Deformation of Nanostructures

I.A. Ovid’ko

Materials based on nanometer-sized structural elements exhibit unique electronic, optical, magnetic, and mechanical properties, opening up a range of new applications (1, 2). The mechanical behavior of nanocrystalline materials—solids composed of nanometer-scale crystallites divided by interfaces (see the figure)—is of particular interest. Such materials are often extremely hard and brittle, but several examples of substantial ductility under mechanical load have been reported (3). Some nanocrystalline metals, ceramics, and alloys even exhibit superplasticity—the ability of a solid to endure large elongations (100% or more) without failure—at relatively low temperatures and high strain rates (4, 5).

These remarkable mechanical properties of nanocrystalline materials are highly desirable for structural applications. To optimize the mechanical behavior, it is important to identify its underlying mechanisms. One of these mechanisms has now been revealed in an atomic-level experiment. On page 2433 of this issue, Murayama et al. (6) provide evidence for a rotational deformation mechanism (see the figure), considered in theoretical models (7, 8), which resembles turbulence in fluids as well as the formation of rotational vortices in liquid crystals, superfluids, and magnetic and biological systems (9).

The appearance of rotational phenomena in deformed nanocrystalline materials can be understood in terms of their structural peculiarities. The materials are composed of nanometer-scale crystallites (grains) divided by interfaces (grain boundaries) (see the figure). Each crystallite is intermediate in size between individual atoms and conventional microstructures, leading to distinct properties. In addition, each crystallite is so small that a large fraction of its atoms (up to 50%) are located at interfaces. These combined nanometer-scale and interface effects are responsible for the unique properties of nanocrystalline materials (1, 2) and give rise to their rotational deformation.

The primary carriers of the rotational plastic deformation in solids are believed to be dipoles of grain boundary disclinations (7, 8). A disclination is a line defect characterized by a rotation of the crystallite lattice around its line (7). A disclination dipole consists of two disclinations causing crystal lattice rotation between them; such dipoles are energetically permitted only for disclinations that are close to each other.

Motion of a disclination dipole along grain boundaries causes plastic flow accompanied by crystal lattice rotation behind the disclinations (see the figure). The disclination dipole motion has been suggested to be intensive in nanocrystalline materials, where the volume fraction of grain boundaries is high and disclinations are close to each other (6). Murayama et al.’s atomic-level observation of disclination dipoles in deformed nanocrystalline materials (6) provides experimental support for this suggestion.

In addition to the rotational deformation, other deformation mechanisms can occur effectively in nanocrystalline materials that usually do not play an important role in conventional materials. Examples are grain boundary sliding and stress-induced mass transfer, which occurs via enhanced diffusion along grain boundaries (10–12). These mechanisms are conducted by grain boundaries and compete effectively with conventional dislocation slip (shear) in crystals, the mechanism that dominates in conventional materials.

Unusual deformation mechanisms also occur in strained semiconductor nanocrystals, called quantum dots, whose deformation behavior is essential for their functional stability as laser elements (13). For instance, as a result of nanoscale and interface effects, nonconventional, extended dislocations cause effective strain relaxation in such nanocrystallites (14).

Different deformation mechanisms, most of which only occur in nanostructured matter, thus compete in mechanically loaded nanocrystalline materials. This competition causes the unique deformation behavior of nanocrystalline materials. Further research focusing on the fundamental laws that govern the competition is crucial for progress in fabrication, design, and processing of nanocrystalline materials with enhanced mechanical characteristics. Some of the remaining experimental and theoretical challenges include identifying (new) deformation mechanisms, elucidating the influence of plastic deformation on structural transformations (including structural stability against grain growth), and understanding the role of distinct structural elements of grain boundaries in deformation processes in nanocrystalline materials.

References and Notes

15. Supported by U.S. Office of Naval Research grant N00014-01-1-0500.

The author is at the Institute of Problems of Mechanical Engineering, Russian Academy of Sciences, Bolshoj 61, Vos. Ostrov, St. Petersburg 199178, Russia. E-mail: ovidko@ifpm.ras.ru