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Manufacturing of Novel Continuous Nanocrystalline Ceramic Nanofibers with Superior Mechanical Properties

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Project Objectives and Summary: This project is in the area of nanomanufacturing of advanced nanostructured materials. Nanostructured materials (NSMs) with unusual and extreme properties will play a key role in many emerging technologies. However, manufacturing of NSMs with the desired properties is highly complex and currently is over-reliant on empirical data. In this project, a novel manufacturing process producing a new class of ceramic materials, i.e. continuous ceramic nanofibers, is addressed. The novel sol-gel electrospinning technique (patents pending), invented recently by two of the PI's (Dzenis and Larsen), produces ceramic fibers of submicron diameters with potentially extreme thermomechanical properties. This technique is being analyzed and further optimized for the production of nanocrystalline ceramic nanofibers with superior mechanical properties, based on a comprehensive, multidisciplinary research effort. The research team develops an efficient and robust computational methodology for simulating realistic nanocrystalline nanofibers and their mechanical response at finite temperatures. A novel atomistic-continuum modeling approach based on a hybrid Monte-Carlo finite element technique is being developed and used. These models will be applied to design strong nanofibers by predicting the effects of the chemical composition and atomic structures of grain boundaries and defects on mechanical properties. The results will be used to develop chemistry and to direct manufacturing of strong nanocrystalline nanofibers. The achievement of the enhanced mechanical properties of the resulting nanofibers will be demonstrated experimentally utilizing novel mechanical characterization techniques based on scanning probe microscopy.

Notable Results to Date: Based on the analytical results from a related project, a numerical model of the electrospinning process has been developed. The model incorporates jet instabilities that have been shown important for nanofiber manufacturing. The model has been modified and used for modeling-based control of nanofiber deposition. The results have shown good agreement with experimental data. Pioneering methods of nanofiber alignment and controlled nanomanufacturing of 3D nanofiber assemblies have also been developed and are now being used to produce quantities of nanofibers. The new ceramic nanomanufacturing process has been used to produce nanofibers from multiple new ceramic systems including zirconia, alumina, and titania. World's first nanocrystalline ceramic nanofibers have been produced and are being evaluated. First principle-based method of calculation of mechanical properties of nanocrystalline fibers is being developed. A potential function of zirconia for large-scale molecular simulation of nanocrystalline zirconia has been developed and used to calculate elastic constants of single-crystal cubic, tetragonal and monoclinic zirconia. As elastic constants of monoclinic zirconia have not yet been reported, these first-principle data will be valuable as a benchmark for various simulation studies. The results have been used in conjunction with a model of polycrystalline fiber to compute properties of nanocrystalline nanofibers. Novel AFM-based characterization method, Atomic Force Acoustic Microscopy, has been further augmented

and used to evaluate elastic properties of ceramic nanofiber composites. A power series expansion has been used to derive simple expressions related to the vibrations of nonuniform cantilevers. The use of this expression for experimental data reduction is now underway.

Collaborations and Broader Impact: This highly interdisciplinary project is being performed by faculty from the Departments of Engineering Mechanics, Chemical Engineering, and Chemistry. In addition, collaboration has been established with NIST. Also, international collaborations have been established with researchers from Greece, Russia, Germany, China, and Spain. As a result of this research, the new nanomanufacturing method will be further developed based on the atomistic-continuum modeling. New nanocrystalline ceramic nanofibers with superior mechanical properties will be produced. The combined manufacturing and model-based optimization will allow the mechanical properties of the nanofibers to be tailored to specific needs of the end user. This general, modeling-driven approach will be applicable to other nanomanufacturing processes and nanomaterials. This technology will be a significant part of future nanotechnology efforts. This research program will impact other key areas of nanotechnology where radical improvement of mechanical properties is critical, *e.g.*, nanostructured membranes for ultrafiltration and other separation processes, nanoreinforcing elements for nanocomposites, supports for nanostructured catalysts, and many others. Several interdisciplinary graduate courses that are being developed by the PIs will further enhance multidisciplinary education of graduate students on materials synthesis technology, computational materials science, and nanoscale materials characterization. Collaboration of graduate and undergraduate research assistants from different research groups on computational and experimental aspects of the research further contributes to their interdisciplinary training. Interactions with researchers at national laboratories and international partners provide graduate and undergraduate students with additional educational exposure.

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