in the FIB-SEM. Real-time observation using secondary electron imaging allowed assessment of the evolving grain microstructure with resolution down to a few nanometers and imaging increments as small as a few seconds. Statistical grain size distributions are currently used as a measurement of microstructural evolution over time and temperature. Coupled with feed-back control of the individual heater line resistances, we are aiming to experimentally show the ability to control the evolving microstructure in-situ. We also target creating unique microstructures based on specific thermal gradients and real-time feedback from imaging.

Preliminary in-situ control of the temperature in each channel of the micro-heater arrays has been established through the characterization of the electrical resistances of the ten channels. Measured temperatures between the heater lines and the chip surface differ only by a few degrees Celsius from the FEM calculations of the temperature distribution. Real-time grain growth at uniform temperature has also been characterized in bulk polycrystalline films between 300 and 500 degrees Celsius and compared to Monte Carlo grain-growth simulation results. The simulated microstructure is initialized to that observed experimentally at room temperature and then annealed until the mean grain size is equivalent to the annealed experimental structures. Results show that the standard deviations of the simulated annealed grain structures are within 10-15% of the corresponding experimental standard deviations.

The initial results from these grain growth studies are used to develop a methodology for control of microstructural evolution in polycrystalline films deposited on micro-heater arrays with designed temperature profiles. While the current model material is polycrystalline copper, we believe this technique has potential to application to other material systems.

Computational Analysis of Low Voltage Tunable Silicon Optical Modulator

Young Hwa Kim1, Lingjun Jiang1, Stephen Anderson1, Zhaoran Huang1
1 Electrical Engineering and Computer and System Engineering, Rensselaer Polytechnic Institute, Troy NY, 12180
contact: kimy15@rpi.edu

Optical interconnect based on silicon photonics has been one of the leading technology candidates that spearheads next generation of electronic circuit interconnects that strives to go beyond the speed of electrons. Si electro-optical (EO) modulator is one of key devices in achieving high performance chip-scale optical interconnect applications. The modulators have been improved dramatically in recent years, especially increasing its bandwidths range to the multi GHz regime and getting closer to the THz regime.

With increasing advancements, the device performance parameters of the optical modulator such as lower energy consumption, smaller device structure, maximum bandwidth and modulation depth, have become more crucial than ever. All of the above must be achieved with acceptable thermal tolerance and optical spectral width, using CMOS compatible fabrication processes.

The state of art silicon optical modulator is limited to 200 nm pitch of the critical dimensions and its size is far from comparable to the smallest lateral CMOS FET. The new fabrication scheme is required to scale down the device structure. In this poster, computational analyses on the fabrication process and the device performance for the interleaved silicon optical modulator will be presented. For the process modeling, two crucial processes of ion implantation and thermal annealing will be analyzed through the analytical Gaussian and the Monte Carlo calculation methods to characterize the effect of junction profile on the performance. As for the device performance modeling, the computational analysis through the Plane Wave Expansion and Finite Difference Time Domain method demonstrate the improved performance through low voltage operating with high efficiency.

Acknowledgements: ARL
Evolution and Structural Investigation of RNA Aptamers for Glycosaminoglycans Heparosan, Hyaluronic Acid and Chondroitin

Megan Kizer1,4, Peiqin Li2,4, Brady Cress3,4, Xing Wang1,4, Robert Linhardt1,3,4
1 Department of Chemistry, Rensselaer Polytechnic Institute, Troy, 12180, 2 Department of Forest Pathology, College of Forestry, Northwest A&F University, Yangling, 712100, China, 3 Department of Chemical and Biological Engineering, Rensselaer Polytechnic Institute, Troy, 12180, 4 Center for Biotechnology & Interdisciplinary Studies, Rensselaer Polytechnic Institute, Troy, 12180

goal: To develop a stable RNA biosensor, and a multivalent aptamer-based, GAG selective purification device. As the RNA aptamers evolved in the lab have shown selectivity among different GAG classes, they therefore hold promise for the development of more robust, efficient, and selective biodetection and separation methods.


A Foldable Lithium Sulfur Battery

Lu Li1, Hao Sun2, Chandra Veer Singh1, Nikhil Koratkar2
1. Rensselaer Polytechnic Institute, Troy, NY, United States. 2. University of Toronto, Toronto, ON, Canada.

