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Plenary Talks

Irradiation resistant materials for extreme environments

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The strategy for developing radiation resistant materials has long been recognized: introduce high concentrations of traps and unbiased sinks into the microstructure to enhance recombination and bubble nucleation. While these methods have been attempted in the past, they suffer from the fact that such nanostructured materials are generally unstable under irradiation. Nevertheless, progress is being made in developing new nanostructures materials that are showing remarkable stability. In this lecture, I will discuss these various directions, with emphasis on work at Illinois that explores immiscible alloys that self organize under irradiation. I will also discuss how these materials might be processed using the similar concepts of self organization during severe plastic deformation.

Modeling Failure, Fatigue and Fragmentation

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Failure of heterogeneous due to fatigue and subsequent fragmentation are ideally modelled by stochastic networks made of beams, springs or similar elements. Fibre models are the simplest description for failure. They are based on the probability distribution of broken fibres. The load redistribution after a fibre yields can be global or local and the first case can often be solved analytically. We will present an interpolation between these the local and the global case and apply it to experimental situations like the compression of granular packings. Introducing viscoelastic fibres allows to describe the creep of wood. It is even possible to deal analytically with a gradual degradation of fibres and consider damage as well as healing. In this way Basquin's law of fatigue can be reproduced giving good agreement with measurements of asphalt samples in Brazil tests. The histograms of bursts and waiting times reveal universal laws that are independent on the material. The fragmentation of solids is important in industry and geoscience. Using a combination of Discrete Element Method and beam networks it becomes possible to simulate the cracking and detachments of fragments in diverse geometries. We studied impacts against walls, particle-particle collisions, explosions of bulk objects and of shells, milling and crushing under cyclic load. Besides purely brittle failure under traction or bending we also studied plasticity under compression or under shear. We find the existence of a critical energy below above which no fragment having a size of the order of the original sample survives. This critical point is dominated by power laws in the fragment size distribution and a divergence of the ratio between the second largest and the largest fragment. This exponent depends among others on the dimension of the object. We also study the distribution of velocities and directions of the fragments and the dependence of their shape on the material. Later question is of relevance for space debris. The numerical results are compared to experiments.

Molecular Organization, Dynamics and Dissipation in Nanojunctions, Nanofluids and Membranes

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The arrangements of molecules in thin films confined in a gap between solid boundaries, layering transitions, solvation forces versus gap width, and segregation effects in mixtures of long and short molecules, as well as straight chain and branched alkane films, will be discussed. The effects of surface morphology, that is smooth versus rough confining surfaces, on the structure, dynamics, diffusional characteristics, and tribological properties of the confined films, with and without shearing motion, will be highlighted. In the second part of the lecture we discuss structural, dynamical, and rheological properties of water films of variable thickness confined between a solid tip and a lipid bilayer membrane (DPPC), as well as force vs. distance curves in this system. Finally, we describe trans-membrane transport processes investigated with large-scale molecular dynamics simulations of immersed capillary nanojet injection of a liquid through a lipid bilayer membrane, illustrating membrane puncture and subsequent self healing processes.

Energy barriers and hysteresis in martensitic phase transformations

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joint work with R.D. James and Z.Y. Zhang

We report results from a systematic program of alloy development in the system TiNiX , $X = \text{Cu, Pt, Pd, Au}$, to pursue certain special lattice parameters that have been identified previously with low hysteresis. We achieve $\lambda(2) = 1$, where $\lambda(2)$ is the middle eigenvalue of the transformation stretch matrix, for alloys with $X = \text{Pt, Pd, Au}$. In all cases there is a sharp drop in the graph of hysteresis vs. composition at the composition where; $\lambda(2) = 1$. When the size of the hysteresis is replotted vs. $\lambda(2)$ we obtain a universal graph for these alloys. Motivated by these experimental results, we present a new theory for the size of the hysteresis based on the growth from a small scale of fully developed austenite martensite needles. The energy of the transition layer plays a critical role in this theory. Overall, the results point to a simple systematic method of achieving low hysteresis and a high degree of reversibility in transforming materials.

