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Grain coarsening in nanocrystalline copper with very small grain size during tensile deformation

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ABSTRACT

Molecular dynamics (MD) simulation has been used to study tensile deformation of nanocrystalline copper with mean grain sizes from 2.1 to 11.5 nm. The flow stress, yield stress and Young's modulus are proportional to the reciprocal of the square root of grain size. They decrease as the grain size is reduced. Grain rotation and grain boundary migration are observed, which are two major causes of grain coarsening during the deformation. Notable grain coarsening is only observed at mean grain sizes below a critical grain size which is dependent on the strain rate. This coarsening is due to the extensive ordering of atoms in grain boundaries induced by grain boundary migration. Deformation twin forms much easily in very small grains.

1. Introduction

MD simulations have been extensively performed to investigate the deformation of nanocrystalline metals [1–3]. These simulations suggest that the deformation mechanism of nanocrystalline metals is not mainly dominated by dislocation activities but the grain boundary sliding or migration. The grain boundary mediated mechanism is used to explain the experimental results, such as leveling off of the hardness at very small grain sizes [4] or even decreasing in some cases [5,6]. Usually, the hardness, yield stress and flow stress of metals increase with reduction of the grain size, which is experimentally established from millimeter-sized grains down to the submicron regime. This relation is caused by the fact that the grain boundaries in the conventional polycrystal can hinder dislocation activities, thereby making plastic deformation more difficult at smaller grain sizes. However, when the grain size is smaller than about 12 nm the relation is reversed, indicating the grain boundary mediated mechanism operates due to a large fraction of atoms in grain boundaries at the grain size.

MD simulation is not only used to explain the experimental results but also a useful tool to show the microstructure developments at atomic level, such as grain boundary sliding, migration and dislocation motion during the deformation. MD simulation can avoid the effect of various defects in experimental samples on the plastic deformation and reveal the substantial physical process.

In this work, grain growth during tensile deformation of nanocrystalline copper with very small grain size is shown by MD simulation. In addition, the decrease of yield stress, flow stress and Young's modulus with the reduction of grain size is observed.

2. Model and methods

Nanocrystalline copper samples with various mean grain sizes from 2.1 to 11.5 nm have been constructed by a computer code which is originally used to produce samples with voids in Ref. [7]. The number of atoms in the samples was about 7×10^5. Grain orientations were randomly arranged in the samples.

Molecular dynamics simulations were carried out with LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) [8]. An EAM (Embedded-Atom Method) potential suggested by Zhou et al. [9] was used in the simulations. Periodic boundary conditions are applied in three dimensions to mimic the situation that is deep within the bulk of a larger sample.

Before deformation the samples were annealed by running an equilibration simulation at 300 K, allowing unfavorable configurations in the grain boundaries to relax. Uniaxial tensile deformation was simulated at a strain rate of 10^8–10^{10} s^{-1} at 300 K until the strain up to 14% or 20%. A program OVITO [10] was employed to visualize or analyze the simulation results.

3. Results and discussion

Stress–strain curves for eight simulations with varying grain sizes are shown in Fig. 1. At the linear elastic region, the slope of the curve generally increases with increasing grain size. This is caused by the reduction of the fraction of atoms in grain

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boundaries. Large fraction of atoms in grain boundaries would lower Young's modulus of the nanocrystalline sample. The stress–strain curves for grain sizes of 2.6 nm, 2.8 nm and 3.2 nm are similar. They are different from the curves for grain sizes between 4.5 and 11.5 nm. After a fast increase at the strain below 8%, the stress of samples with grain sizes of 2.6–3.2 nm still increases slowly without a maximum which appears in the curves of samples with grain sizes larger than 4.5 nm at the strain of about 5%. Furthermore, there are no steady states in the curves for grain sizes of 2.6–3.2 nm, whereas in the curves for grain sizes of 4.5–11.5 nm flat region appears at above 10% strain.

The yield stress, flow stress and Young's modulus calculated from the stress–strain curves are presented in Fig. 2. The yield stress and flow stress are proportional to the reciprocal of the square root of grain size. The slope of the lines is minus, which means that the yield stress and flow stress increase with increasing grain size. This relation is opposite to that of the conventional metals.

Experimental results of the yield stress of nanocrystalline copper prepared by various methods were plotted together by Swygenhoven et al. [2]. An increase in yield stress with decreasing grain size from micrometer scale to about 12 nm is presented in their paper. The experimental result of even smaller grain size is not available, therefore the relation between the yield stress and grain size is uncertainty at the scale below 12 nm. However, the experimental yield stress of a sample with grain size of about 12 nm shown in Fig. 2 of Ref. [2] is very close to our simulation value. Hence we infer that the strongest grain size is about 12 nm for nanocrystalline copper, and further decrease in grain size will induce the reduction of yield stress as demonstrated in Fig. 2.

