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Strain rate effect on plastic deformation of nanocrystalline copper investigated by molecular dynamics

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ABSTRACT

The strain rate effect on the plastic deformation of nanocrystalline copper with mean grain sizes in the range of 3.8–27.3 nm has been investigated by using molecular dynamics simulation. The simulated results indicate that the critical mean grain size corresponding to the transition of plastic deformation mechanism is little influenced by the strain rate in the strain-rate range of 1×10^{7}–1×10^{10} s^{-1}. The simulated grain-size dependence of the strain rate sensitivity for strain rate below 1×10^{8} s^{-1} is in agreement with the experimental results of nanocrystalline copper reported in literatures. The strain rate sensitivity values for the simulated samples with mean grain sizes of 3.8 and 5.5 nm are 0.073 and 0.065 respectively. These results reveal that the stress-driven grain-boundary plastic deformation mechanisms such as grain-boundary sliding and migration are not as sensitive to strain rate as that expected for the thermally assisted mechanisms. Furthermore it is found that if the stacking faults act as obstacles to the motion of partial dislocations the strain rate sensitivity will increase.

1. Introduction

Experiments on strain rate changes are very useful in revealing deformation mechanisms in metals, from which two primary parameters, the strain rate sensitivity m and the activation volume V^* for the flow stress, can be calculated. The m and V^* are defined as [1,2]

$$m = \frac{\partial \ln \sigma}{\partial \ln \dot{\varepsilon}}, \tag{1}$$

$$V^* = \sqrt{3}kT\frac{\partial \ln \dot{\varepsilon}}{\partial \sigma}, \tag{2}$$

where σ is the flow stress, $\dot{\varepsilon}$ is the strain rate, k is Boltzmann's constant and T is absolute temperature. The experimental m values for coarse grained copper with the grain size larger than 10 μm are between 0.004 and 0.009 [1]. The m values for copper samples with mean grain sizes of about 200 nm are reported to be 0.02 [1,3], though the measurement methods are different in these two references which are nanoindentation method and strain-rate change test respectively. For nanocrystalline copper with a mean grain size of 10 nm, the m value reaches 0.06 [1] which is approximate ten times larger than that for coarse grained copper. According to the summaries of the m values of copper in a large range of mean grain size [1,3,4,5], m shows a clear increase with decreasing the mean grain size, especially when the mean grain size is below a couple of hundred nanometers. The activation volume V^* is inter-related with m and thus decreases with the decrease of mean grain size. With the decrease of mean grain size from the micron to submicron region, the V^* reduces fast from around $1000b^3$ [6] to about $50b^3$. Further decrease of mean grain size to 10 nm leads a slight decrease of V^* to $8b^3$ [1].

The grain size dependence of m and V^* is qualitatively interpreted in terms of thermally activated process of overcoming of the obstacles to the motion of glissile dislocations [3,5]. For coarse grained copper the moving dislocations interact with short-range obstacles, such as forest dislocations and impurity atoms, which results in weak strain rate sensitivities on the flow stress. When the grain size decreases to submicron regime, especially below 100 nm, the large mount of grain boundaries serve as significant obstacles to dislocation motions. In this case the m value increases fast with decreasing mean grain size, for example, which is 0.026 for mean grain size of 54 nm [5] and increases to 0.06 for mean grain size of 10 nm [1]. Huang et al. [7] also measured $m=0.103$ for Cu film with a mean grain size of 9.1 nm using nanoindentation method. Moreover, a fitting curve calculated using dislocation-kinetics approach [8] achieves a good agreement with the experimental results with mean grain sizes in the range of about 10–

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190 nm. However the experimental m value for nanocrystalline copper with mean grain sizes below 10 nm is still absent at present. Molecular dynamics (MD) simulations performed on nanocrystalline copper [9,10] indicate that the plastic deformation mechanism transits from the dislocation-mediated plasticity in the coarse-grained material to grain boundary sliding in the nanocrystalline region around the mean grain size of 10 nm. At mean grain sizes below 10 nm the interaction between dislocation and grain boundary should not be the main contribution to the strain rate sensitivity because the plastic deformation is dominated by grain-boundary activities. Hence the dislocation-kinetics approach can not cover this mean grain size range.

The m value should be 0.5 corresponding to the grain boundary sliding mechanism [1,11]. However the experimental value $m=0.06$ at the mean grain size of 10 nm is still much smaller than the expected value. MD simulation is well suitable to investigate the mechanical properties and plastic deformation mechanism of nanocrystalline metals with mean grain sizes around 10 nm [12,13,14,15,16]. In addition, in MD simulation the strain rate can be easily controlled to study the strain rate effect on the plastic deformation, although the strain rate is usually very high in order to achieve large strain. A MD simulation on nanocrystalline copper [17] showed that a decrease of strain rate from $5\times10^8\ s^{-1}$ to $5\times10^7\ s^{-1}$ results in a 15% reduction in the flow stress, however a systematic study of the strain rate effect on plastic deformation is needed. Furthermore, the strain rate may also influence the critical grain size where the plastic deformation mechanism transits.

