2013 OSU MATERIALS RESEARCH SEED GRANT PROGRAM AWARDS

The **OSU Materials Research Seed Grant Program** provides internal research funding opportunities through three distinct Funding Tiers designed to achieve the greatest impact for seeding and advancing excellence in materials research of varying scopes. The OSU Materials Research Seed Grant Program is jointly funded and managed by the Center for Emergent Materials (CEM), the Center for Electronic and Magnetic Nanoscale Composite Multifunctional Materials (ENCOMM), and the Institute for Materials Research (IMR).

We are excited to announce that after a thorough internal and external review process, six awards have been made to fund innovative and exciting materials research on campus through the OSU Materials Research Seed Grant Program. These awards total $280,000 in internal research funding to 17 OSU researchers in six departments.

2013 Multidisciplinary Team Building Grants

Multidisciplinary Team Building Grants provide funds up to $60,000/year per award in direct costs, require one PI and one Co-PI, and may have unfunded collaborators. The goal of the Multidisciplinary Team Building Grants is to form multidisciplinary materials research teams that can compete effectively for federal block-funding opportunities. Two Multidisciplinary Team Building Grants were awarded this year:

Towards an Atomic Scale Understanding of CO_2 Photocatalysis

Principal Investigator: Jay Gupta, Physics; Co-Investigator: Aravaind Ashtagiri, Chemical and Biomolecular Engineering

We propose a combined experimental / theoretical study of photoreduction of CO_2 on thin oxide films. CO_2 reduction to fuels such as alkanes and alcohols is a promising approach to an anthropogenic carbon cycle that could convert renewable energy sources to high-energy density, easy to store and transport fuels. Recent research in photocatalysis has focused on developing nanostructured oxide thin films in part to reduce electron-hole recombination, but a fundamental understanding of the surface photochemistry remains to be developed. The work proposed for the seed grant will focus on Cu_2O thin films on Cu(111) and Cu(100) surfaces. Scanning tunneling microscopy of CO_2 and relevant products in the photoreduction cycle (e.g., MeOH) will be conducted at temperatures ranging from 5-300K. Atomic-resolution imaging will directly determine adsorption sites, and tunneling spectroscopy will probe molecular orbitals and charge transfer to the oxide substrate. The experimental data will be directly compared with Density Functional Theory (DFT) calculations of the local density of states, lowest-energy molecular structure, vibrational modes and likely reaction mechanisms. The synergy of STM and DFT will provide a framework for future study aimed at building an atomic-scale understanding of

CO_2 photoreduction, a grand challenge for future energy needs and climate change, and place the team to examine other nanostructured oxide materials as candidates for photoelectroreduction or photocatalysis. This work will help in nucleating a broader team of catalysis researchers at OSU that can tackle problems in heterogeneous, electro- and photo-catalysis spanning fundamental studies to reactor-scale implementation.

Next Generation 2D Semiconductor Heterostructures

Principal Investigator: Siddharth Rajan, Electrical and Computer Engineering; Co-Investigator: Yiying Wu, Chemistry; Collaborators: Roberto Myers, Materials Science and Engineering; Wu Lu, Electrical and Computer Engineering; Wolfgang Windl, Materials Science and Engineering

The objective of the proposed work is to investigate synthesis, electronic properties, and device applications of 2D materials based on the metal dichalcogenides. We seek to build on our recent pathbreaking results on the first synthesis of large area single crystal MoS_2 with excellent optical and electronic properties. Our aim is to investigate synthesis of the entire new class of semiconductors including HfS_2, TiS_2, ReS_2, NbS_2, WS_2, as well as their heterostructures for the first time. This will be combined with the first detailed study of their electronic and optical properties, as well as demonstration of new device structures.

2013 Exploratory Materials Research Grants

Exploratory Materials Research Grants provide funds up to $40,000/year per award in direct costs, require one PI, and may have Co-PIs and/or unfunded collaborators. The goal of the Exploratory Materials Research Grants is to enable nascent materials research to emerge to the point of being competitive for external funding. Four Exploratory Materials Research Grants were awarded this year:

Enabling High-Efficiency Thin-Film CIGS Photovoltaics through Nanometer-Scale Defect Identification

Principal Investigator: Aaron Arehart, Electrical and Computer Engineering; Co-Investigators: Tyler Grassman, Materials Science and Engineering; Jonathan Pelz, Physics; Collaborators: David McComb, Materials Science and Engineering; Sylvain Marsillac, Electrical and Computer Engineering, Old Dominion University