The next generation of deformable and shape-conformable electronics devices will need to be powered by batteries that are not only flexible but also foldable. Here we report a foldable Lithium-Sulfur (Li-S) rechargeable battery, with the highest areal capacity (~3 mAh cm^-2) reported to date among all types of foldable energy-storage devices. The key to this result lies in the use of fully-foldable and super-elastic carbon nanotube current-collector films and impregnation of the active materials (S and Li) into the current-collectors in a checkerboard pattern, enabling the battery to be folded along two mutually orthogonal directions. The carbon nanotube films also serve as the sulfur entrapment layer in the Li-S battery. The foldable battery showed < 12% loss in specific capacity over 100 continuous folding and unfolding cycles. Such shape-conformable Li-S batteries with significantly greater energy density than traditional lithium-ion batteries could power the flexible and foldable devices of the future including laptops, cell-phones, tablet computers, surgical tools and implantable bio-medical devices.
Single crystalline graphene is always desirable for electronic applications because the grain boundaries would undermine the extraordinary properties from a single crystal graphene. To date, chemical vapor deposition (CVD) is the most widely used method to produce high quality graphene. Among those graphene growing catalysts, the Cu(111) surface has been a favorable choice due to its advantages in symmetry matching with graphene, effectiveness of catalyzing, and the low carbon solubility. However, 60° in-plane rotational twinning in these Cu films have caused graphene growth direction rotation of 30° across the Cu twin boundaries and also served as the carbon segregation and nucleation sites. Methods have been explored to remove the twinning since it appears to be a concern for the growth of single-crystal graphene. On the other hand, the symmetry of graphene is usually determined by low-energy electron diffraction (LEED) method when the graphene is on the conductive substrates. But LEED cannot handle graphene transferred to SiO$_2$/Si substrates due to the charging effect.

Herein, we employed a novel azimuthal reflection high-energy electron diffraction (RHEED) method to construct the reciprocal space mapping and determine the symmetry of wafer size graphene both pre- and post-transfer. In this work, the graphene was epitaxially grown on single-crystalline Cu(111) films with a low pressure chemical vapor deposition. The reciprocal space mapping using azimuthal RHEED confirmed that the graphene grown on Cu(111) films was single-crystalline, in the form of either monolayer or multilayer structure. While the Cu(111) film grown on sapphire(0001) may occasionally consist of 60° in-plane rotational twinning, the reciprocal space mapping revealed that the in-plane orientation of graphene grown atop was not affected in this work. The proposed structural characterization of the post-transferred graphene sheets is an important step in the realization of the graphene as a platform to fabricate electronic and optoelectronic devices.

**Acknowledgements:** This work is supported by the NYSTAR Focus Center at RPI, C130117 and by NSF Award under DMR 1305293. The authors would also like to thank RPI MNCR clean room staff for their great help on this project!
Resistivity Size Effect in Epitaxial Ru(0001) Layers
Erik Milosevic, Daniel Gall
Department of Materials Science & Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180
Contact: milose@rpi.edu

Ruthenium is a promising candidate for replacing copper as a conductor in confined dimensions due to its small predicted mean free path of 6.7 nm. Epitaxial Ru(0001) layers are sputter deposited onto Al₂O₃(0001) and their resistivity is measured as a function of sample thickness $d = 5-80$ nm both in situ and ex situ at 295K and 77K for the purpose of quantifying electron scattering at the surfaces and experimentally determining the mean free path without confounding impact from grain boundary scattering. X-ray diffraction analyses show an epitaxial layer-substrate relationship with Ru[0001] || Al₂O₃[0001] and Ru[1010] || Al₂O₃[1120]. Fitting the resistivity data with the semiclassical model of Fuchs and Sondheimer yields a room temperature mean free path of $6.7 \pm 0.3$ nm, in excellent agreement with predictions from first principal calculations. Ru interfaces are determined to scatter diffusively, and the Ru surface shows no specularity change upon exposure to an oxidative environment. Atomic force microscopy and X-ray reflectivity are used to determine the surface roughness, which is < 1nm and therefore has a negligible impact on the measured resistivity. Transport measurements at 77K show an unexpected and highly favorable resistivity size effect with a mean free path that is 39% lower than expected based on the temperature dependence of the bulk resistivity. In-plane Boltzmann transport simulations done by integrating over real and reciprocal space of the thin film and the Brillouin zone, respectively, show agreement with experimental results. Transport simulations suggest a reduced resistivity increase for transport perpendicular to the basal plane, with, for example, a 3.59 μΩcm lower resistivity for a 2 nm thick film. This study confirms Ru as a promising candidate for future back and middle of line applications.
Effect of graphene buffer layer on the van der Waals epitaxy of CdTe thin films

