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Effect of twist boundary angle on deformation behavior of ⟨1 0 0⟩ FCC copper nanowires

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ABSTRACT

Uniaxial tensile deformation behavior of nano-scale bicrystal copper nanowire with different twist grain boundary which comprises several twist angles is investigated via molecular dynamics simulation to obtain the influence of twist angle on deformation mechanism. The grain boundary twist angle has a significant effect on mechanisms of tensile deformation. Highest amount of twinning activity and creation of staking faults, formation of dislocation locks such as Stair-rod 1/6 ⟨1 1 0⟩ dislocation, and Hirth1/3 ⟨0 1 0⟩ dislocation are witnessed during tensile deformation of Cu nanowire with twist grain boundary angle of ± 15°, whereas amount of twinning and creation of staking faults are comparatively less, and dislocation locks are not evident for Cu nanowire with twist grain boundary angle of ± 30°.

1. Introduction

Unique mechanical properties of metallic nanowires/nanopillars attract research interest due to their potential applications in future nano/micro electromechanical systems (NEMS/MEMS) [1,2]. The nanowires hold an inherent surface stresses as high as tens of GPa due to very small lateral dimensions. The nanowires display unique structural transformations and thermo-mechanical behavior due to its high surface stresses [3–6] and potential candidate for novel and flexible NEMS/MEMS [1]. Cu nanowires is a potential candidate for resonators, smart sensors, transparent electrodes, inter-connectors, organic solar cells and other components of electronic circuits of NEMS/MEMS [7,8]. Understanding the deformation behavior of nanowires is essential for effective potential practical applications.

Researchers found through experimentation and atomistic simulation that the slip of partial/full dislocations is the cause of plastic deformation in many FCC/BCC metallic nanowires [9–18]. Perfect dislocations 1/2 ⟨1 0 1⟩ dissociated in two 1/6 ⟨1 2 1⟩ Shockley partials in {1 1 1} slip planes during plastic deformation of face centered cubic (FCC) materials. In bulk FCC materials, deformation twinning resulting from the glide of Shockley partials in adjacent planes can also contributes to plastic deformation, but limited to low temperature deformation of low stacking fault energy materials [19–22]. Same plastic deformation mechanisms can takes place for high stacking fault energy FCC materials with nano scale characteristic dimensions. The nucleation of Shockley partial dislocations and hence mechanical twinning takes place more frequently for the decreasing grain size [23], size of nanowires [24] or film thickness [25]. Deformation twinning also dominates the plastic deformation for defect-free nanowires and as a consequence amazing properties can be achieved, such as super-plasticity [26,27] or pseudo-elasticity [4,28].

Deformation twinning generally takes place for FCC materials with low stacking fault energy, and for other materials it is limited for high strain rates or low temperatures [29] where high local stresses are generated. A number of experimental [30,31] and atomistic simulation investigations [9–11,13,32,33] have revealed that both FCC and BCC (body centered cubic) metallic nanowires with favorable orientations can plastically deformed by twinning mechanism. Because of small size and the exhaustion of dislocation sources, generation of local high stresses is possible in perfect nanowires [34,35]. It is shown through using in situ scanning electron microscopy and high-resolution transmission electron microscopy for defect-free Au nanowire with ⟨1 1 0⟩ orientation that the plastic deformation takes place by twinning mechanism [30]. It is also reported by different research groups that twinning takes place in ⟨1 0 0⟩ Cu, Au and Ni nanowires under tensile loading [5,9,32] as well as compressive loading [32]. Deformation by twinning leads to reorientation, pseudo-elasticity, shape memory and super-elasticity for both FCC and BCC nanowires [4–6,33,36,37]. The majority of these investigations were conducted on perfect nanowires, but plastic deformation mechanism may alter in the presence of defects such as twist grain boundary.