The difference of the relation between the yield stress and grain size implies the change of the deformation mechanism. For larger grains the dislocation-mediated plastic deformation dominates, and for smaller grains the grain-boundary sliding or migration plays a major role [1,11]. In the latter situation grain rotation will be driven by grain boundary sliding. We can see from Fig. 3 that grains with similar orientation rotate into identical direction and then coalesce to a large grain in the sample with grain size of 2.8 nm. For instance, grains G1 and G2 with misorientation angle of 9.2° coalesce to grain G9 at 4% strain (Fig. 3 (a) and (b)). In addition, grain rotation is found to be a successive process with the plastic deformation because grains G3 and G6 rotate 4.7° and 3.6° from the initial state to 12% strain respectively (Fig. 3(a) and (d)). Correlated with the observation that grain G3 is

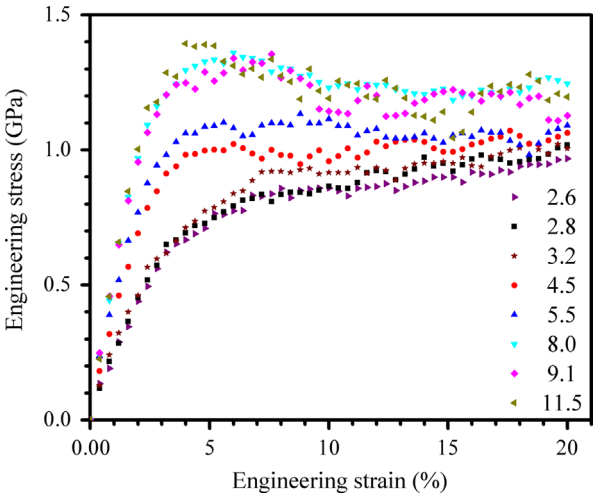

Fig. 1. Stress–strain curve for each mean grain size. The unit of the grain size shown in the figure is nanometer (nm).

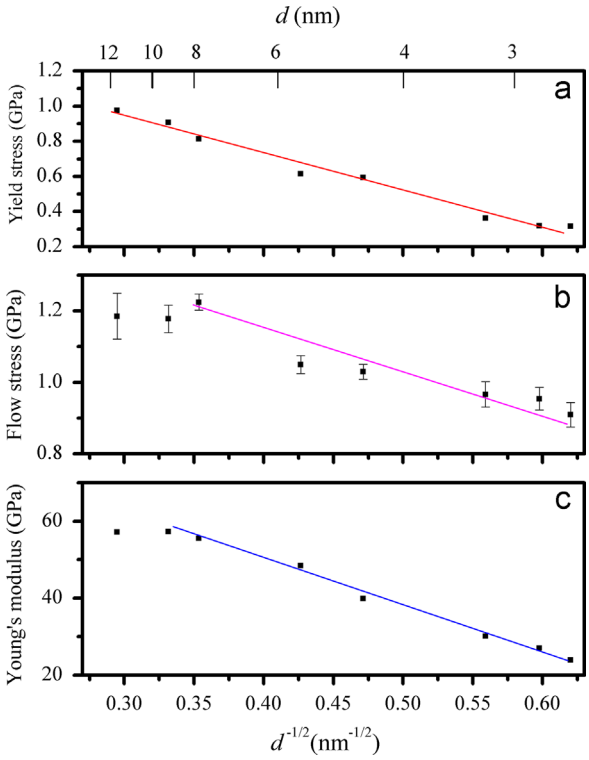

Fig. 2. The flow stress, yield stress and Young's modulus as a function of grain size. The letter *d* represents the mean grain size. Lines are used to guide the eye. The yield stress is defined as the stress where the strain departs 0.2% from linearity. The flow stress is defined as the average stress in the strain interval from 12% to 20% deformation.

apparently smaller than grain G6, we can conclude that small grains rotate somewhat easily. A successive coalescence is also observed in Fig. 3. Grains G7 and G8 firstly combine to G10 from the initial state to 4% strain, and then grains G4 and G10 coalesce to G11 at 12% strain. Grains G5 and G6 coalesce gradually to grain G12 from strains of 0% to 16%. It needs to be noticed that the misorientation angle of G5 and G6 is 13.0° at the strain of 12%, which means that grains with relative large misorientation angle also can combine to a large grain. This phenomenon is also observed in the sample with 9.1 nm grain size. Grains G1 and G2 of this sample (Fig. 4(a)) with misorientation angle of 11.7° coalesce to grain G3 in Fig. 4(d) at 12% strain.

In addition to the grain rotation discussed above, grain boundary migration is also observed. Some grain boundaries disappear and atoms in them become ordered as a face-centered-cubic (fcc) structure, for example, the adjacent region of grain G5 in Fig. 3. This ordering is caused by grain boundary migration. Some atoms in grain boundaries move to lattice positions on grains nearby to reduce the total system energy during the grain boundary migration. The ordering of some grain boundaries promotes the grain coarsening. On the contrary, the grain coarsening in the sample with grain size of 9.1 nm is not much notable (see Fig. 4).

As the deformation proceeds, stacking faults appear as partial dislocations move through the grains (see Figs. 3 and 4). With increasing the strain more stacking faults appear as more partial dislocation nucleates in grain boundaries, although some stacking faults also disappear during deformation. The increase of stacking faults induces the decrease of the fraction of atoms in fcc structure. It can be seen from Figs. 3 and 4 that both grain boundary activities and partial dislocation process operate during the deformation of samples with grain size of 2.8 and 9.1 nm. In addition, a small amount of deformation twin is observed in the