Dibyajyoti Mohanty1,*, Zonghuan Lu1, Xin Sun1, Shengbai Zhang1, Morris Washington1, Gwo-Ching Wang1, Toh-Ming Lu2 and Ishwara B. Bhat1

1 Center for Materials, Devices, and Integrated Systems
2 Physics, Applied Physics and Astronomy Department, Rensselaer Polytechnic Institute, Troy, NY 12180
* mohan@rpi.edu

Conventional heteroepitaxy requires well matched crystalline symmetry, lattice constant, and expansion coefficient between the grown film and the substrate to produce a strain and defect free film [1]. However, in van der Waals epitaxy, the bonding between the over layer and substrate is due to weak van der Waals forces instead of strong covalent bonds. As a result, not only the lattice matching requirement is relaxed, but also significantly fewer defects are present in the grown film, due to the dangling bond free interface [2]. Traditionally, layered materials, have been successfully used as substrates to grow other layered materials epitaxially, i.e., 2D on 2D. But the growth of 3D materials on layered materials such as graphene has found little success until recently [3,4]. Among II-VI semiconductor materials, CdTe has invoked intense interest in recent years due to its applicability in photovoltaics, aerospace, and radiation detection related applications. Hence, it is highly desirable to produce low cost, epitaxially grown CdTe films on various substrates, which can be fulfilled by vdWE. We have studied 3D CdTe film on graphene buffer layer owing to graphene’s inherent advantages such as high thermal stability, high mechanical strength, high decomposition temperature, ease of producing high quality graphene and transferring to any substrate of interest. In this study, we found that the nature of the graphene film influences the quality of CdTe film grown on it.

References

Adaptation of CMOS oriented Auto Placement and Route to Asynchronous RSFQ Logic with emphasis on a 32 bit ARM

Sagnik Nath1, Alex Derrickson2, John F. McDonald1
1 Electrical, Computer and Systems Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180
contact: naths3@rpi.edu

Rapid Single Flux Quantum (RSFQ) Logic, employing the superconducting device Josephson Junctions, holds considerable promise in creating computer architectures for fast processing of data. The two main attributes of RSFQ allowing this are the Josephson Junctions that can act as picosecond switches and, the use of superconducting microstrip transmission lines capable of transferring picosecond waveforms over virtually any interchip distance while exhibiting low attenuation and dispersion. However, commercial EDA tools to handle complex RSFQ designs do not yet directly support RSFQ technology for Auto Place and Route of complex designs.

The current research work describes a methodology to attempt to Auto Place and Route an asynchronous RSFQ Binary Decision Diagram (BDD) based dual rail processor design using the EDA tool Innovus and then move towards laying out an ARM processor. Dual rail logic is used in writing the Verilog code. The asynchronous BDD, confluence buffer and Josephson Transmission Line are the only RSFQ cells whose layouts are made by hand. The layouts are then optimised and inserted with Passive Transmission Line receivers and transmitters at the input and output end. Single rail structural verilog, corresponding to the desired circuit design, is outputted by dc_shell. This is then passed through a Python script that converts it to dual rail. Finally, the finished dual rail structural verilog design is ready for Auto Place and Route through Innovus.

Currently, Auto Place and Route of RSFQ designs of the architectures: SCRAM2, MIPS and 32 bit single cycle ARM have been accomplished following the proposed methodology. Subsequent evaluation of these designs in terms of timing, power supply and pin connect are being currently investigated.

