

2014 OSU MATERIALS RESEARCH SEED GRANT PROGRAM AWARDS

We are pleased to announce that after a thorough internal and external review process, ten awards have been made to fund innovative and exciting materials research on campus through the 2014 OSU Materials Research Seed Grant Program. This year's awards include three Multidisciplinary Team Building Grants and seven Exploratory Materials Research Grants – the most awarded in the program's four years! These awards total \$460,000 in research funding to 25 OSU researchers in ten departments from four colleges, as well as two external collaborators.

Congratulations to the ten research teams whose projects were selected this year for seed grant funding.

2014 Multidisciplinary Team Building Grants

Multidisciplinary Team Building Grants form multidisciplinary materials research teams that can compete effectively for federal block-funding opportunities. Three Multidisciplinary Team Building Grants were awarded \$60,000 each this year:

Ultrastructural and Ultrasensitive Characterization of Iron-overload

PI: Gunjan Agarwal, Biomedical Engineering; Co-Investigators: Dana McTigue, Neuroscience; David McComb, Materials Science and Engineering; Collaborators: Eric Kraut, Hematology; John Moreland, National Institute of Standards and Technology

This proposal aims to develop novel high-resolution microscopy techniques for clinical pathology, in particular for iron detection. Ferritin is the major constituent of iron deposits found in iron overload. Current tests for ferritin content rely on antibody-based assays which measure ferritin concentration irrespective of iron ligation. Biochemical assays used to measure iron have limited sensitivity and spatial resolution. The ability to distinguish ferritin from apoferritin (non-iron-bound ferritin) at single particle level in small aliquots of samples may help improve diagnostics and treatment of imbalanced iron homeostasis. We plan to develop a novel *indirect* magnetic force microscopy technique to detect the iron-bound, superparamagnetic protein, ferritin in biological tissue with very high sensitivity and spatial resolution. In addition we will bring forth the liquid STEM capability to OSU to detect ferritin in biological fluids.

In-situ Solid-State NMR for Battery Studies

PI: Anne Co, Chemistry; Co-Investigator: Philip Grandinetti, Chemistry

The demand for inherently safe, large capacity, high-rate capability energy storage has led to the investigation of a class of metallic and semi-metallic elements that form stable intermetallics with lithium, providing Li⁺ storage capacities of 3 to 10 times that of Li⁺ intercalation into graphite sheets. Unfortunately, such high capacity intermetallic anodes undergo large volume expansions upon intercalation, changing the anodes microstructure and local chemical environments, which leads to reduced capacity. Our goal is to seek a fundamental understanding of material properties during dynamic changes that occur throughout the lithiation (charging) and de-lithiation (discharging) processes, commencing with Sn and other Sn-based anode materials. Our previous work has shown that a range of lithium-tin intermetallics can be formed electrochemically as a function of applied potential; however, preliminary data suggest that these intermetallics may be amorphous in nature

depending on the rate at which they are formed. The condition at which the material transforms from a crystalline to an amorphous phase has great implications on their rate capability and stability over time. Lithium and Tin solid-state NMR is an ideal technique to probe amorphous materials and understand how kinetically driven compositional changes affect the material microstructure and the local chemical environment. The scope of this seed proposal is to obtain preliminary data on the structural transformations of what seems to be an amorphous Li_xSn_y , starting with ex-situ measurements of these air-sensitive samples as a function of lithiation. We also seek to establish collaborative relationships to pursue future block funding opportunities from NSF and DOE to develop in-situ solid-state NMR and perhaps NMR imaging methodologies to probe the dynamics or chemical reactions in charge storage materials.

Group-III Nitride Nanowires for High-Efficiency Hydrogen Production via Photocatalytic Water Splitting

PI: Tyler Grassman, Materials Science and Engineering; Co-Investigators: Roberto Myers, Materials Science and Engineering; Patrick Woodward, Chemistry

InGaN is the only material system known to exhibit a band gap that can be tuned deep into the visible spectrum while maintaining the fundamental ability to split water into hydrogen and oxygen, without the need for separate or additional electrodes. This is due to InGaN having conduction and valence bands that effectively straddle the relevant redox potentials for much of the compositional range. Recent work has provided initial demonstrations of this capability, using InGaN/GaN nanowires to perform one-step overall photocatalytic water splitting (with the assistance of metal/metal-oxide co-catalysts). We propose to greatly improve upon these initial demonstrations by taking advantage of the full potential of the InGaN nanowire materials system. We will utilize advanced band gap, polarization, and device structure engineering to design and synthesize InGaN nanowires that exhibit optimal electronic structures specifically tailored to maximize every aspect of the water splitting reaction. Additionally, since the nanowires can be grown on silicon wafers, there is potential for the development of novel hybrid power generation systems that integrate traditional photovoltaics with photocatalyzed hydrogen fuel production. Along the way, we will develop a deeper understanding of such nanowire related catalytic processes, coupling the worlds of semiconductor band engineering with electrochemistry and catalysis.

