

Phase transformations and thermodynamics

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Several broad trends have emerged as we explore the mechanical behavior of nanostructures. The studies of phase transformation, fracture and deformation are converging. These phenomena appear to be distinct at the macroscopic scale. At a microscopic scale, however, they are variations of a single theme: the collective behavior of atoms. Also convergent are traditionally different disciplines such as thermodynamics, kinetics and mechanics. A unifying concept is the energy landscape, which contains both thermodynamic and kinetic information. External forces modify the energy landscape. Another unifying concept is to view structural evolution as a sequence of configurational changes driven by thermodynamic forces. In addition to more familiar forces of push and pull, other thermodynamic forces come from entropy, elasticity, electrostatics, phase separation, phase boundaries, van der Waals interactions, etc.

The presentations at the workshop sampled recent advances in the field. The energy landscape is a function of a large number of coordinates. A construction of the full energy landscape is prohibitively time-consuming for most phenomena of interest. Techniques now exist to compute the minimum energy path on the energy landscape, which connects one local minimum, via a saddle point, to another local minimum. Dislocation nucleation and crack extension have been studied this way. Thermodynamics and mechanics, in combination, have

been used to study self-assembling nanostructures. The phase field model can now simulate realistic microstructures in alloys. Efforts are underway to link such microstructural simulations to thermodynamic data banks, and to the mechanical behavior of alloys. First principles methods have been used to study the energetics of atomic clusters, the structures that are far beyond the reach of continuum mechanics. Stress-induced phase transformations have been studied experimentally and theoretically. Phase transformation can give rise to large deformation, and is a basis for active structures. A continuum theory is presented to couple Stokes's creep with Herring's diffusion. In nanostructures, surface energy and surface stress often play prominent roles, as the fraction of atoms on the surface is large.

The participants also speculated on likely progress in coming years. Deformation localization will be studied at the atomic scale. First principles calculations will be more widely used to study electronic effects on mechanical behavior. We will see more coupled actions of mechanics and chemistry. Few engineering problems are solved by computation alone. The pragmatic approach is to divide the labor between computation and measurement. Some quantities are easier to compute, others are easier to measure. A combination of computation and measurement solves problems economically. Of course what is easy changes with circumstances. As new tools and applications emerge, it behooves us to renegotiate a more economical division of labor. This is a time of renegotiation. Great progress will be made to link computations more intelligently across scales, and with experiments.

In a traditional mechanics education, thermodynamics and kinetics rarely play a part. This situation will change in coming years. The impetus comes from a confluence of new tools, new questions, and new applications. The affordable computers have opened new ways to study most phenomena. The new instruments, such as the scanning tunneling microscope, have

brought us to an intimate contact with individual atoms. Like traditional mechanics, traditional thermodynamics studies macroscopic structures. For nanostructures, we are interested in local processes. Many thermodynamic properties become size and shape dependent. Both mechanics and thermodynamics have long played active roles in manufacturing, such as metal forming, ceramic sintering, and rapid prototyping. Together, mechanics and thermodynamics will play active roles in nano-manufacturing.