Acknowledgements: This research is based on a subcontract under IBM for IARPA under the Cryogenic Computing Complexity (C3) program.
Structure and Properties of Crystalline Polymer Nanocomposites: Filler Dispersion and Crystallization Behavior
Xin Ning
Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, 12180
contact: ningx3@rpi.edu

Polymer nanocomposites (PNC), mixtures of polymer matrixes and inorganic/organic nanoscale particles, have received tremendous attention over the last few decades. Recent work has focused on the assembly of ligand-grafted nanoparticles in amorphous polymer matrices. It has been found that the molecular weight and graft density of the ligands can be used to control spatial dispersion and interface interaction. A new approach to nanofiller organization using crystallization kinetics has been demonstrated but not fully explored. In addition, organizing nanofillers in the melt (i.e. aggregation, sheet, strings) and using that to control polymer heterogeneous nucleation and crystal growth is also unknown. This work will focus on kinetically organizing spherical nanoparticles using polymer crystallization across multiple length scales and conversely organizing nanoparticles in a polymer melt to subsequently control crystal morphology. The issues that determine NPs dispersion and crystal morphology will be addressed along with aspects of mechanical properties (i.e. elastic modulus).
Peierls stresses of dislocations in HMX
Anirban Pal and Catalin R. Picu
Department of Mechanical, Aerospace and Nuclear Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180

Being an energetic material, HMX (cyclotetramethylene-tetranitramine) has a high energy-release rate upon decomposition. In this molecular crystal, the role of defects and deformation in causing initiation following mechanical shock or impact is not well understood. Owing to the effect of crystal orientation to initiation sensitivity in such materials, it is hypothesized that dislocation mediated plastic deformation plays a central role, where higher impact sensitivity in a crystalline direction can be associated with limited slip along sterically hindered slip planes. In this work, we investigate and characterize slip systems in β-HMX using computational tools. We use a geometric overlap procedure to infer geometric-gamma surfaces for various slip planes. Using the Smith-Bharadwaj potential calibrated for HMX, we estimate the Peierls stresses for dislocation motion for these slip systems. Slip is highly asymmetric and anisotropic. We conclude that there are enough slip systems available for supporting a generalized state of plastic strain.

3D Printing Implications for Breast Cancer Research
James Nowak1, Kristen Mills1,2, Assad Oberai1, Johnson Samuel1
1 Mechanical, Aerospace, and Nuclear Engineering Department, Rensselaer Polytechnic Institute, Troy, NY, 12180
2 Center for Biotechnology and Interdisciplinary Studies, Rensselaer Polytechnic Institute, Troy, NY, 12180
Contact: nowakj2@rpi.edu

Breast cancer, and other soft tissue cancers, are being studied extensively by biomedical researchers and tissue engineering. However, the environments and manufacturing processes to create these environments are not indicative of the actual environment seen in the human body. Manufacturing solutions, such as 3D printing, need to be developed in order to create environments that better replicate these environments. Therefore, the objective of this research is to develop innovative 3D printing processes that enable the biomedical community to effectively diagnose and treat cancerous diseases affecting soft tissues. In light of this objective, we provide two main research thrusts, viz. (1) Patient-specific phantom tissue models for surgeon training and patient education, and (2) Fibrous networks for tumor cell morphology and growth.

For Thrust 1, we developed a 3D printing process that converts the stiffness map taken from an ultrasound scan, to a two-material model that can be printed using a custom-built silicone-extrusion process. Models were printed of both benign and malignant tumor models. Preliminary compression testing was performed on the printed samples, to show the tumorous regions to provide a detectable difference.

For Thrust 2, we developed a hybrid process that involves far-field electrospinning of polymer fibers and syringe deposition of hydrogel solution. Combined, these two processes provide a 3D reinforcement in the hydrogel, that better replicates the environment seen in breast tissue. Cross-sectional views of the fiber-reinforced hydrogels show the fiber density within the sample can be varied, which will directly correlate to the stiffness of the gel. It is hypothesized that these stiffness variations will have a direct variation on the cell morphology and growth patterns of the tumor cells.
PP.25 | Scott Peters
12:00 – 1:30
Solution Thermodynamics of DNA templated Nanoparticle Lattices based on an expanded complementary contact model
Scott Peters¹, Neha Chauhan¹, Xing Wang²,³,⁴, Chaitanya Ulla⁺,⁵ and Daniel J. Lewis¹,⁵
1 Department of Materials Science & Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180
2 Department of Chemistry and Chemical Biology, Rensselaer Polytechnic Institute, Troy, NY 12180
3 Center for Biotechnology and Interdisciplinary Studies, Rensselaer Polytechnic Institute, Troy, NY 12180
4 Center for Materials, Devices, and Integrated Systems, Rensselaer Polytechnic Institute, Troy, NY 12180
5 Center for Lighting Enabled Systems & Applications, Rensselaer Polytechnic Institute, Troy, NY 12180

