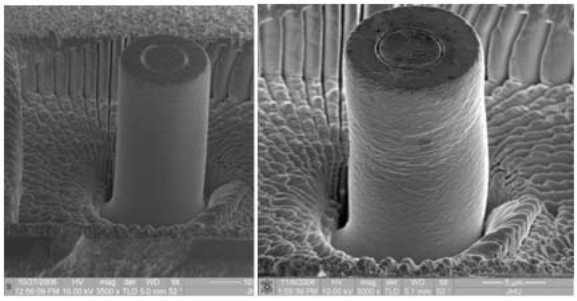
Nanomechanics of Metal Plasticity of Thin Films and Cylinders

Just as small-scale flying machines and microfluidic channels behave far differently than their large-scale counterparts, microscopic mechanical parts and metal films present unique design challenges not observed at a larger scale. Properties such as particle size, microstructural features, and film thickness take on a greater importance with respect to mechanical properties, impact resistance (or impact effectiveness), behavior under stress, and modes of failure. Thus, microscopic devices cannot be designed simply by scaling down their macroscale counterparts, even if they are made from the same materials.

Material properties, including yield stress and defect propagation, at or below the micron scale (0.001 mm; a human hair is about 25 microns across) are not well understood, especially under rapid deformation and high strain rates, where experimental data is difficult to obtain. Particle sizes and surfaces play a greater role in components that are on the same size scale as individual grains. High-performance computer modeling and simulation offer capabilities for predicting and understanding such behaviors, which in turn, can guide the rational design of new materials and configurations.

Wei Cai, assistant professor of mechanical engineering at Stanford University, is working with research associate Sylvie Aubry and graduate students Christopher Weinberger and Jie Yin to develop metal microstructure modeling capabilities under the AHPCRC program. Their research follows two main directions: the response of metal micropillars under tensile and compressive deformation, and thin metal films that undergo tensile or cyclic (fatigue) loading conditions.

Cai and his group are developing modeling capabilities using a method called dislocation dynamics (DD), which tracks defect motion through a crystal lattice. They are comparing their results with those obtained using molecular dynamics (MD) modeling, which characterizes the behavior of atoms and small ensembles of atoms, with the intent of bridging these two methods and the length scales to which they apply.



Scanning electron micrographs of nanocrystal BCC tantalum micro-pillars (about 5 microns diameter) before and after a compression test. Courtesy Qiuming WEI, University of North Carolina at Charlotte, Department of Mechanical Engineering, in collaboration with ARL's Brian Schuster.

Shear Banding

Impact studies on metal parts, including vehicle panels and projectile tips, have turned up a microscale phenomenon called adiabatic shear banding (ASB). This, in turn, has provided important insights into why metallic parts bend and break. Shear bands act as sites for future failures. Voids and other defects appear in the shear bands after a shock event, as the material recovers in its deformed state.

Shear bands form in metal when the stress and deformation are localized into a small area. "Adiabatic" refers to the absence of heat transfer: strain rates are so high that there is not enough time for the heat to diffuse away from the deforming zone, causing a local softening of the metal. Formation of ASBs helps the tip of a projectile tip penetrator stay sharp during impact, because thin layers of metal shear off as the projectile penetrates the target. Shear bands are a detrimental feature for armor parts or machine parts that experience repeated shocks (forging, impact, electromagnetic forming, etc).

ARL-sponsored research found that ASBs form in certain body-centered-cubic (BCC) metals when their grain size is below 1 micron (*See "Anatomy of a Dislocation," page 16*). FCC metals do not exhibit this property. The origin of this size effect is still under debate.

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Nanomechanics of Metals

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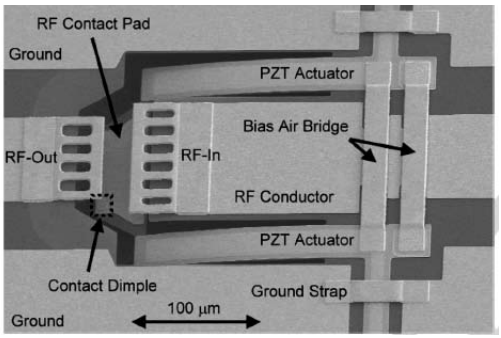
Researchers Brian Schuster and Reuben Kraft (ARL Weapons and Materials Research Directorate) want to understand the mechanical properties of BCC metal nanocrystals, in order to design better armor materials. As a way to characterize these materials, they perform compression and tensile tests on micro-pillars cut from BCC metal nanocrystals. They are searching for material systems that combine high strength, the ASB mechanism, and tensile ductility. They are studying the effect of the grain boundaries on mechanical strength, and they have observed that fine-grained metals experience more ASB than do more coarse-grained metals.

