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Effects of grain size and temperature on mechanical response of nanocrystalline copper

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ABSTRACT

Molecular dynamics simulation is utilized to study the effects of grain size and temperature on the mechanical properties of quasi-two-dimensional (2D) nanocrystalline Cu with grain sizes of 3–8 nm under uniaxial tensile tests. Our results show that the grain growth is caused by the grain rotation and leads to strain hardening at 300 K for a grain size of <5 nm and at 100 K for a grain size of <4 nm. For a grain size of ≤ 7 nm, the inverse Hall–Petch relation was observed in the yield stress. The Young's modulus for the quasi-2D system is higher than that for the three-dimensional (3D) system.

1. Introduction

Nanocrystalline metals comprise crystalline grains of different sizes and orientations with a grain size of less than 100 nm. In nanocrystalline metals, the yield stress, flow stress, and hardness are significantly influenced by the grain size. The increase in the flow stress, yield stress, and hardness is inversely proportional to the square root of the grain size known as the Hall–Petch (H–P) relation [1–3]. Previous studies using molecular dynamics (MD) simulations [4–7] and bubble raft models [8] show that the maximum value is observed at a mean grain size of 7–15 nm. An inverse H–P relation is observed beyond the critical grain size. This phenomenon results due to the transition of the plastic deformation mechanism from the dislocation-mediated hardening to the grain boundary-mediated softening.

Chokshi et al. [9] were the first to report experimentally determined reverse k values for nanocrystalline Cu and Pt. Numerous studies [10–13] show that the critical value might be less than 20 nm. However, it is extremely difficult to process the high-quality homogeneous nanocrystalline specimens with a grain size less than 15 nm [13]. Recently, Zhou et al. [14] used MD simulations to mark the existence of a transition region (grain size of approximately 8–20 nm). In this region, the (inverse) H–P relation is not evident. However, at a grain size of <8 nm, the inverse H–P relation is evident. Further, at small grain sizes, several studies [15–18] provide experimental evidence for significant grain growth and rotation in deformation tests. Recently, Wang et al. [19] observed that grain rotation becomes the most prevalent mode at a grain size of <6 nm. The deformation-induced grain rotation and grain growth have been evaluated using MD simulations [20–23] and theoretical model calculations [24,25].

Using MD simulations, we observed a stress-enhanced grain growth in quasi-two-dimensional (2D) nanocrystalline Cu, with a grain size of <5 nm, at 300 K in a nanoindentation process [23]. We performed uniaxial tensile tests on a quasi-2D thin film of nanocrystalline Cu with grain sizes varying from 3 nm to 8 nm. Structural characterization techniques, such as the bond angle analysis (BAA) [26], shear strain tensor [27], and slip vector [28], were used to identify the deformations at atomic resolution detail. With $d<5$ nm at T $=300$ K and $d<4$ nm at T $=100$ K the strain hardening is followed by the strain-induced grain growth, which is caused by the grain rotation. At a grain size of ≤ 7 nm, the inverse H–P relation was observed in the yield stress. However, it is very difficult to define a reliable flow stress, which varies extremely in our system. In addition, the Young's modulus in a quasi-2D system is higher than that in a three-dimensional (3D) system.

The article is organized as follows. Section 2 describes the simulation method and model. The relative potential and atomic stress are introduced in this section. The BAA method, which is used to identify the structure of atoms, is described in Section 3.1. In Section 3.2, the tensile stress–strain curves and deformation mechanics for different grain sizes are discussed in detail. In Section 3.3, the yield stress and Young's modulus are discussed. The conclusions from our study are presented in Section 4.

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2. Simulation method and model

The dimensions of the model shown in Fig. 1 are approximately 20 Å (width) × 225 Å (length) × 130 Å (height) in the *x*, *y*, and *z* axes, respectively. A periodic boundary condition (PBC) was imposed in the *x* direction. The simulation was performed considering a quasi-2D system. Six samples with the grain sizes (*d*) of 3, 4, 5, 6, 7, and 8.0 nm were used. The nanocrystalline Cu comprises hexagonal columnar grains with orientation angles of 0°, 30°, and −30° along the *x* direction. The crystal unit is a face-centered cubic (FCC) structure and the orientation angle of 0° is defined with respect to the *x*, *y*, and *z* axes in the [100], [010], and [001] directions, respectively.

The system contains boundary atoms and thermostat atoms. The number of thermostat atoms is approximately 50,000. The boundary atoms are located at the left and right surfaces in the *y* direction and the thickness is approximately 5 Å. In the tensile test, the left and right boundary atoms move at a velocity of 10 m/s along the left and right direction, respectively (see Fig. 1). In other words, the strain rate is $10^9\ s^{-1}$. The velocity rescaling method comprising 40,000 time steps (80 ps) was used to establish equilibrium at a specific temperature. During the tensile tests, the Berendsen weak coupling method was used to allow temperature fluctuation at a relaxation time of 0.3 ps. The motion was integrated using the velocity Verlet algorithm with a time step of 2 fs.