2014 Exploratory Materials Research Grants

Exploratory Materials Research Grants enable nascent materials research to emerge to the point of being competitive for external funding. Seven Exploratory Materials Research Grants were awarded \$40,000 each this year:

Self-Patterned Oxide Nano-Structures: Laser Material Interaction

PI: Sheikh Akbar, Materials Science and Engineering; Co-Investigator: Enam Choudhury, Physics

The proposed research is based on previous work in the PI's laboratory which has led to the development of a low-cost and high throughput process by which self-assembled nanostructures can be produced on single crystal ceramic oxide surfaces. These nanostructures are formed due to a morphological instability created by intermixing of rare earth oxides on yttria-stabilized zirconia (YSZ) single crystal surfaces leading to the formation of nanoislands or nanobars to relieve strain energy. The most remarkable feature of this type of self-assembly is that it does not require lithography or any other process to guide the nanostructure formation. Furthermore, the nanostructures tend to align along certain crystallographic directions on the substrate surface, a process dictated by the elastic modulus anisotropy of the substrate. The major focus of the proposed research is to improve the ordering of these nanostructures by surface engineering while further deepening our understanding of the mechanism by which this self-assembly phenomenon takes place. Along with mechanistic studies, exploratory research will be conducted on the coupling of femtosecond laser on these

surfaces to study novel effects such as metastable state formation, enhancement of ordering of nanostructures, field confinement, collective motion and plasmon coupling.

Enabling High Efficiency Thin-Film Photovoltaics through Nanometer-Scale Defect Characterization (second year renewal)

PI: 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, Old Dominion University

We propose a renewal grant to develop and demonstrate a defect spectroscopy technique to investigate defects in thin-film photovoltaic materials. By providing nanometer-scale spatially-resolved trap spectroscopy measurements with a custom, high-speed, scanning Kelvin probe microscope (SKPM) with controllable temperature and monochromated photoexcitation, the complex structures in polycrystalline thin-film materials can be characterized and the trap associated with specific types of grain boundaries, microstructure, impurities, or composition. Atomic-resolution scanning transmission electron microscopy (STEM), STEM-based electron energy loss spectroscopy, and energy dispersive X-ray analysis will further elucidate the physical sources of such defect states and the role of impurities. This suite of proposed 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 and quantify the impact of specific defect structures have on solar cell terminal characteristics (i.e. fill factor, efficiency). This will be demonstrated in $\text{Cu}(\text{In,Ga})\text{Se}_2$ (CIGS) because it is more understood and controllable, but ultimately this will be applied to a wide range of thin-film materials including novel materials like $\text{Cu}_2\text{ZnSnS}_4$ (CZTS) and organic-inorganic hybrid lead-halide perovskites. This approach is aligned with OSU's Discovery Theme's "Energy and Environment" challenge, is strong step to provide a sustainable path for continued thin-film photovoltaics research at OSU, and will enable new collaborations within OSU where this research is growing.

Electric Field-Induced Effects on Defects in Complex Oxides

PI: Leonard Brillson, Electrical and Computer Engineering; Co-Investigator: Wolfgang Windl, Materials Science and Engineering

We have discovered that defects related to oxygen vacancies diffuse under electric fields of $> \sim 2 \times 10^4$ V/cm. Nanoscale depth-resolved defect measurements of complex oxides under room temperature and 80K applied electric field bias reveal that these fields can drive the movement of native point defects in real time. These preliminary results suggest an exciting new direction for understanding and controlling the properties of perovskites envisioned for a wide range of electronic and magnetic applications. Native point defects with energy levels within the band gap of complex oxides act as traps, recombination centers, dopants, and sources of RF dielectric loss. We now know that many of these imperfections are charged as well as mobile on a scale of hundreds of nanometers or more. The ability to measure these defects using nanoscale depth-resolved techniques and move these imperfections within complex oxides under electric fields enables a novel method to "refine" these materials, either removing them to improve interface transport and RF properties or to intentionally populate interface regions to increase doping densities. This exploratory work combining theory and experiment will establish a base on which to build proposals for, e.g., NSF Materials Engineering & Processing, DOE BES, and ONR.

