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Effects of grain size and shape on mechanical properties of nanocrystalline copper investigated by molecular dynamics

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ABSTRACT

Molecular dynamics (MD) simulation has been used to study effects of grain size and shape on mechanical properties of nanocrystalline copper with mean grain size varying from 2.6 to 53.1 nm. Three grain size regions are identified according to the plot of flow stress versus mean grain size d. In region I ($d \approx 20$–53 nm) flow stress increases with the decrease of d. Deformation twinning process and extended dislocation are observed in this region. In region II ($d \approx 8$–20 nm) detwinning process appears as a competitive deformation mechanism with the twinning process. The flow stress begins to decrease slightly in this region. In region III ($d < 8$ nm) plastic deformation mainly occurs in grain boundaries and grain rotation is observed to accommodate the stress buildup induced by the grain boundary sliding. Deformation twin formed by sequent emission of partial dislocations at nearby sliding planes is not observed in this region. Young's modulus has a linear relation with d^{-1} in the simulated range of mean grain size, and it directly depends on the volume fraction of grain boundaries. The Young's modulus of the grain boundary component is found to be ~25% of that of the grain interior. MD simulations on samples with spherical and cylindrical grain shapes are also carried out. The influence of grain shape on flow stress is hardly observed, indicating that for different grain shapes the plastic deformation mechanism is the same. The grain shape has an obvious effect on Young's modulus, which is attributed to the difference of the volume fraction of grain boundaries for samples with the different grain shapes.

1. Introduction

MD simulation has already provided illuminating insight into the atomic scale processes that occur during plastic deformation [1–3]. Some simulations reveal the ability of the grain boundary network in nanocrystalline sample to accommodate an external applied stress by means of grain boundary sliding [4] and emission of partial dislocations [5] involving local structural changes in the network. By varying the mean grain size between 5 and 50 nm, a maximum in the flow stress of nanocrystalline copper is observed at a mean grain size of 10–15 nm [2]. Below this mean grain size the flow stress decreases with decreasing mean grain size, which is reverse when mean grain size is above the critical value. A shift in the microscopic deformation mechanism from dislocation-mediated plasticity in the coarse-grained material to grain boundary sliding in the nanocrystalline region is suggested to explain the change of the relation between flow stress and mean grain size [2]. Both mechanisms are dependent on grain size, and usually in nanocrystalline materials the grain size is not uniform but has some distribution. Therefore, in the crossover region both mechanisms would operate in grains with different sizes separately and the relation between flow stress and mean grain size in this region should be different to that for dislocation mediated mechanism or grain boundary sliding mechanism.

Zheng et al. [6] have studied the roles of grain boundary and dislocations at different deformation stages of nanocrystalline copper under tension using MD method. They have found that in the early stage of deformation grain boundary sliding together with the rotation of small grains is dominant and partial dislocations emitting from grain boundaries propagate inside grains leaving stacking faults behind. With further loading, extended dislocations can form in large grains and the rotation of small grains is suppressed. Li et al. [7] have performed MD simulations of plastic deformation in nanocrystalline Al with mean grain sizes of 10, 20, and 30 nm. Competing grain-boundary- and dislocation-mediated mechanisms during plastic strain recovery have been observed and the fractional contributions by these mechanisms to the overall recovered strain have been quantified. They have found that both mechanisms operate in the mean grain sizes of 10–30 nm, and the fractional strains due to grain boundary processes increase with decreasing mean grain size. These investigations indicate that a change in deformation mechanism has occurred, however this is not a sharp transition.

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Conrad [8,9] has analyzed the influence of mean grain size on flow stress of copper with mean grain size from nanometers to millimeters according to the published experimental data. Three grain size regimes were identified using the plot of flow stress versus inverse square root of grain size. The rate-controlling mechanisms were determined for each regime. The transition grain size which distinguishes one regime from another was found to depend on temperature and strain rate. Because there is few experimental data on nanocrystalline copper with grain size less than 20 nm, the detailed relation between flow stress and mean grain size in this region is not well established experimentally. MD simulation has been proved to be a useful tool in investigating the mechanical properties of nanocrystalline metals with mean grain size in nanometer scale. Furthermore, it can provide an atomic view of the plastic deformation process.

Until now those computer simulations are usually performed on three-dimensional nanocrystalline samples with equiaxed grains in uniaxial tensile deformation. Grain shape may have some influence on mechanical response of nanocrystalline metals.

In this paper, the dependence of mechanical properties such as flow stress and Young's modulus on mean grain size varying from 2.6 nm to 53.1 nm is studied by MD simulation. Additionally, the effect of grain shape on mechanical properties of nanocrystalline copper is discussed.