The programmable nature of DNA bonds has been exploited to direct the assembly of nanoparticles functionalized with dense brushes of DNA into lattices with an unprecedented level of control over crystal structure. Much of this success results from the treatment of the DNA mediated interactions as analogous to the concepts of valency and bonds in atomic crystal lattices. The treatment of bonds from a solutions thermodynamics perspective raises the prospect of control over microstructure. Here we present predictions of the solution thermodynamic behavior of two component nanoparticle lattices based on a simple complementary contact model. Such models have been demonstrated to capture the essential behavior of DNA templated nanoparticle lattices. We expand the standard complementary contact model to include an important elastic bending energy term, discuss the importance of other energy terms and present the predicted phase space. We also summarize recent efforts to create two component DNA coated nanoparticles that will validate the predicted solution behavior.

PP.26 | Baiwei Wang
12:00 – 1:30
Optical and Electronic Properties of Epitaxial Tiₓ−Mg Nx Layers Grown on MgO(001)
Baiwei Wang, Sit Kerdsongpanya, Erik Milosevic, Mary McGahay, Daniel Gall
Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180
contact: wangb12@rpi.edu

Epitaxial single-crystal Tiₓ−Mg Nx (001) ternary alloy layers were deposited on MgO (001) by reactive magnetron co-sputtering from titanium and magnesium targets in 15 mTorr pure N₂ at 600°C. X-ray diffraction (XRD) indicates that the deposited alloy layers exhibit a solid solution rock-salt phase for x = 0 - 0.67. Increasing the Mg concentration leads to an increase in the lattice constant from 4.25Å for TiN to 4.28Å for Tiₓ−MgNx, and a decrease in the crystalline quality as quantified by the Full Width of Half Maxima (FWHM) of the ω rocking-curve XRD peak which increases from 0.25° to 0.80°. XRD φ-scans verify that all Tiₓ−Mg Nx layers are single crystals with a cube-on-cube epitaxial relationship to the substrate: [001]_{Ti−Mg Nx} || [001]_{MgO} and [100]_{Ti−Mg Nx} || [100]_{MgO}. The electrical resistivity increases from 14.5 μΩ·cm for x = 0 to 554 and 3197 μΩ·cm for x = 0.29 and 0.61, respectively. Ti₁₋Mg Nx layers with x ≥ 0.61 show a negative temperature coefficient of resistivity which is attributed to the decreasing electron density of states at the Fermi level and a weak localization of free carriers. Optical transmission measurements indicate the onset of interband transitions at 2.0 and 1.7 eV for Ti₁₋Mg₀.₂₉ N and Ti₁₋Mg₀.₆₃ N, respectively.
This paper selects the metal Mo as the infrared reflective layer, Mo-Al_2O_3 as the absorbing layer and Al_2O_3 as the anti-reflective layer. Mo-Mo-Al_2O_3/Al_2O_3 selective absorbing coatings with double absorption layers were fabricated on polished 316L stainless steel by using a hybrid magnetron sputtering. The influences of the volume fraction of Mo and the thickness of anti-reflective layer and absorbing layer on the selective absorption performance of the obtained Mo-Mo-Al_2O_3/Al_2O_3 selective absorbing coatings were studied. The results show that the thickness of anti-reflective layer exerts an obvious effect on absorption edge and the location of the absorption peak. When the sputtering time for the anti-reflective layer is 10 min, the absorption performance of the coating is the best. With increasing the thickness of high metal absorbing layer, the surge threshold wavelength of the reflectance will red-shift, and the emittance will also increase, however, if the thickness is too high, it will affect the interference effect. With increasing the thickness of high metal absorbing layer, the visible absorption ratio will increase and the surge threshold wavelength of the reflectance will red-shift, but the emittance will gradually increase. With increasing metal content of high metal absorbing layer, its square resistance reduces, resulting that the emittance gradually declines. With increasing metal content of low metal absorbing layer, it will increase the absorption over long wave spectrum and decrease the infrared interference, resulting in a rising emittance.