We propose to study defects in Cu(In,Ga)Se_2 (CIGS) thin-film materials via the adaptation of a newly-developed high-speed, nm-scale scanning Kelvin probe microscope with variable temperature and monochromated photoexcitation systems, enabling the correlation of defect states to microstructure and impurities, and quantification of their impact on photovoltaic efficacy. Such measurements are non-trivial, but the successful demonstration of this technique for the characterization of complex defects in III-N high-speed electronics provides strong motivation to explore its application toward nm-scale defect distributions in thin-film chalcogenides. In these materials, issues such as grain boundaries and impurities are known to impact device performance, but the precise mechanisms are unknown. Along with these nm-scale defect spectroscopy measurements, atomic-resolution scanning transmission electron microscopy (STEM) and STEM-based electron energy loss spectroscopy, energy dispersive X-ray analysis, and cathodoluminescence will be employed to further elucidate the physical sources of the observed defects. This suite of distinctive techniques will provide unique insight into defect-mediated

recombination, transport, and photovoltaic performance, informing the question of why CIGS photovoltaics perform well below the Shockley-Queisser limit. This approach will ultimately be applicable to many thin-film materials, including earth-abundant photovoltaics, such as $Cu_2ZnSn(S,Se)_4$ and FeS_2, providing a sustainable path for continued thin-film photovoltaics research at OSU.

A New Approach for Contactless Transport Measurements

Principal Investigator: Thomas Gramila, Physics

We propose development of a transport measurement method free from the need for ohmic contacts. The method provides access to longitudinal resistance as well as the transverse resistance that is so important in the presence of magnetic fields. It is ideally suited to systems where ohmic contacts are unfeasible, such as the low density two-dimensional electron gas at very high magnetic fields, or for novel systems where suitable contacts are not yet developed. The technique mimics the topology of a conventional transport measurement, but utilizes capacitive coupling for both inducing sample currents and for signal detection. This manner of electrical connection introduces experimental challenges that must be overcome. One involves the small signal size, another is the elimination of stray signals. Our work will capitalize on the low noise measurement expertise present in our laboratory to develop the technique into a powerful measurement approach for probing a wide range of electronic systems.

Engineering the Morphology of Ionenes for Self-Healing and Self-Destructing Materials

Principal Investigator: Lisa Hall, Chemical and Biomolecular Engineering; Co-Investigator: Vishnu Baba Sundaresan, Mechanical and Aerospace Engineering; Collaborator: Timothy Long, Chemistry, Virginia Tech

Ionenes, polymers with ions in their backbone, are of interest as self-healing materials because their ionic aggregates act like reversible crosslinks. We will study poly(propylene glycol)-based ammonium ionenes containing varying amounts of hard segments, using molecular simulations and experimental characterization. The hard segments are composed of alkyl groups with quarternary ammonium cations and bromide counterions. Previously, the healing of such materials after damage and heating was found to depend strongly on the percent of hard segments. Because healing is thought to depend on the aggregates and their ability to break and reform, which depends on their microscopic structure, we hypothesize that the structure and dynamics of these ionenes are noticeably different at the molecular level as a function of percent of hard segments. Prior simulations of different ionomers showed that varying the ionic content does drastically change the aggregate morphology. We thus propose to use molecular simulations to quantify the aggregate morphology and dynamics as a function of hard segment content in these ionenes, and to relate the observations to experimental trends in morphology and healing behavior. This will elucidate the relationship between morphology and healing behavior and enable further studies to design materials that reliably heal or destruct.

Pulsed Laser Deposition Synthesized Heterostructures, Nanostructures, and Graded Nanostructure Engineered Materials

Principal Investigator: Michael Sumption, Materials Science and Engineering; Co-Investigator: Roberto Myers, Materials Science and Engineering

We propose to study Pulsed Laser Deposition (PLD) synthesized heterostructures with a goal of using strain and modified PLD rastering to generate materials with nanophase and graded nanophase components and enhanced and/or novel properties. Previous work from our group, starting with PLD grown c-axis oriented MgB_2 thin films, has used a sequential rastering deposition technique incorporating secondary ZrB_2, SiC, and TiB_2 targets to generate multilayer structures with modified superconducting critical fields and temperatures. We propose to use sequential rastering to produce self-assembled secondary phases in the form of uniform-chemistry nano-columns through strain engineering of the structures, aiming for coherent boundaries between the phases with a residual lattice mismatch. Beyond the possibilities of materials modification available with uniform nanophase in-a-matrix assemblages with various morphologies, we can explore the extra degree of freedom accessible by grading the chemistry of the nanophase. As one example, we have recently worked to generate strain engineered structures in graded ZnO-MgO nanowires in a bid to take advantage of the band gap of ZnO (band gap 3.2 eV) for electronic devices. Graded chemistry (and thus polarization) in the ZnO-MgO system may allow p-type doping of the ZnO semiconductor without the need for impurity donors/acceptors by utilizing the asymmetry of ionic positions in the non-centrosymmetric Wurtzite crystal structure. The formation of graded nanocolumns or nanowires wires via PLD may find interesting possibilities in a variety of systems and applications.