Development of a Tactile-Sensing Bio-Complex Material for Engineering of Electronic Skin

PI: Liang Guo, Electrical and Computer Engineering

Complex materials are widespread in nature, and their intricate structure entails sophisticated functions. The objective of this project is to develop and characterize an artificial complex material, which incorporates the mechanoreceptor cells from *Mimosa pudica*, a sensitive plant famous for its rapid leaf movements when touched, as a tactile-sensing component, for fabrication of electronic skin. This tactile-sensing bio-complex material will be formed by crosslinking an aqueous mixture of

alginate and mechanoreceptor protoplasts. The protoplast's density and the alginate's porosity, pore size and stiffness will be tuned to meet the electronic skin design requirements. Mechano-electrical transducing dynamics of the mechanoreceptor protoplasts in alginate will be characterized with respect to desirable properties of a tactile sensor. This project will provide a framework for future materials research aimed at developing smart materials for a variety of applications, and motivate the team to examine other biological components as potential candidates for engineering novel bio-complex materials. This work will also enable further collaborative efforts at OSU to apply the tactile-sensing electronic skin to robotics, prosthetics, non-invasive physiological measurements, and wearable electronics.

Nanoscale Materials for Oxygen Sensing with Optically Detected Electron Paramagnetic Resonance

PI: Michael Poirier, Physics; Co-Investigators: Ramasamy P. Pandian, Physics; Vidya P. Bhallamudi, Physics; Chris Hammel, Physics

We propose to employ lithium-based naphthalocyanine, a material whose magnetic resonance linewidth varies with oxygen content, for much-needed, high spatial resolution mapping of oxygen content within cells. We are currently using optically detected magnetic resonance (ODMR) employing nitrogen-vacancy (NV) defect centers in nanodiamond, a technique that can sensitively resolve small magnetic fields. We request funding to develop the high resolution pulsed NV ODMR techniques needed to detect the weak magnetic fields generated in the vicinity of these micron-scale, ESR active, naphthalocyanine crystals. These techniques could enable spatially resolved oximetry by placing these crystals within cells.

Advanced Finite Element Approach for the Virtual Design of Functionally Graded Al/Al₂O₃ Reinforced Composites

PI: Soheil Soghrati, Mechanical and Aerospace Engineering; Co-Investigators: Marcelo Dapino, Mechanical and Aerospace Engineering

A new hierarchical interface-enriched generalized finite element method (hierarchical IGFEM) together with the genetic algorithm (GA) will be implemented for the virtual design of Al/Al₂O₃ reinforced composites fabricated using the ultrasonic additive manufacturing (UAM) process. UAM allows additively consolidating dissimilar materials such as Al foils and reinforced metallic prepregs via producing full-density metallurgical bonds between each layer. By tailoring the alumina content in the prepreg layers it is possible to achieve lightweight structures with selective reinforcement and functionally graded microstructure. The key challenge in the optimization and digital manufacturing of metal matrix composites using conventional approaches such as the standard FEM is to create finite element (FE) meshes that conform to the evolving morphology of the material throughout the computational design optimization process. To address this challenge, the hierarchical IGFEM will be employed as the main computational engine in this project, which will provide an automated framework for conducting high fidelity simulations using FE meshes that are independent of the composite heterostructure. A unique feature of this mesh-independent technique is the ability to accurately quantify stress discontinuities associated with modeling multi-phase problems with materials interfaces that are in a close proximity or contact. During the term of this project, a 2D hierarchical IGFEM solver will be expanded to 3D and equipped with a ductile elasto-plastic model to simulate the multi-scale nonlinear deformation of the metallic-matrix composite as it is being processed. This mesh-independent technique will then be integrated with a multi-objective GA code to evaluate the optimal design of the composite microstructure for potential application in brake rotors and armor sheets.

Fabrication of Patterned Protein Molecules Using Living Magnetic Microbes

PI: R. Sooryakumar, Physics; Co-Investigators: Steven Lower, Earth Sciences; Brian Lower, Environment and Natural Resources

We will develop a protein lithography system using magnetotactic bacteria, microorganisms with intracellular nanomagnets, as living pens that create and secrete protein ink. Placement of the ink will be controlled by exploiting the innate bacterial magnetite nanocrystals through a remotely activated

mobile magnetic tweezers system developed in the PI's laboratory. An effective system must be nontoxic, safeguard protein functionality, preserve biocatalytic properties, allow precisely patterned architectures, and enable time and dose-dependent placement of protein. Our approach is based on three principles: structure of designed magnetic domains, superparamagnetic properties of the microbe nanoparticles for positioning, and focused momentary electric fields for precise cell transfection. Expression of specific fluorescent proteins (colored inks) on the outer membrane of the organism (the pen) will be based on protocols of gene transfection and signaling within living organisms that were developed by the co-PIs. This hybrid system would allow fabrication of tailored submicron-scale biosensors and bioelectronics.

About the OSU Materials Research Seed Grant Program

The OSU Materials Research Seed Grant Program provides 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).