![Reflectance graph](image_url)
AUTHOR INDEX

Andersen, D., 13(AIS.01), 29(OP.01)
Anderson, N., 29(OP.02)
Anderson, S., 44(OP.12)
Arbanas, G., 41(OP.06)
Bae, C., 43(OP.09)
Baltazar, T., 13(AIS.02), 39(OP.01)
Baskaran, A., 36(OP.16), 39(OP.02)
Basu, S., 31(OP.06)
Bewersdorf, J., 33(OP.09)
Bhat, I., 48(OP.19)
Bhatt, S., 30(OP.03)
Carabis, D., 40(OP.03)
Catarino, C., 39(OP.01)
Chandra, A., 15(AIS.03)
Chauhan, N., 51(OP.25)
Chen, Y., 31(OP.06)
Chen, Z., 38(OP.19)
Cheng, H., 33(OP.10)
Cherniak, D., 30(OP.04), 35(OP.14)
Chow, P., 32(OP.08)
Clifton, Z., 41(OP.06)
Cress, B., 45(OP.13)
Danon, Y., 41(OP.06)
De, S., 37(OP.17)
Deagen, M., 15(AIS.04), 31(OP.05)
Derrickson, A., 48(OP.20)
Dinolfo, P., 29(OP.02), 41(OP.05)
Dudney, N., 35(OP.14)
Duquette, D., 35(OP.13)
Engler, B., 40(OP.04)
Ergene, C., 17(AIS.05)
Erickson, J., 42(OP.08)
Esposito, T., 41(OP.05)
Feng, J., 41(OP.06)
Fox, P., 42(OP.08)
Gall, D., 47(OP.18), 51(OP.26), 52(OP.27)
Gao, J., 33(OP.10)
Ghoshal, D., 17(AIS.06), 31(OP.06)
Giovino, M., 19(AIS.07)
Goldberg, M., 42(OP.08)
Gross, R., 46(OP.16), 47(OP.17)
Guo, Z., 32(OP.08)
Gupta, T., 31(OP.06), 32(OP.07)
Han, J., 43(OP.09)
Hao, X., 33(OP.09)
Hendler, J., 42(OP.08)
Holcomb, A., 41(OP.06)
Hollingsworth, A., 42(OP.07)
Howell-Clark, J., 32(OP.08)
Huang, L., 36(OP.15)
Huang, Z., 42(OP.07), 43(OP.10), 44(OP.12)
Hull, R., 29(OP.01), 35(OP.13), 36(OP.14), 36(OP.16), 40(OP.04), 42(OP.08), 44(OP.11)
Hynes, A., 42(OP.08)
Ispas, S., 36(OP.15)
Jeon, J., 43(OP.09)
Jiang, L., 43(OP.10), 44(OP.12)
Kane, G., 36(OP.16), 44(OP.11)
Karanastasis, A., 33(OP.09)
Karande, P., 39(OP.01)
Keblinski, P., 34(OP.12), 49(OP.21)
Kenath, G., 33(OP.09) McGuinness, D., 42(PP.08)
Kercher, A., 35(OP.14) McMaster, M., 46(PP.16), 47(PP.17)
Kerdsongpanaya, S., 51(PP.26) Mekala, S., 46(PP.16)
Kim, Y., 44(PP.12) Merola, J., 39(PP.01)
Kisslinger, K., 34(OP.11) Meunier, V., 30(OP.04), 31(OP.06)
Kizer, M., 45(PP.13) Mills, K., 50(PP.23)
Kob, W., 36(OP.15) Milosevic, E., 47(PP.18), 51(PP.26)
Koratkar, N., 31(OP.06), 33(OP.10), 45(PP.14) Mohanty, A., 43(PP.09)
Lee, W., 43(PP.09) Mohanty, D., 48(PP.19)
Lewis, D., 36(OP.16), 39(PP.02), 51(PP.25) Nath, S., 21(AIS.10), 23(AIS.11), 48(PP.20)
Lewis, K., 41(PP.05) Nie, J., 49(PP.21)
Li, F., 33(OP.10) Ning, X., 23(AIS.12), 49(PP.22)
Li, L., 19(AIS.08), 33(OP.10), 45(PP.14) Nowak, J., 50(PP.23)
Li, P., 45(PP.13) Oberai, A., 50(PP.23)
Li, Y., 52(PP.27) Ozisik, R., 34(PP.12)
Li, Z., 34(OP.11) Pal, A., 50(PP.24)
Liang, Z., 49(PP.21) Palermo, E., 37(OP.18)
Linhardt, R., 45(PP.13) Pan, F., 42(PP.08)