Multiscale Analysis as an Approximation Scheme

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The development of microstructure and the attendant effective or macroscopic behavior of materials may often be understood as the material's ultimately futile attempt to minimize a certain functional which has no minimizer. In the pursuit of this unattainable objective, the material develops fine nested structures often spanning the atomistic and many continuum scales. A number of 'multiscale' analytical and computational tools have been devised in order to study these material systems. For the most part, such schemes are computational in nature and ad hoc, in the sense that they offer no clear notion and guarantee of convergence to an exact solution. For systems with well-separated lengthscales, a well-developed mathematical theory, the 'modern calculus of variations', offers scientists and engineers a radically different and powerful way of thinking about what it means to 'solve' multiscale problems and approximate their 'solutions'. In particular, within this modern calculus of variations framework multiscale analysis is a rigorous approximation scheme with a well-defined notion of convergence. I plan to illustrate the challenges and opportunities that this analysis framework offers by way of selected examples of application, including: the atomistic-to-continuum transition in molecular statics; discrete-to-continuum transition in dislocation dynamics; subgrain dislocation structures in polycrystals; and the time-evolution of surface roughness in thin films.

Theory of dynamical response of live cells to mechanical stresses

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Recent research at the interface of physics and biology has shown that cellular processes such as proliferation, differentiation and tissue development, are controlled by the mechanical properties of cells and their environment. This talk reviews current experiments on cell mechanics in the context of theoretical models in which cells are treated in terms of active force dipoles. The theory includes non-equilibrium cell activity (related to the fact that the cell is “alive”), local mechanical equilibrium, and random forces to determine cell response to static and dynamic stress, as well as the curvature of the substrate. To understand how substrate rigidity determines the polarization of cells, we have generalized the treatment of elastic inclusions in solids to “living” inclusions whose active polarizability, analogous to that of non-living matter, results in feedback in response to matrix stresses. We use this to explain recent observations of the non-monotonic dependence of stem cell polarization on matrix rigidity. Similar considerations are used to study the ordering of dipoles and are applied to the dependence of muscle striation on substrate properties. These findings provide a mechanical correlate for the existence of an optimal substrate elasticity for cell differentiation and function.

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The Role of van der Waals Interactions in Physics, Chemistry, and Biology; Insights from DFT and Beyond

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Van der Waals (vdW) forces are crucial for the formation, stability, and function of molecules and materials. At present, ubiquitous vdW interactions are absent from essentially all local-, gradient-corrected, and hybrid functionals of density-functional theory (DFT). Recently we have developed an efficient method to obtain an accurate description of the long-range vdW interactions in terms of adding simple, pair wise $C6[n]/R6$ terms, where $C6[n]$ is a functional, calculated from either DFT or Hartree-Fock: The so called DFT+vdW [1] and the MP2+ Δ vdW [2] approach. In particular the latter has an accuracy close to that of the “gold standard” of quantum chemistry, namely CCSD(T).

We will briefly sketch the theory, also comparing it to other methodology, as for example Møller-Plesset perturbation theory, the vdW-DF (density functional) [3], and the highest level DFT approach, namely exact exchange plus correlation treated in the random phase approximation (EX+cRPA).

Examples to be discussed include bulk crystals, surfaces, organic/organic and organic/inorganic interfaces, and the unfolding dynamics of polyalanine helices.[4]

In all case it is found that vdW interactions play a noticeable if not crucial role, not just for quantitative values but also for the qualitative behavior.

[1] A. Tkatchenko and M. Scheffler, Phys. Rev. Lett. 102, 073005 (2009).

[2] A. Tkatchenko, et al., J. Chem. Phys. 131, 094106 (2009).

[3] M. Dion, et al., Phys. Rev. Lett. 92, 246401 (2004).

[4] A. Tkatchenko, M. Rossi, V. Blum, J. Ireta, M. Scheffler, to be published.

Computations and Experiments in Four Dimensions

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Recent advances in computational and experimental techniques now permit the evolution of a microstructure to be determined in three dimensions and as a function of time. Since x-ray tomography is nondestructive, it is possible to employ an experimentally measured microstructure as an initial condition in a simulation and to then compare the predicted structure to that measured experimentally at some later time. The comparison between simulation and experiment therefore does not require the use of statistically averaged quantities. Such an approach is thus a particularly stringent test of simulation and can be used to identify important phenomena that are lost in the averaging process. We shall illustrate this approach using experiments and simulations of solid-state grain growth and the evolution of solid-liquid mixtures during coarsening.