The tensile stress was calculated from the virial atomic stress using the following equation:

$$\sigma_{i,\alpha\beta} = \frac{1}{\Omega_i}\left(-m_i v_{i,\alpha} \otimes v_{i,\beta} + \frac{1}{2}\sum_{j\neq i} r_{ij,\alpha} f_{ij,\beta}\right) \quad (1)$$

here, $\sigma_{i,\alpha\beta}$ represent the components of the tensor. Ω_i is the average volume of one atom, m_i is the mass, v_i is the velocity, f_{ij} is the interatomic force, and r_{ij} is the distance between the atoms *i* and *j*. The stress–strain curves are calculated by averaging the atomic stresses along the tensile direction, which is the average of σ_{yy} over the thermostat atoms.

The interaction was modeled using the second-moment approximation of the many-body tight-binding (TB) potential [29]. The parameters for Cu are r_0 = 2.5 Å, ξ = 1.224 eV, A = 0.855 eV, p = 10.96, and q = 2.278. Additionally, the OVITO program [30] was used to visualize the atomistic configurations.

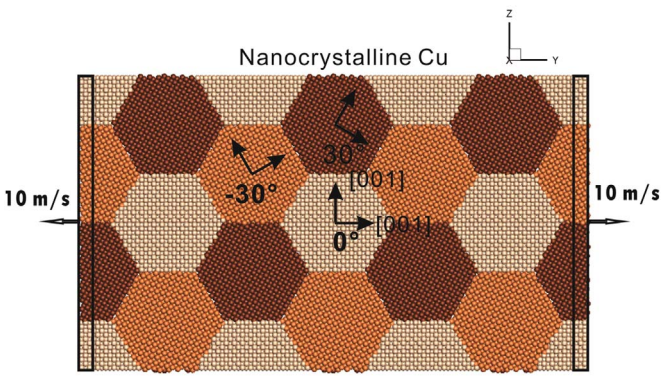

Fig. 1. Show the molecular model of nanocrystalline Cu structure under uniaxial tensile test.

3. Results and discussion

3.1. The structure of the nanocrystalline Cu

We used the BAA method to identify the structure of the atoms. The method is based on the analysis of angular distribution functions and is more stable against thermal boost [26,31]. The structures of nanocrystalline Cu with d = 3 and 7 nm following the equilibration process at 300 K, are shown in Fig. 2(a) and (b), respectively. Atoms are colored based on FCC, BCC, or hexagonal close-packed (HCP) classification system. At 300 K and d = 3 nm, some grain boundaries vanish and the grains grow due to the thermally induced grain-rotation coalescence [32]. However, at 100 K we do not observe this behavior.

In general, the atoms can be classified into grain boundary atoms or grain core atoms. Here we define the number fraction of the grain core component, ϕ_{core}, as follows:

$$\phi_{core} = N_{FCC}/N_{all} \quad (2)$$

here, N_{FCC} is the number of atoms belonging to the FCC structure, and N_{all} is the total number of atoms.

Fig. 2(c) shows ϕ_{core} as a function of grain size at 100 K, 300 K, and 450 K. At a large grain size and lower temperature, the system has a higher fraction of grain core. To determine the thickness of the grain boundary in a quasi-2D system, we used a method similar to the one used by Gao et al. [33], which assumes that the fraction of grain core is given by the following expression:

$$\phi_{core} = \left(\frac{d}{d + d_{GB}}\right)^2 \quad (3)$$

here, d_{GB} is the average thickness of the grain boundary. Since the number of atoms is proportional to the area in a quasi-2D system, the square of the ratio is used. From Eqs. (2) and (3), the grain boundary thickness was determined to be approximately 0.47 nm (BAA calculation). This result is similar to the value of 0.5 nm reported in other studies [34–36].

3.2. Deformation mechanics

The tensile stress and the average of σ_{yy} over the thermostat atoms in nanocrystalline Cu with various grain sizes at 300 K and 100 K are shown in Fig. 3(a) and (b), respectively. At 300 K, there are two types of stress-strain behavior depending on the grain size. When the grain size is > 5 nm, the tensile stress drops sharply beyond the yield point and shows obvious serrated stress-strain behavior while decreasing gradually. However, when the grain size is < 5 nm the tensile stress decreases relatively smoothly beyond the yield point. This is because the dislocation dominates the deformation at large grain sizes, whereas grain boundary motion dominates the deformation at smaller grain sizes. With a further increase in the stress, strain hardening occurs clearly in case of d = 3 and 4 nm. For example, in grains with d = 3 nm, the stress continues to increase for $\varepsilon\cdot$ ranging from 11% to 16% (see Fig. 3) and reaches a maximum value at ε = 16%. At 100 K the strain hardening occurs only in grains with d = 3 nm because at a higher temperature and lower grain size, the grain growth occurs easily, causing the strain hardening behavior. Similar stress-enhanced grain growth has been observed in previous experiments [15,17,19] and simulations [22,26].

Fig. 4(a)–(d) illustrate the detailed snapshots of shear strain and the structure of atoms in grains with d = 3 and 8 nm under special strain. Frames (a1–d1) correspond to the deformation near the yield point, the frames (a2–d2) correspond to the deformation after the yield point, and frames (a3–d3) correspond to the large strain (ε = 16%). As observed from Fig. 4(a1) and (c1), the