The current study aims to investigate, at the atomic-scale, the influences of twist grain boundary angle on deformation mechanism i.e. dislocations glide and their interaction, twin nucleation- growth and their interaction. Because of the small space and time scales involved, it is difficult to observe experimentally the impact of twist grain boundary

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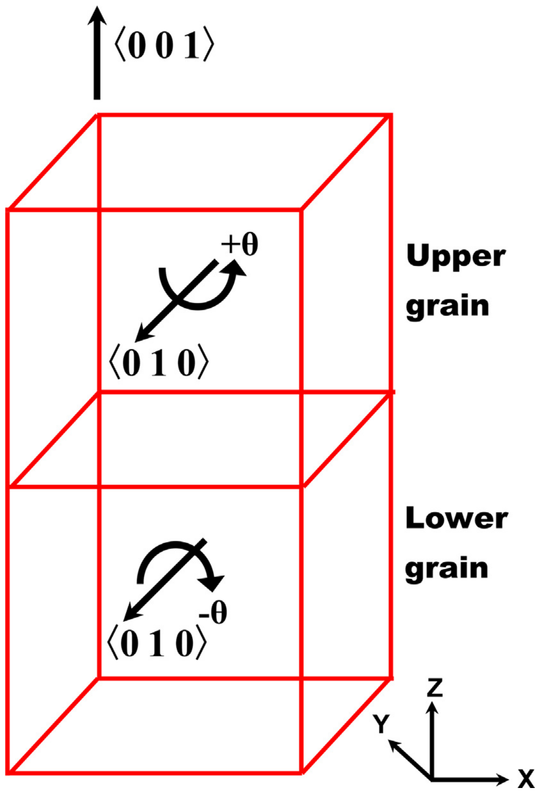

Fig. 1. Schematic of the process of creating a twist grain boundary in ⟨0 1 0⟩ FCC Cu nanowire.

angle on deformation mechanism. On the other hand, atomic-scale simulations used in this study allow for a visualization of plastic deformation mechanisms at the atomic scale and for short time ranges. It is believed that the results obtained could be applicable to other FCC materials with low stacking fault energy and FCC materials with high stacking fault energy at low temperature and high strain rate. This investigation focuses on plastic deformation mechanism in copper which is a good candidate for mechanical twinning at the nano-scale also because of its low stacking fault energy.

Different molecular dynamic simulations of Cu nanowire with and without twist grain boundary at the middle of nanowire are performed. The present work highlights separately the impact of twist grain boundary angle on deformation mechanism of Cu nanowire. Simulation model and procedures are detailed in Section 2. Finally, the influence of twist grain boundary angle on deformation mechanism is discussed in Section 3.

2. MD simulation details

Large-scale atomic/molecular massively parallel simulator (LAMMPS) [38] is used for molecular dynamics simulations. Pre-processing is done in ATOMSK [39]. OVITO [40] is used for post-processing and visualization. Copper (Cu) nanowire with dimensions of $10.8 \times 10.8 \times 11.5\ nm^3$ consisting of about 115,200 atoms arranged in a FCC lattice is created. The single crystal FCC copper nanowires are created such a way that axis is oriented in ⟨0 0 1⟩ with {1 0 0} side surfaces. Three types of twist boundaries are introduced in this study. In order to introduce a twist boundary, the single crystal is divided into two equal half along the axis ⟨0 0 1⟩ and the upper grain is rotated by an angle $+\theta^\circ$ and lower grain by $-\theta^\circ$ around the ⟨0 1 0⟩ axis (Fig. 1). Nanowire with four twist angles (θ) are ± 0°, ± 5°, ± 15° and ± 30° are shown in Fig. 2. Periodic boundary condition is selected along the nanowire length direction (z axis), whereas the other two directions (x and y axis) are kept free to represent infinitely long nanowire. After initial construction of the nanowire in ATOMSK [39], the nanowire is thermally equilibrated to a constant temperature of 300 K in canonical ensemble (constant NPT) with a Nose–Hoover thermostat. To integrate the equations of motion velocity verlet algorithm with a time step of 1 femto second is used. Finally after thermal equilibration, uniaxial tensile deformation is carried out at a constant strain rate of $1 \times 10^9\ s^{-1}$ along the nanowire axis (z-axis).