Littlejohn, A., 21(AIS.09), 34(OP.11) Park, E., 43(PP.09)
Liu, F., 46(PP.16) Patel, A., 47(PP.17)
Liu, L., 41(PP.06) Peng, W., 34(PP.12)
Lu,T., 34(OP.11), 38(OP.19), 46(PP.15), 48(PP.19) Peters, K., 46(PP.16)
Lu, Z., 34(OP.11), 46(PP.15), 48(PP.19) Peters, S., 51(PP.25)
Maiorana, A., 47(PP.17) Picu, C., 50(PP.24)
Manas-Zloczower, I., 47(PP.17) Pinkowitz, A., 25(AIS.13), 35(OP.13)
Maniatty, A., 30(OP.03), 36(OP.16), 44(PP.11) Pober, J., 39(PP.01)
Marschikok, A., 35(OP.14) Rabinowitz, G., 39(PP.02)
McDonald, J., F., 48(PP.20) Ranganathan, R., 34(OP.12), 49(PP.21)
McDonald, N., 42(PP.07) Ren, W., 33(OP.10)
McGahay, M., 51(PP.26) Rende, D., 37(OP.17)
<table>
<thead>
<tr>
<th>Authors</th>
<th>Page Numbers</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ryu, C.</td>
<td>43(PP.09)</td>
</tr>
<tr>
<td>Saltzman, M.</td>
<td>39(PP.01)</td>
</tr>
<tr>
<td>Samuel, J.</td>
<td>42(PP.08), 50(PP.23)</td>
</tr>
<tr>
<td>Sarbada, V.</td>
<td>25(AiS.14), 27(AiS.15), 27(AiS.16), 35(OP.14)</td>
</tr>
<tr>
<td>Schadler, L.</td>
<td>31(OP.05)</td>
</tr>
<tr>
<td>Schwartzberg, A.</td>
<td>42(OP.08)</td>
</tr>
<tr>
<td>Shi, J.</td>
<td>38(OP.19)</td>
</tr>
<tr>
<td>Shi, S.</td>
<td>31(OP.06)</td>
</tr>
<tr>
<td>Shin, D.</td>
<td>43(OP.09)</td>
</tr>
<tr>
<td>Singer, K.</td>
<td>46(OP.16), 47(OP.17)</td>
</tr>
<tr>
<td>Singh, C.</td>
<td>33(OP.10), 45(OP.14)</td>
</tr>
<tr>
<td>Sun, H.</td>
<td>45(OP.14)</td>
</tr>
<tr>
<td>Sun, X.</td>
<td>34(OP.11), 38(OP.19), 46(OP.15), 48(OP.19)</td>
</tr>
<tr>
<td>Sundararaman, S.</td>
<td>36(OP.15)</td>
</tr>
<tr>
<td>Takeuchi, E.</td>
<td>35(OP.14)</td>
</tr>
<tr>
<td>Tan, Y.</td>
<td>36(OP.16), 44(OP.11)</td>
</tr>
<tr>
<td>Teunisse, C.</td>
<td>37(OP.17)</td>
</tr>
<tr>
<td>Turkseven, M.</td>
<td>37(OP.17)</td>
</tr>
<tr>
<td>Uchida, S.</td>
<td>38(OP.20)</td>
</tr>
<tr>
<td>Ulial, C.</td>
<td>31(OP.05), 33(OP.09), 37(OP.18), 51(OP.25)</td>
</tr>
<tr>
<td>Vijayamohanlan, H.</td>
<td>37(OP.18)</td>
</tr>
<tr>
<td>Wang, B.</td>
<td>51(OP.26)</td>
</tr>
<tr>
<td>Wang, G.</td>
<td>34(OP.11), 46(OP.15), 48(OP.19)</td>
</tr>
<tr>
<td>Wang, T.</td>
<td>31(OP.06)</td>
</tr>
<tr>
<td>Wang, X.</td>
<td>29(OP.02), 45(OP.13), 51(OP.25)</td>
</tr>
<tr>
<td>Wang, Y.</td>
<td>38(OP.19)</td>
</tr>
<tr>
<td>Washington, M.</td>
<td>46(OP.15), 48(OP.19)</td>
</tr>
<tr>
<td>Watson, B.</td>
<td>30(OP.04)</td>
</tr>
<tr>
<td>Wen, J.</td>
<td>36(OP.16), 40(OP.03), 44(OP.11)</td>
</tr>
<tr>
<td>Wetzel, C.</td>
<td>32(OP.08)</td>
</tr>
</tbody>
</table>