Mechanical deformation of nanocrystalline materials

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ABSTRACT

The deformation of a nanometer sized wire containing multiple grain boundaries has been studied using molecular dynamics. We observe a splitting of the grain boundaries, followed by the migration of the new grain boundaries, leading to a complete transformation of the original grains. The stress-strain curves obtained from the simulations clearly show the effect of the grain boundaries on the mechanical properties. These simulations show how the grain boundaries in nanocrystalline materials may dominate the mechanical properties.

In recent years investigations of nanocrystalline materials have shown these to have different — and in many cases superior — mechanical properties compared to their macrocrystalline counterparts (Siegel and Fougere, 1994). For fcc metals like copper increases of hardness and tensile strength by a factor of 2–5 are not uncommon (Nieman, Weertman and Siegel, 1991). The mechanical properties of ordinary metals are dominated by dislocations and their interactions with grain boundaries and defects. However, the dislocation density in nanocrystalline materials is expected to be strongly suppressed (Siegel and Fougere, 1994) and the mechanisms active during plastic

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deformations are much less known. In this Letter we present atomic-scale simulations of a nanocrystalline metal under mechanical deformation, and show how the high density of grain boundaries significantly influence the mechanical behavior. The grain boundaries migrate during the plastic deformation, and thus participate actively in the deformation process.

We have performed Molecular Dynamics simulations of copper wires with dimensions 10 nm $\times$ 10nm $\times$ 40nm (361568 atoms), with periodic boundary conditions along the direction of the wire (the z-axis). The inter-atomic interactions are described by the effective medium theory (Jacobsen, Nørskov and Puska, 1987; Jacobsen, 1988; Stoltze, 1990), providing a realistic many-body description of the inter-atomic interactions. The wires contain four grain boundaries (of the $\Sigma 5$ coincidence site type) perpendicular to the z axis in the initial configuration. The grain sizes are thus comparable to the grain sizes of the experimentally investigated nanocrystalline copper (5–50nm) (Nieman *et al.*, 1991). We have also performed simulations of single-crystal wires without any grain boundaries for comparison. The wires are deformed by a tensile strain in the z directions, with a strain rate of $1.0 \times 10^9 \mathrm{s}^{-1}$. This strain rate is high, but the velocities of the atoms are still far below the speed of sound. Due to the absence of dislocation sources, like Frank-Read sources which are operative for metals with more usual grain sizes, a very high strain and stress is reached before any plastic deformation occurs. In the wires without grain boundaries, dislocations are finally nucleated at the surface, but in the wires with grain boundaries a more interesting phenomenon is seen.

As a multigrain wire is pulled, the original grain boundaries split into two and new grains are formed between the old ones. The new grains are nucleated where the grain boundary meets the surface, but quickly grow inwards, and become present everywhere along the original grain boundary. At further strain these new grains grow at the expense of the original grains, until the entire wire is transformed. This transformation process is illustrated in figure 1. A closer look at the atomic motion near the migrating grain boundaries reveals the atomic mechanism behind it. The grain boundary between the old and the new grain can be described as an array of partial dislocations (Shockley partials) with Burgers vectors $\frac{1}{6}\langle 211 \rangle$, gliding on adjacent $\{111\}$ planes. A partial dislocation is present on two out of three planes (figure 2). The dislocations move collectively, causing the grain boundary to move and the crystal to elongate.

If the dislocations were present at every $\{111\}$ plane the grain boundary would be a twin boundary, and fcc stacking would be recovered behind the moving grain boundary. With the current configuration the crystal behind the moving grain boundary contains a stacking fault on every third {111} plane, the crystal structure thus becomes the “9R” phase — a phase having a slightly higher energy than the fcc ground state. The “9R” phase appears stable on the time scale of the simulation if it is performed at very low temperatures (12K). However, we have also performed simulations at 580K and in that case the stacking faults finally anneal out and the fcc crystal structure is recovered.

