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The ability of flow fields to strongly perturb molecular-scale structure in polymers has profound scientific and technological consequences. The nonlinear rheology of polymers is directly attributed to stretching and alignment of polymer molecules under flow. Materials with more complex internal structure?polymer blends, ordered block copolymers, polymer nanocomposites, for example?exhibit even more dramatic modes of flow-structure coupling. Further, polymer technology frequently hinges on the ability of flow fields during processing to impart molecular or microstructural anisotropy in the resulting product. X-ray scattering is a powerful tool for in situ structural studies during both flow and processing. To date, however, x-ray scattering methods have never been applied to well defined, homogenous extensional flows. Since extensional flows involve exponential stretching of fluid elements, they are dramatically more effective than shear flows at inducing molecular or microstructural alignment. These same characteristics make it notoriously difficult to produce homogenous extensional flows for laboratory testing. In this project, researchers at Northwestern will develop unique instrumentation that will allow, for the first time, in situ synchrotron-based studies of polymer structure development in well-defined uniaxial extensional flow. This experiment will be built around a proven, commercially available test fixture designed to facilitate extensional rheometry using conventional rotational rheometers. For synchrotron studies, this fixture will be integrated into a testing platform with computerized motion control and a custom-fabricated convection oven designed to facilitate x-ray access for both small- and wide-angle x-ray scattering. This instrumentation will open new vistas of scientific inquiry in virtually every class of polymer material that has been the object of flow-induced structure studies. Within this project, three specific application areas will be explored: (i) alignment of ordered block copolymers; (ii) particle orientation in polymer nanocomposites; and (iii) flow-induced crystallization of semi-crystalline polymers.

Solid oxide fuel cells (SOFCs) offer an important new option for converting fuels to electricity with increased efficiency, reduced pollution, and reduced greenhouse gas emissions. The race to reap the commercial and environmental benefits of this technology is largely being decided by practical issues, including cost and device reliability. The proposed project seeks to better understand how SOFC performance and reliability are linked to manufacturing methods and constituent materials properties, by the acquisition and analysis of three-dimensional images of the fuel cells. Such images can be used to determine what structures yield improved performance and hence reduced cost, find manufacturing conditions that yield the desired structure/chemistry, and examine the factors causing fuel cells to degrade over time. The improved structural and chemical information will be disseminated to the fuel cell research and development community where it will help enable critical connections, for example between industrial developers ? who need reliable performance/lifetime predictions ? and modelers ? who require good structural/chemical information to make such predictions. A substantial number of graduate and undergraduate students, in many cases from underrepresented groups, will receive training through this project. There are a number of other educational impacts, including high-school science teachers participating in summer research.

Results disseminated via publications could help facilitate a transition to new market structures that may lower the barriers to entry into the wireless services market thereby facilitating competition and

the introduction of new services. The infusion of the cross-disciplinary ideas developed through this project into graduate classes also broadens the training of graduate students.F NeTS: Medium: Design of Dynamic Spectrum Markets for Wireless Networksµ American Recovery and Reinvestment Act funds have significantly aided the research mission of Northwestern University by providing salary and wage compensation for individuals directly involved in ARRA-funded projects, both at Northwestern and at consortium institutions, as well as at the vendor organizations who provide goods and services in support of that mission. Northwestern has employed a standard methodology for determining jobs created or retained, based on revised guidance presented by OMB on 12-18-09 (ref. M-10-08). Jobs are reported in aggregate for the grant, comprised of calculated figures for hourly and salaried employees at Northwestern plus the reported jobs created or retained by subrecipients. The number of Northwestern hourly employees will be calculated as the number of hours charged to the grant during the quarter divided by the standard hours in a full-time schedule for the quarter. The number of Northwestern salaried employees will be calculated based on the salaries charged to the ARRA fund during the quarter. Following is a list of descriptions for jobs created or retained, in whole or in part, by this ARRA funded project:Post Doctoral Fellow,Research Assistant.

The research will study the economic experiences and related social processes of people living with HIV/AIDS (PLWHA), how their financial conditions and economic survival strategies evolve over time, and how these processes shape and are shaped by their health and well-being. This theorized relationship between economic survival strategies and health maintenance raises critical policy, programmatic, and societal questions about how researchers, policymakers, and society will address the epidemic?s next frontier: ensuring that the economic and social factors that increase the risk of HIV infection do not further hinder individuals? abilities to take care of themselves and contribute to their communities after diagnosis. HIV infections have risen particularly alarmingly among African American women in recent years, creating additional post-diagnosis economic and social challenges because of their social locations. This multidisciplinary, comparative ethnographic research project and integrated educational initiative will explore how living with HIV shapes the economic realities and related social experiences of infected women while educating students, the HIV services community, and the public about this important but often ignored facet of the fight against AIDS. The study will focus on 105 women living with HIV/AIDS who represent a diverse sample in terms of race, socioeconomic class, age, reported mode of infection, and time since diagnosis. The PI and a graduate student research team will conduct the in-depth interviews in order to build a large qualitative database on the economic survival strategies of women living with HIV, likely the first of its kind. The educational objectives will be accomplished through (1) the creation of a sociological research lab; (2) course offerings that include a service-learning exercise pairing undergraduate students with local AIDS Service Providers for educational event planning for clients and other stakeholders; and (3) a research dissemination apparatus that utilizes media, Internet technology, and traditional tools such as newsletters, fact sheets, policy briefs, books, and academic papers to inform multiple groups.