2. Simulation model and methods

Three dimensional nanocrystalline copper samples with various mean grain sizes from 2.6 to 53.1 nm have been constructed by a computer code which was originally used to produce samples with voids in Ref. [10]. The number of atoms in the samples varied from about 7×10^5 to 1.2×10^7 according to mean grain size of the samples. Grain orientations were randomly arranged in the samples.

In order to study the effect of grain shape on the mechanical properties, samples with spherical and cylindrical grains were constructed. Fig. 1 shows an example of the configuration of samples with the two types of grains.

MD simulations were carried out with Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [11]. An embedded-atom method (EAM) potential suggested by Zhou et al. [12,13] was used in the simulations. Periodic boundary conditions were applied in three dimensions to mimic the situation that is deep within the bulk of a larger sample. The time step used in the simulation was 1 fs.

Before deformation simulation the samples were annealed by running an equilibration process at 300 K, allowing unfavorable configurations in the grain boundaries to relax. Uniaxial tensile deformation along x-axis was simulated at a strain rate of 10^8 s^{-1} at 300 K until the strain up to 20%. A program OVITO [14] was employed to visualize or analyze the simulation results. Mechanical properties such as flow stress and Young's modulus were calculated from engineering stress–strain curves.

3. Results and discussion

3.1. Effect of grain size on mechanical properties

3.1.1. Flow stress

Fig. 2 presents the relation between flow stress and mean grain size d of nanocrystalline copper samples. The maximum flow stress appears at a mean grain size of 8–20 nm. Three regions can be identified in Fig. 2, and in each region the flow stress has a linear relation of different slopes with $d^{-1/2}$. In region I ($d \approx 20$–53 nm) the flow stress increases with decreasing mean grain size, which is the same as that of conventional polycrystalline metal. In regions II ($d \approx 8$–20 nm) and III ($d < 8$ nm) the flow stress

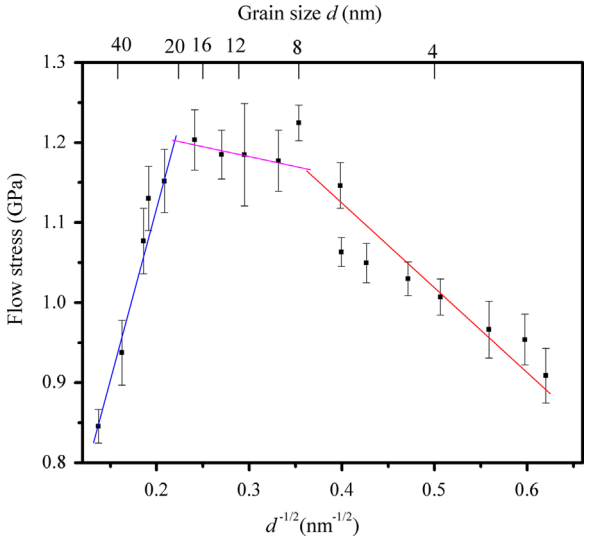

Fig. 2. Flow stress as a function of mean grain size d. The flow stress is defined as the average stress in the strain interval from 12% to 20%. Three regions of mean grain size are indicated by lines with different slopes.

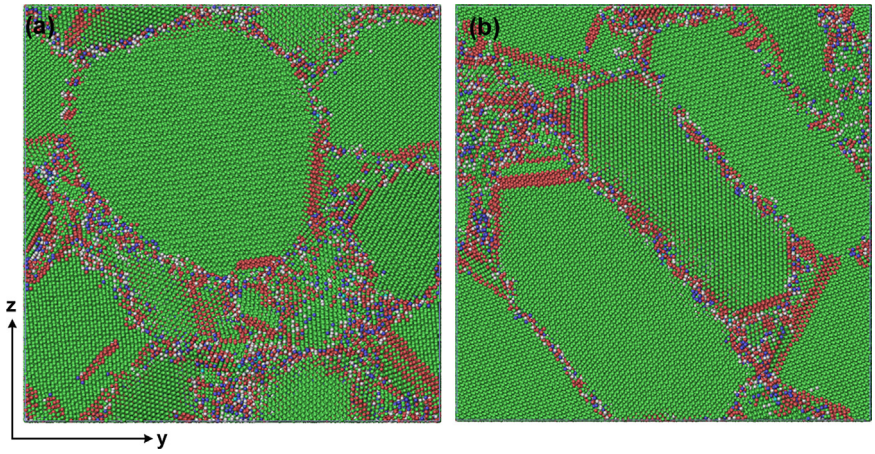

Fig. 1. Initial configurations of samples with spherical (a) and cylindrical (b) grain shapes. The two samples have the same mean grain size, which is 9.1 nm. Only y–z plane is presented in this figure. Red atoms are at stacking faults and twin boundaries; green atoms are inside grains; others are mostly at grain boundaries and dislocation cores. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)