Report of the Discussion on Plasticity and Modeling
Workshop on Nanomechanics
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1. Progress in nanoscience and nanotechnology needs contributions from *all* the natural sciences: physics, chemistry, biology, and engineering. For researchers in materials science and in applied mechanics there are many new opportunities and they bring *unique* expertise to the enterprise. These are some of the contributions that only they can provide:
(i) an understanding of microstructure and its relation to properties;
(ii) developing a phenomenological and theoretical understanding of the constitutive relations of mechanical behavior on the nanoscale;
(iii) connecting phenomena on the nanoscale, through the intervening scales, up to the macroscopic scale.

2. The strong activity in analysis (theory and simulation) needs to be balanced by an increase in ***experimental*** work. Needed are experiments specifically designed to reveal underlying mechanics. Mechanical testing on the nanoscale is a challenge. New ways of fabricating samples (lithography, focused ion beam,...), new ways of loading them (AFM, optical tweezers, ...), new and more precise ways of measuring stress and strain, and new ways of observing the samples (high-resolution electron microscopy, AFM, atom probe, ...) *in* or *ex situ*, should be broadly considered. Different modes of deformation (tension, compression, shear, bending, wear) give complementary information. There is much room for clever and innovative experimentation.

There should be more testing as a function of strain rate and temperature to reveal underlying mechanisms. Nanoscale testing at elevated or low temperature is difficult, but solution of the experimental problems is particularly worthwhile given the broad kinetic window offered by variation in temperature.

Nanoindentation remains one of the main tools of the field. New ways should be found to make direct observations or *in situ* measurements of the area of contact between indenter and sample. Much can be learned as well from detailed comparison of the experimental load-displacement curves with the results of discrete dislocation simulations.

3. Some aspects in the ***modeling*** of plasticity in nanostructured materials have received insufficient attention. An example is the modeling of "nonlinear" events in the kinetics of dislocation motion: formation of nodes, entanglement, or formation of cells. In the interest of computational efficiency, such events are treated as "black boxes": the initial and final states are specified, but the specific path between them is left unspecified. More specific rules and computational exploration of the kinetic path inside these "boxes" are highly desirable.

A further example is the use of dislocation theory with continuous space- and time-dependent variables, such as the dislocation density tensor and the velocity vector. This approach represents a length scale intermediate between those of discrete dislocation modeling and continuum mechanics. The main issue in the development of continuum dislocation theory is the appropriate averaging of the quantities in discrete dislocation modeling.

4. As sample size or microstructural length decrease, ***surfaces and interfaces*** become increasingly important, and they can have substantial effects on plasticity. For example: How is the nucleation of dislocations affected by the topology (roughness, steps), energy (including orientation), chemistry (including contamination) and stress of the surface ? Is subsurface plasticity distinct from that in the bulk (e.g., is there a dislocation-free zone) ? Under what conditions does the formation of stacking faults or twin boundaries become important alternative responses to shear loading ?

5. The small ***volume*** of a sample or a grain limits the nucleation probability of dislocations. For quantum structures, which need to be defect-free to function, understanding these probabilities in detail is essential. In polycrystalline systems, nucleation of dislocations at grain boundaries, especially with limited area, remains largely unexplored. The shear of an entire small grain by the passing of the dislocation can be usefully considered as a "quantum event" in a description of the overall plasticity of nanosize polycrystals.

6. The ***fabrication*** of nanostructures is often a mechanical process or contains important mechanical steps. Clear examples are the production of very small grains by comminution or abrasive wear. The study of plasticity at very high strain rates can contribute to a quantitative understanding of these processes. Planarization is an essential ingredient of contemporary microfabrication; the chemical and mechanical processes in nanoplanarization remain a fruitful areas of technological and scientific research. There are many fascinating new areas of nanofabrication where the exploration of the mechanics has only just begun, such as nanowelding, nano-imprinting and stamping, and the many forms of adhesion on the nanoscale.

7. The study of the plasticity of ***soft materials*** is well developed for polymers, but is only just beginning for colloids, membranes and many biological materials. It should be explored to what degree the insights from the more mature study of plasticity (experiments, theory, simulations) in metals and semiconductors can be transferred usefully to some of those soft materials.