Novel experimental techniques are developed to investigate size-scale plasticity in one dimensional metallic nanostructures. Additionally, atomistic models of the experiments are proposed to pursue one-to-one comparison of deformation fields and fracture. The proposed research involves in-situ tensile experiments in the transmission electron microscope (TEM) on one-dimensional fcc crystal nanostructures which are characterized in terms of their atomic structure by high-resolution TEM. Atomic scale modeling of tested specimens will be used to validate existing EAM potentials. A computational framework will be formulated to identify criteria for yielding and failure of metallic fcc nanostructures under uniaxial loading given their initial atomic structure. Limitations in testing specimens of suitable size and atomic structure will be overcome by employing a previously developed nanoscale-material testing system based on micro-electro-mechanical systems sensing (MEM< S) and actuation, using protocols for sample fabrication and manipulation. Dislocation nucleation and/or activation will be identified and modeled atomistically for comparison. In order to address temporal and spatial resolution issues, high-speed TEM imaging will be carried out. Likewise, in order to capture material instabilities and failure, the MEMS technology will be extended to achieve load sensing with feedback control, which will ensure testing under displacement control. Boundary conditions on the atomistic models will be imposed in the form of displacement fields

obtained from TEM images taken during the experiments. The atomic rearrangement predicted will then be directly compared with the TEM observations at different strain levels. Deformation of the nanowires will then be modeled including the surface and internal defects experimentally observed. A systematic study will be carried out to develop a criterion capable of predicting nanowire strength and failure, given its size and atomic structure. Although very challenging, if successful this research will constitute a major step in the quest for connecting experiments and simulations at the atomic level.

This work promises to improve the state of the art in contract checking. Specifically, the PI will study the interaction between statically and dynamically verified portions of systems, in a manner similar to hybrid and gradual types. Building on this integration, the PI will also study how to integrate theorem provers into software systems in a way that the theorem prover's scope can be limited to just the most mission-critical parts of the system. The PI will also study how to add contracts to more sophisticated modularity mechanisms like traits and the ML module system, and explore how contracts can help generalize existing techniques for automatic test case and test oracle generation to support higher-order functions and unknown classes. All the while, the PI will ensure that these new techniques are practically viable by using them in a 500,000 line software system that the he maintains, as well as conducting detailed studies of how contracts are used in other settings, including JML and Eiffel.2 CAREER: Lightweight, Blame-Aware Contract Checking SP0004616 Franks,John M DMS-0901122 SP0004616-60024176¸ This is a project to investigate aspects of low-dimensional dynamical systems. The proposed research addresses the connection between algebraic properties of a group that acts on a surface in an area-preserving way and the possible topological nature of the dynamics of the action. One theme is to try to find global fixed points for a smooth group action and use the induced representation of the group into the automorphisms of the tangent space at the fixed point to conclude information about the action. Anticipated results from this project will advance our knowledge of dynamical systems and will explore new relationships between dynamics and algebra.

Broader Impacts: The project will prepare future researchers through the training of undergraduate and graduate students, and the mentoring of post-doctoral associates.K Collaborative Research: Semiclassical Methods for the Study of Spin Systems SP0004530 Geiger,Franz M ATM-0856428 SP0004530-60023981µ Understanding the chemistry of organic compounds that are part of atmospheric aerosols is crucial for assessing the impact that aerosols have on climate and the chemical composition of the atmosphere. Given the rich, well documented organic C=C double bond oxidation chemistry, and given the abundance of stereocenters in atmospherically important organic compounds, stereochemistry could play an important role in tropospheric chemical processing, including heterogeneous reactions on aerosol surfaces. However, surprisingly little is known about atmospheric stereochemistry. This project begins to fill this void by applying nonlinear optical spectroscopies, specifically second harmonic generation (SHG) and vibrational sum frequency generation (VSFG) to study the interaction of ozone with surface-active, tropospherically relevant chiral organic compounds, as they yield not only important spectroscopic, structural, and thermodynamic information with surface and molecular specificity, but also the kinetic parameters that are vitally needed for obtaining reliable climate change models. Real-time kinetic measurements, combined with surface spectroscopic studies, allow elucidation of < heterogeneous organic oxidation reaction mechanisms.

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