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Atomistic simulation study of deformation twinning of nanocrystalline body-centered cubic Mo

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ABSTRACT

Deformation twinning of nanocrystalline body-centered cubic Mo was studied using molecular dynamics simulations, and the effects of grain sizes and temperatures on the deformation were evaluated. With small grain size, grain rotation accompanying grain growth was found to play important role in nanocrystalline Mo during tensile deformation. Additionally, grain rotation and the deformation controlled by GB-mediated processes induce to the difficulty of creating crack. Twin was formed by successive emission of twinning partials from grain boundaries in small grain size systems. However, the twin mechanisms of GB splitting and overlapping of two extended dislocations were also found in larger size grain. Twin induced crack tips were observed in our simulation, and this confirmed the results of previous molecular dynamics simulations. At higher temperatures, GB activities can be thermally activated, resulting in suppression of twinning tendency and improvement of ductility of nanocrystalline Mo.

1. Introduction

Nanocrystalline (NC) metals have attracted intensive research interests due to their enhanced mechanical properties compared with coarse-grained materials [1]. Reduction of grain size lead to novel and unique mechanical properties of polycrystalline metals, such as increased strength and hardness, reduced elastic moduli and ductility [2], weakening, or even breakdown, of the Hall-Petch effect [3,4]. As the grain size reduces to nanoscale, the grain boundaries take up a relatively large volume fraction of the system and inherently act as strong barriers to dislocation motions. Additionally, deformation twinning often competes with dislocation slip in the plastically deformed nanocrystalline metals and alloys, especially with low stacking fault energy, low deformation temperatures and high strain rates [5–7]. The activated twinning enriches the possibilities of the material to respond to external load. Twin boundaries can serve as pre-existing dislocation nucleation sites [8], and therefore enhances the ductility in structures with a relatively small number of slip systems. On the other hand, twinning can also degrade the ductility of nanocrystalline materials through facilitating grain boundary (GB) failure [8].

Experimental results show that smaller grain sizes make the deformation twinning more difficult in coarse-grained metals and alloys [9–11], but such grain size dependence fails when the grain size reaches the nanoscale due to that the deformation mechanisms of twinning in nanocrystalline materials are dramatically different from those in coarse-grained scale [5,12]. Twinning can be observed in FCC nanocrystalline with very small grain size. In nanocrystalline materials, several twinning mechanisms have been proposed. Experimental observations and molecular dynamics simulations suggested that the significance of each mechanism changes with grain size [13]. Temperature and strain rate are two important factors affecting the propensity of deformation twinning. It has been verified that low temperature and high strain rate usually promote deformation twinning in nanostructured materials [14]. Generally, the tendency for twinning increases rather slowly with decreasing temperature but much faster with increasing strain rate [5], but there are debates on this issue [15].

Up to data, deformation mechanisms in nanocrystalline FCC are predominantly and extensively studied through experiments and molecular dynamics simulations. Little knowledge has been gained in the past few decades about the deformation mechanisms of NC BCC metals and alloys. So, our current limited knowledge about mechanical properties, particularly plastic deformation of NC bcc structure, merit further investigation. Molecular dynamics (MD) simulation is a power-

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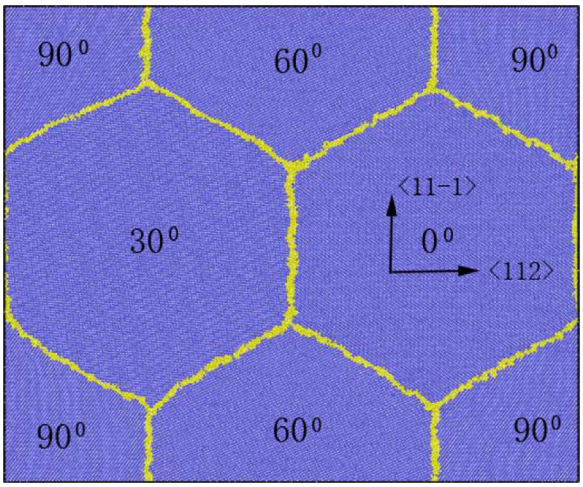

Fig. 1. Snapshot of the fully equilibrated nanocrystalline Mo microstructure with grain size of 24 nm at 300 K prior to loading. The viewing direction is along the [110] columnar axis; the simulation cell contains 12 (110) atomic planes in this direction. In the tensile simulations, loading is applied along the x-direction.

ful tool and has some advantages over experiment for studying plastic deformation in NC materials. By molecular dynamics simulations, deformation twinning in BCC Fe [16], Mo [17] and Ta [18] have been investigated as a secondary deformation mechanism. Recently, MD results by Zhang et al. [8] show that twinning could be the dominant deformation mechanism in NC Mo with a certain orientation. Besides, they give the relationship between grain crack and twinning [8,12].

In the present work, we follow up on the investigation of deformation twinning in NC Mo metal through atomistic simulations, while we are interested in the effects of grain size and temperature. We provide details on molecular dynamics (MD) simulations in Section 2, in Section 3, we present our simulated results and discuss in detail. Conclusions are given in Section 4.

