Reduced Degree of Freedom Predictive Methods for Control and Design of Interfaces in Nanofeatured Systems

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Research Background: The promise of nanofeatured systems is being realized in critical technologies that include

- Tough nanocrystalline metals,
- nanotemplated Li / V_2O_5 nanocomposite batteries,
- fuel cells with nanostructured electrocatalytic materials,
- computing/sensing systems using quantum dots.

A common feature of these technologies is the presence of nanoscale solid interfaces. For quantum dots, stresses at interfaces drive self-assembly. For nanocrystalline solids, interfaces trap dislocations while allowing grain boundary sliding. For energy storage, interfaces produce large surface areas and channels for ion motion, as well as separate regions with different electrical properties that can control conductivity.

Taking further advantage of the unique functionalities of nanofeatured solids requires accurate, predictive computational tools that span multiple time and length scales. Our work is focusing on developing limited degree of freedom (LDF) models that connect quantum to continuum mechanics across disparate time and length scales.

Research Team: Our NIRT is an interdisciplinary effort between theoreticians and modelers from the NC State Departments of Physics, Materials Science, Mechanical Engineering, and Electrical and Computer Engineering. Our team embodies the inter-disciplinary nature of the NIRT program in several crucial ways. Our team

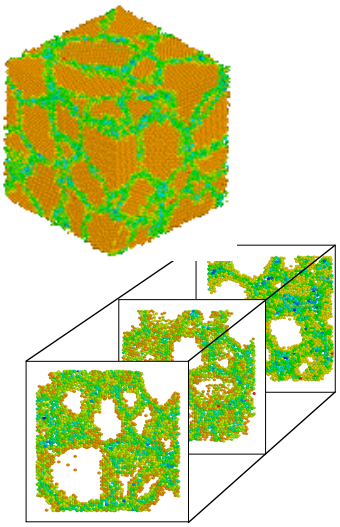
- has complementary expertise spanning accurate state-of-the-art DFT calculations and quantum formalisms to continuum-based materials modeling methodologies;
- comes from 2 colleges & 4 departments, and has an outlook that embodies both engineering and basic science interests;
- is composed of two senior faculty, a new faculty member, and two rising mid-career PIs. Members bring different levels of experience and career perspective.

Education: We are developing an educational program that trains students to link and implement computational methods **independent of discipline** to relevant spatial and time scales. The basic science community has focused on a "materials by design" goal in which total energy methods predict atomic arrangements/compositions for desirable properties. The engineering community has focused on phenomenological models that naturally span engineering time and length scales. These communities and their associated methods must converge in an effective manner to make meaningful advances in LDF models. To this end a web-based graduate course designed to train the next generation of scientists and engineers in the principles

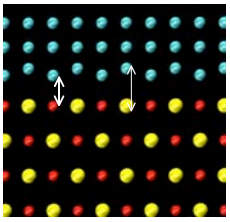
of modeling methods across length scales has been developed. The topics covered, which range from fundamental quantum mechanics to continuum models of dynamic plasticity, provide a more comprehensive overview of modeling methods than can be taught within a single discipline, thereby giving students the broad outlook needed to attack modern problems in materials science and engineering. The course is taught as part of the NC State distance education effort and is available through the web. Educational materials associated with this course include ~30 hours of streaming lectures and almost 800 associated overheads, plus assignments and spreadsheet simulations that provide hands-on experience with example calculations.

Research Projects: The following sections describe some of the current research efforts that are being carried out by our NIRT.

Nanostructure Solids: Our experimental collaborators have recently produced copper with nanometer-sized grains that has a yield strength almost twice that of high-strength low-alloy steels. To better understand the deformation mechanisms that lead to this unique property, we are using molecular and continuum simulations to model the yielding of copper and aluminum samples with microstructures that are representative of nanocrystalline materials. Parameters and validation data for the analytic force expressions are generated from first principles calculations. The figures to the right illustrate a structure created by simulated grain growth. The atoms in each figure are colored by their coordination. The bottom figure illustrates "slices" through the material that allow visualization of the interior. In these images atoms whose number of nearest neighbors match the pure lattice have been removed, allowing better visualization of the grain boundaries. The competing roles of grain sliding vs. dislocation motion, the effect of grain orientation and grain size, and the influence of trace impurities on deformation mechanisms and the resulting mechanical properties of these systems are being characterized.

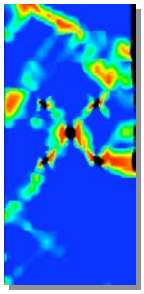


Metal-Oxide Interfaces for Novel Structural and Electronic Materials: Studying metal-oxide interfaces is fundamental to understanding the behavior of nanosized metal particles embedded in a dielectric matrix. The search for novel mechanical and electronic properties of these systems is intrinsically a multi-scale problem. Prof. Marco Buongiorno-Nardelli and graduate student Matias Nunez are using first principles methods to determine the geometry and electronic behavior of interfacial structures in metal-oxide complexes. The figure to the right illustrates a SrO/Cu interface. The results of this study are being integrated into atomistic and mesoscale models to explore novel mechanical and optical properties of composites containing this class of nanofeatured material.



Multiscale Prediction of Material Failure using Hierarchical Coupling of Modeling Methods: A hierarchical approach combining a multiple-slip dislocation-density based crystalline constitutive formulation, grain boundary interfacial kinematics, failure criteria, and specialized finite-element modeling techniques together with molecular dynamics predictions of local grain boundary structure and dislocation nucleation is being developed to

- predict and validate failure paths in porous aggregates with grain boundaries/subgrains at different scales
- identify transmission and pile-up regions that lead to bands of strain accumulation and stress concentration
- engineer and control grain-boundaries in nanocrystalline materials for regimes ranging from nanoporosity nucleation to specimen rupture.



The figure to the right illustrates porosity contours at 8% normal strain for a small-sized void cluster calculated at the continuum scale using our modeling approach.

Quantum Studies: Our team has been studying the quantum-mechanical behavior of nanocomponents embedded in a dissipative environment. An interacting harmonic oscillator and angular momentum oscillator are utilized to simulate the interaction of an electromagnetic field mode with an atom in an embedded micro or nano cavity to provide atomic transitions in absorption and emission; as the cavity boundaries are influenced by a surrounding environment, the cavity modes are perturbed thus influencing the transition characteristics. The objectives are to study the nanocomponent-environment interaction, and to provide adequate modeling capability for elucidating the robustness of the nanocomponent quantum characteristics due to the interaction with the environment

References

[1] For further information about this project link to **<www.mse.ncsu/nirt/>** or email **<brenner@eos.ncsu.edu>**