In this work MD simulations are used to investigate the strain rate sensitivity of nanocrystalline copper with mean grain sizes between 3.8 and 27.3 nm. The dependence of strain rate sensitivity on the mean grain size is discussed based on the simulation results. The atomic processes behind the dependence will be observed by virtue of the ability of MD simulation to show the atom motion in real time.

2. Simulation model and methods

Three dimensional nanocrystalline copper samples with various mean grain sizes from 3.8 to 27.3 nm were constructed by a computer code [18] using Voronoi construction. The number of atoms in the samples varied from about 7×10^5 to 5.5×10^6 according to the mean grain size of the samples. Grain orientations were randomly arranged in the samples. Fig. 1 presents a sample with a mean grain size of 5.5 nm.

MD simulations were carried out with LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator)[19]. An EAM (embedded-atom method) potential suggested by Zhou et al.[20] 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 deformations along x-axis were simulated at strain rates of 10^7–$10^{10}\ s^{-1}$ at 300 K. During the tensile simulations the y- and z-direction boundaries were allowed to vary to keep the corresponding components of the stress to zero.

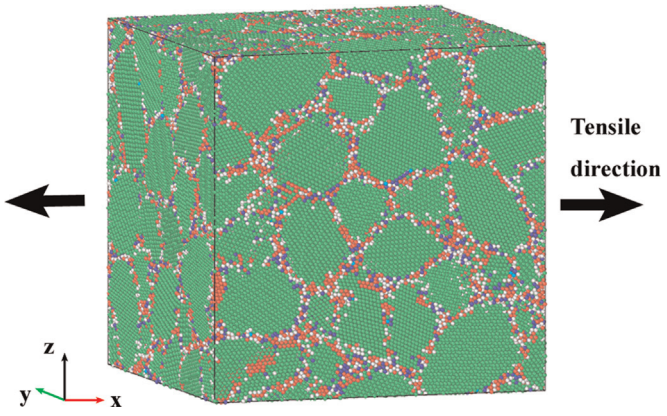

Fig. 1. Atomic configuration of a sample with a mean grain size of 5.5 nm after relaxation at 300 K. Tensile direction is along the x-axis. Simulation cell boundaries in y-axis and z-axis directions are set to stress free during the deformation simulations.

A program OVITO [21] was employed to visualize and analyze the simulation results. Structural characterization of the simulated nanocrystalline system was performed by using bond angle method [22]. The atoms with perfect fcc coordination are shown as green, while those with perfect hcp coordination are shown as red. A single plane of hcp atoms represents a twin boundary, two adjacent hcp planes stand for an intrinsic stacking fault and two hcp planes with an fcc plane between them stand for an extrinsic stacking fault.

3. Results and discussion

True stress–strain curves for nanocrystalline copper with different mean grain sizes are shown in Fig.2. Strain rate is varied in the range of 1×10^7–$1\times10^{10}\ s^{-1}$ to investigate the rate dependence of the stress–strain curves. For each nanocrystalline copper, the flow stress increases apparently with the increase of the strain rate; the slope of the elastic region shows little difference for different strain rates expect the highest strain rate of $1\times10^{10}\ s^{-1}$. At the highest strain rate, some kind of plastic deformation may occur in the linear elastic region. Schiøtz et al. [23] confirmed this by stopping a simulation while the system is still in the elastic region and allowing it to contract, but the system can not return to the original length. This plastic deformation occurs in grain boundaries because no dislocation activities can be observed in grains at the early stage of the deformation simulation at the strain rate of $1\times10^{10}\ s^{-1}$ in the present work.

For large mean grain sizes, bumps can be seen in the stress–strain curves (Fig. 2(c)–(e)), particularly at higher strain rates and larger mean grain sizes. At lower strain rates these bumps disappear. This can be explained by that for the simulated sample with large mean grain size, at higher strain rates there is not enough time to nucleated dislocations at the onset of plastic deformation. For small mean grain sizes (3.8 and 5.5 nm) there are no bumps in the stress–strain curves even at the highest strain rate used in the simulations. This observation apparently indicates dislocations are not the dominant deformation mechanism in nanocrystalline copper with small mean grain sizes. Hence the difficulty of creating them is irrelevant, and consequently the bump is absent in the stress–strain curves.

A transition of the dependence of the flow stress on mean grain size can be seen in Fig. 2(f). The maximum in the flow stress is corresponding to 17.2 nm for strain rates of $1\times10^8\ s^{-1}$ and $1\times10^9\ s^{-1}$, and 11.5 nm for strain rate of $1\times10^{10}\ s^{-1}$, respectively. This kind of transition has already been observed in nanocrystalline copper by using MD simulations [9,10,17]. The maximum of flow stress was reported at a mean grain size of 10–15 nm with the strain rate of $5\times10^8\ s^{-1}$ [9] and at a mean grain size between 8 and 20 nm with the strain rate of $1\times10^8\ s^{-1}$ [10]. The maximum of flow stress is caused by a shift from grain-boundary mediated to dislocation mediated plasticity. The present result in Fig. 2(f) shows that the value of flow stress increases with the increase of the strain rate, but the mean grain size for the