2. Methodology

Our simulations used a periodic 3D < 110 > textured (or columnar) polycrystalline model consisting of four grains of identical size and regular hexagonal shape with a sample thickness of 1.34 nm. The grains are oriented through rotations about the texture axis [1 1 0] with angles of 0°, 30°, 60°, and 90°, which are shown in Fig. 1. The same hexagonal grain structure was adopted to obtain samples with grain sizes from 8 nm to 32 nm (the distance between two parallel GBs). A recently developed embedded-atom method (EAM) interatomic potential for Mo by Smirnova et al. [19] was used to describe the interatomic interactions. Before loading, simulation block was equilibrated at target temperatures and zero pressure in an NPT ensemble to ensure that the system has adequate time to sample a suitable local equilibrium structure. Temperature and pressure of the system were corrected by Nose/Hoover thermostat [20] and Nose/Hoover barostat [21,22] respectively. Fig. 1 shows a relaxed structure at 300 K with grain size of 24 nm.

After equilibration, uniaxial tensile loading was applied by a tiny scaling of the x- coordinate at each time step, and at the same time NPT simulation was performed in the y- and z-directions. The imposed strain rate is $1\times10^{8}\,s^{-1}$ in all simulations of tensile deformation. Common neighbor analysis (CNA) method [23,24] was employed to study the defects evolution during tensile process. All the simulations were performed by the code LAMMPS [25], and all images of atomic configurations in this work are exported using the visualization tool OVITO [26].

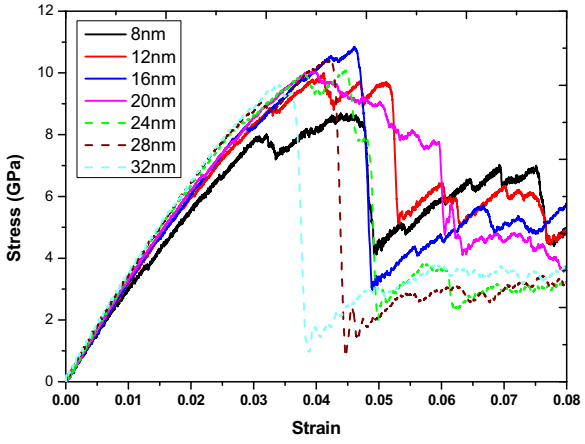

Fig. 2. Stress-strain curves of NC-Mo vs. grain size at temperature of 300 K.

3. Results and discussion

We evaluated the elastic moduli of the samples of various grain sizes from the stress-strain curves, as shown in Fig. 2. Theoretically, the elastic modulus is the slope of the linear portion of a stress-strain curve obtained on an infinitely hard machine [18]. Fig. 2 shows that the elastic limit of the polycrystalline reaches at about 3% strain, which is seems to be independent of the grain size. As shown in Fig. 3, the elastic modulus calculated by fitting linear stress-strain region up to 2% strain varies linearly with the relative density, which is similar to the nanocrystalline Ta [18]. For the polycrystalline system with smaller grain size, the fraction of atoms in grain boundary is larger, which leads to a relative lower density compared with bulk Mo. Within the elastic deformation region, the elastic moduli of nanocrystalline Mo in our simulations are 266.5–311.7 GPa, which is well in agreement with experimental values of 265 GPa by Simmons et al. [27] and 300–330 GPa by Srivatsan et al. [28]. However, it is should be noted that the elastic moduli varies slightly with the tensile orientation. The anisotropy of the elastic moduli has been confirmed by MD simulations [12].

Before reaching the maximum of stress, a zigzag of increase-decrease in stress was found in the stress-strain curves of nanocrystalline Mo with smaller grain sizes. This phenomenon is especially obvious for the grain size of 8 nm and 12 nm, as can be seen in Fig. 2. In the simulations of polycrystalline Mo nanowires under uniaxial tensile loading, a similar zigzag curve was also been observed

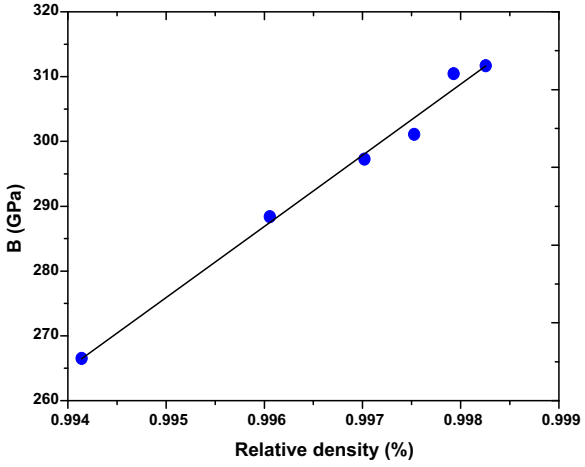

Fig. 3. Linear variation of elastic modulus of NC-Mo as a function of the relative density for each grain size at temperature of 300 K.