Cai's group is doing dislocation dynamics simulations for micro-pillars made of single crystals. Both research groups are coordinating their studies on micro-pillar deformation, so that the computer simulations and experimental measurements can be compared to each other.

MEMS Actuators

Microelectromechanical systems (MEMS)—tiny machines made of sensors and actuators a few microns in size—have been finding increased application as switching devices, components in consumer electronics devices, miniature sensors, and telecommunications equipment. Because of the small size of MEMS devices, electrostatic and surface effects take precedence over such macroscale properties as inertia or thermal mass. MEMS devices can be manufactured using technologies similar to those used for computer chips. Multiple thin-film layers are deposited on a rigid substrate, then etched or micromachined into gears, cantilevers, and channels.



Multilayer MEMS device with piezoelectric lead zirconium titanate (PZT) actuators coated above and below with thin platinum films. Micrograph courtesy Dr. Madan Dubey, ARL.

Dr. Madan Dubey's group at ARL is developing a multilayer MEMS that uses thin films of PZT (lead zirconium titanate, a piezoelectric material) as the actuating material and platinum metal as the electrode. The thickness of the platinum film layers determines how many actuation (bend-and-release) cycles they can undergo before an accumulation of dislocation defects causes metal fatigue and failure. Understanding dislocation dynamics in metal and semiconductor thin films is important for ensuring the reliability of these novel MEMS and electronic devices.

Modeling Tools

Micro-compression experiments on individual pillars have shown that the amount of stress necessary to sustain plastic deformation increases dramatically from the bulk value once the pillar diameter drops below one micron. That is, it takes more force applied to a given cross-sectional area to induce plastic deformation of a micro-pillar than for a macroscopic pillar. This is a size effect that is beyond the scope of conventional plasticity theory and constitutive models (which describe the response of a material to external forces). The physical basis for this effect is not well understood, but it is widely accepted that explicit large-scale defect dynamics simulations are more faithful to the underlying physics, provided that the computer program is able to handle a sufficient number of defects for a long enough time.

The main challenge in predicting materials strength by computation lies in the gap, roughly 10^{-9} to 10^{-3} m, between the fundamental physics of atoms and phenomenological models of a continuum. To this end, the dislocation dynamics (DD) simulation method was invented, with the goal of directly computing the plastic strength of crystals in terms of the motion of their dislocations. This vision has not yet been realized because of the tremendous number of dislocation seg-

ments that must be included in a statistically meaningful simulation.

The main challenge in applying DD simulation to metal micro-samples is the need to account for the image stress produced by the free surfaces. Existing DD simulations in micropillars and thin films do not have an efficient image stress solver and do not scale well on large number of processors.

Cai and his co-workers at Lawrence Livermore National Laboratory have developed a publicly available, massively parallel dislocation dynamics simulator called ParaDiS (Parallel Dislocation Simulator, http://paradis.stanford.edu), with the intention of overcoming many of the problems associated with conventional dislocation dynamics programs. By using thousands of processors simultaneously, ParaDiS has, for the first time, successfully captured the strain hardening behavior of a 10μm^3 representative volume in a bulk metal. It runs routinely on 100–1000 processors, including Stanford's local cluster SU-AHPCRC and the Navy DSRC Cray XT5 EINSTEIN. The scalability of ParaDiS has been demonstrated on the 132,000 processors of the BlueGene/L supercomputer. Thus, ParaDiS can take advantage of more parallel computing power as it becomes more readily available in the near future.

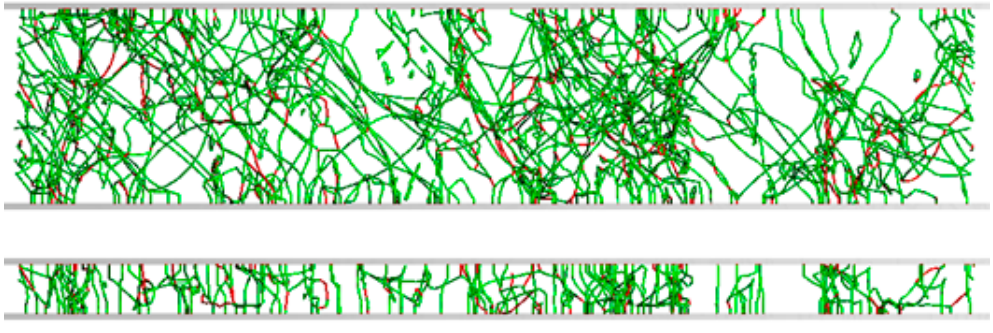
Under the AHPCRC program, Cai is developing numerical algorithms and computer programs (implemented in ParaDiS) that allows DD simulation of thin films and micro-cylinders. An efficient image stress algorithm has been implemented in ParaDiS for thin film and cylinder geometries. The thin film algorithm is also working in parallel.