The formation of twins at grain boundaries during deformation has also been observed experimentally, e.g. by Inoko and Yoshikawa (1993). In the experiment a copper bicrystal is deformed under tensile strain parallel to the grain boundary, and a new grain in twin relation with one of the original grains is formed. The main difference between the experiment and our simulations is that the experimental sample has undergone significant plastic deformation, the twin appears after work hardening has increased the stress levels in the sample, whereas in our simulation the lack of dislocations and dislocation sources prevent plastic deformation until stresses are sufficiently high to initiate grain boundary migration.

The formation of the 9R phase is another interesting phenomenon. In many fcc metals exhibiting twinning, the twin boundary reconstructs and a thin layer (a few lattice constants) of 9R phase is formed (Ernst, Finnis, Hofmann, Muschik, Schönberger and Wolf, 1992). The creation of such a reconstructed layer indicates that the energy of the interface between the 9R phase and the ordinary fcc phase is less than half the energy of a twin boundary. This may explain why the 9R phase forms here. When the 9R phase grows further it will be energetically favorable to nucleate a new fcc grain in twin relation to the original grain.

A different but related splitting of tilt grain boundaries has recently been observed in fcc metals, both in simulations and experimentally. Under some circumstances a tilt boundary lowers its energy by emitting stacking faults ending in partial dislocations (Rittner, Seidman and Merkle, 1996). The dislocations form a low angle grain boundary parallel to the original boundary, separated by a region of stacking faults.

The influence of the grain boundaries is clearly seen on the stress-strain behavior of the wires. Figure 3 shows the stress versus strain curves for wires both with and without grain boundaries at two different temperatures. Due to the lack of low-stress dislocation sources, very high stresses and strains are seen. Experimentally very high stresses and strains can also be realized in for example dislocation-free whiskers (Kelly, 1973). The grain boundaries lower the yield point significantly compared to the simulation with the single crystal, however, it is still rather high for a direct comparison with the observed yield strength for nanocrystalline copper (approx. 200MPa for 25nm grain size (Nieman *et al.*, 1991)). This difference may be caused by the high strain rate and the very idealized geometry used in the simulation, and possibly also by porosity and other types of defects/impurities in the experiments (Siegel and Fougere, 1994, and references therein).

The simulations clearly illustrate the importance of including the motion of grain boundaries in an understanding of plastic deformation in nanocrystalline materials, and shows the feasibility of treating the mechanical behavior of these materials on the atomic scale with simulation techniques. The heterogeneous nucleation of the deformation process at the free surfaces show the importance of including surfaces, be it external or internal surfaces (voids), in the simulations. In a material containing 5% voids (Siegel and Fougere, 1994) most grains are at or near internal surfaces.

Acknowledgments

The authors would like to thank Jens K. Nørskov for many interesting discussions, and Anders E. Carlsson for reading the manuscript. We would also like to acknowledge computing facilities at JRCAT Supercomputer System as financially supported by New Energy and Industrial Technology Development Organization (NEDO). We also acknowledge computing resources from the Center for Parallel Computer Research as funded by the Danish Research Councils. Center for Atomic-scale Materials Physics is sponsored by the Danish National Research Foundation.

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Figure 1: The development of new grains. Atoms at grain boundaries and other crystal defects are colored. The left row shows cuts through the system; the right row shows the same cuts, but only surface atoms and atoms at grain boundaries and dislocation cores are shown. (a) $\epsilon = 4.7\%$ (ϵ is the strain): The formation of new grains has just begun. (b) $\epsilon = 5.2\%$: At this strain new grains have formed at the original grain boundaries. The new grains grow by grain boundary migration. (c) $\epsilon = 5.7\%$: The new grains grow at the expense of the original grains, thus relieving the elastic stress. (d) $\epsilon = 6.3\%$: Two of the original grains have been completely transformed. As the simulation is continued the two larger original grains are completely transformed as well.

Figure 2: Grain boundary migration at the microscopic scale. The grain boundary can be considered an array of partial dislocations. As they move collectively, the fcc phase is transformed to a 9R phase. The actual grain boundary contains a few "defects" where there are either three dislocations on adjacent planes, or only one. The (111) planes and the [100] direction of the original grain are indicated.

Figure 3: Stress versus strain for a single crystalline and a nanocrystalline wire. At both temperatures the yield point is seen to be significantly lowered by the grain boundaries.