3. Results and discussion

The uniaxial tensile stress-strain responses of ⟨1 0 0⟩ FCC Cu nanowires with various {0 1 0} twist boundary along with perfect nanowire are shown in Fig. 3. The nanowires with twist grain boundary angle of ± 0°, ± 5° and ± 15° displayed similar elastic deformation at low strains having elastic modulus of 53.5 GPa, while ± 30° twist boundary displayed 82.8GPa elastic modulus. The perfect FCC Cu nanowire (without any twist boundary) exhibited large elastic deformation and higher yield strength in comparison to nanowires with twist boundary. The tensile yield strength of 8.33 GPa obtained for perfect nanowire is close to the theoretical strength of FCC Cu in ⟨1 0 0⟩ direction and the yielding leads to an abrupt large drop in flow stress to about 1 GPa. FCC Cu nanowires with {0 1 0} twist boundaries of ± 5° and ± 15°, ± 30° displayed comparatively small elastic deformation and lower yield strength of 5.1 GPa, 5.4 GPa, and 5.1 GPa respectively. After yielding for all nanowire with twist boundaries along with perfect nanowire are shown flow stress fluctuations at level of 1–2 GPa.

In order to understand the tensile deformation mechanisms of FCC Cu nanowires with various {0 1 0} twist boundaries along with perfect nanowire, the details dislocation evolution have been analyzed at various strain levels using dislocation analysis (DXA) in Ovito [40] and the results are presented in Figs. 4–12. Dislocation evolution during tensile deformation on ⟨0 0 1⟩ Cu nanowire without any twist boundary is shown in Figs. 4, 5 and 6. It can be observed that the original ⟨0 0 1⟩ Cu nanowire (without any twist boundary) yields through the nucleation of multiple 1/6 ⟨1 1 2⟩ Shockley partial dislocation on {1 1 1} plane from the corners of free surfaces (Figs. 4b and 5a). Multiple numbers of Shockley partial dislocation nucleate on the adjacent planes from corners of the free surfaces (Fig. 5a and e). Twin nucleation and growth is shown in details in Fig. 6 at various tensile strain levels. Two Shockley partials on the adjacent planes represent one layer of twin (Fig. 6). This means that twins nucleate from corners of free surfaces and propagate towards the center of the original ⟨0 0 1⟩ Cu nanowire (without any twist boundary) (Fig. 5) with increasing tensile deformation. In this case, the twin boundaries are not able to sweep across the nanowire and as a consequence, the nanowire does not undergo full reorientation. This arises primarily from the initiation of twins from various corners of free surfaces and also the glide of extended dislocations within the twinned region disrupting the twin growth and the reorientation process. The twin-twin interactions lead to the formation of different dislocation locks (example, formation of Stair-rod dislocation), which hinders the motion of twin boundaries. Rohith et al. [13] also observed similar type of dislocation lock formation during tensile deformation of ⟨1 1 0⟩ Cu nanowires. Fig. 4d and 5c show interactions among Shockley partials. Two Shockley partials with 1/6 ⟨−2 −1 −1⟩ and 1/6 ⟨1 2 1⟩ interact with each other and formed a Stair-rod 1/6 ⟨−1 1 0⟩ dislocation. Formation of Stair-rod dislocation acts as a hardening mechanism. Two Shockley partials with 1/6 ⟨−2 −1 1⟩ and 1/6 ⟨−1 −2 −1⟩ interact with each other and formed a 1/2 ⟨−1 0 1⟩ perfect dislocation. Formation of perfect dislocation acts as a softening mechanism as perfect dislocation easily glides along slip planes. With increasing