Cai is conducting a quantitative comparison between DD and MD simulations of dislocation behavior in thin films and micro-cylinders. The DD and MD predictions on dislocation equilibrium angles in thin films agree well with each other. DD and MD predictions also converge on dislocation behavior (self-multiplication) in micro-cylinders.

Future work

Efforts are underway to understand the size effect in plasticity of thin films and micro-pillars undergoing uniaxial loading and bending, using large-scale DD and MD simulations. Dislocation–grain boundary interactions are being incorporated into the DD model, assisted by insights from MD simulations. Another observation from MD simulations, the kink pair mechanism of dislocation motion in BCC metals, will also be incorporated into DD. A quantitative comparison between DD and MD simulation predictions and laboratory micro-tensile tests of single-crystal and bicrystal BCC pillars is planned for the coming year.

ARL scientists are constructing a lab setup for tensile and compression tests of micron-sized metal pillars to enable direct comparison between model predictions and experiments. ✯



Dislocation models for metal films under tension. Top: thicker film has dislocations in many directions. Bottom: dislocations are preferentially aligned in a thinner film. ParaDis simulation courtesy Dr. Wei Cai, Stanford University.

Anatomy of a Dislocation

Metallic elements and alloys exist as crystalline materials: orderly three-dimensional arrays of atoms that form small particles called grains. Metallic grains adhere to one another to form the macroscale structures we recognize as paper clips, coins, gears, and sheet metal. Thin metal films and microscopic metal devices are only a few grains across, and they behave very differently from their larger counterparts.

Metals differ from other crystalline materials such as ceramics or gemstones in their ability to deform—bend, flatten, or be drawn into wires—without breaking. Planes of metal atoms glide past each other like layers of ball bearings and settle into new positions that maintain the overall integrity of the crystal structure.

This process is not perfect, however. Each time a piece of metal bends, planes of atoms slip past each other. In the process, some of these planes become misaligned to form structures called dislocations. Dislocations can travel through the structure, and when enough of them accumulate, a crack forms. In thin metal films, the distance from the interior to the surface is small, so the interaction of dislocations with the surface becomes a driving factor. Dislocations that reach the surface of the metal disappear, or "exit," but can leave behind various types of structural imperfections, depending on the metal's crystal lattice structure.

Two common structures for metallic crystals are body-centered cubic (BCC) and face-centered cubic (FCC). Metals with a BCC structure, including tungsten, chromium, and molybdenum, tend to be strong and moderately ductile. Soft, ductile metals such as aluminum, copper, nickel, and platinum assume an FCC configuration. (Brittle metals such as zinc, titanium, and magnesium take on a third structure, not addressed under the current AHPCRC project, known as hexagonal close packing.)

A moving dislocation (pinned at both ends) encounters an immobile dislocation near its glide plane. The moving dislocation cross-slips to a different glide plane to bypass the obstacle. Image courtesy Dr. Wei Cai, Stanford University.

Metal micropillars are convenient stand-ins for macroscale test bars when the compression tests are performed at a very small scale. "Forests" of micropillars can be grown and cut from a thin film on a substrate using focused ion beams. Micro-tensile tests are much more challenging because one has to machine "grips" on top of the micro-pillar so that a holder can grab the pillar and pull on it.

Using Molecular Dynamics and Dislocation Dynamics simulations, Wei Cai's group has discovered a counter-intuitive behavior of dislocations in BCC pillars. When stress is applied to BCC pillars, dislocations do not simply exit the pillar (as they do for FCC pillars). Instead, the dislocations self-replicate and send other dislocation moving in the opposite direction before the first one exits the surface. This means that a single dislocation nucleation event in a BCC pillar can produce a larger amount of plastic deformation than for a corresponding FCC pillar.

It is very difficult to verify these simulation results directly from in situ experiments, but some research groups have started to design experiments that could ultimately test this prediction.

Reference

Surface Controlled Dislocation Multiplication in Metal Micro-Pillars. C.R. Weinberger and W. Cai, *Proceedings of the National Academy of Sciences, 105,* 14304–14307, 2008. doi:10.1073/pnas.0806118105