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Effect of coherent twin boundary and stacking fault on deformation behaviors of copper nanowires

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ABSTRACT

The effect of coherent twin boundary (TB) spacing and stacking fault (SF) spacing on the deformation behaviors of copper nanowires (NWs) is investigated using molecular dynamics simulation. The study indicates that there is a pronounced shift in the mechanical behavior of nanotwinned copper NWs when TB spacing is smaller than 10.23 nm, which declares that there exists an optimal TB spacing, and that the peak stress decreases with decreasing coherent TB spacing, which reveals a reverse Hall–Petch relationship. The results also show that for the specimens with various SF spacing, the peak stress turns out to be a similar trend with those of nanotwinned specimens. When the SF spacing is rather fine, the SF acts as strong barrier like TB. In addition, the deformation behavior of crystalline copper containing parallel alternate TB and SF are also investigated. The results indicate that this model has higher peak stress and potential high peak strain. The general conclusions derived from this work may provide a guideline for the design of high-performance metal NWs.

1. Introduction

Generally, most face-centered cubic (FCC) nanocrystalline metal is produced in polycrystalline forms due to its instinctive isotropy. It is well accepted that the yield strength of conventional polycrystalline metals increases as the grain size decreases, which is known as the Hall–Petch effect [1]. Hence, reducing the grain size to nanometer scale is an effective approach to the production of metals with ultra high strength. However, people soon realize that compared with their coarse-grained counterparts, nanocrystalline metals produced by plastic deformation usually have low ductility. Fortunately, research [2] has shown that by introducing twin boundaries (TB) into nanocrystalline copper, material with simultaneous high strength and high ductility can be achieved. In addition, engineering internal boundaries at nanoscale into ultra-fined-grained copper could obtain better electric conductivity and ductility than conventional coarse-grained copper or ultra-fined-grained copper without the embedded nanotwins as counterparts [3–5]. Therefore, it is very necessary to understand how TB spacing determines the properties of nanocrystalline metal for realizing their future applications in nanotechnology.

TB is known to be as effective as conventional grain boundaries (GB) in strengthening material, offering us a feasible approach to optimize nanoscale material by introducing internal defects so as to obstruct the motion of dislocation and maintain the substantial tensile ductility and electrical conductivity of material [6]. It is convinced that TB in nanowires (NWs) will strongly affect the physical properties of NWs, a lot of researches [7–13] are carried out to investigate the insights of twin structure and its role in metal NWs. One of the main motivations for the research comes from the expectation of remarkable mechanical properties. Zhang et al. [14] argued that whether the coherent TBs strengthen NWs depends on the necessary stress for dislocation nucleation. When the cross-section of NWs changes from square to circular, the TB-induced strengthening effects completely disappear in twinned copper NWs. Deng et al. [15] have shown that when balancing NW diameter and TB spacing, a significant strain hardening effect and a fundamental transition are observed due to the site-specific dislocation nucleation and cross-slip mechanisms. Guo et al. [16] reported that the TB spacing takes control of two competing mechanisms in initial yield of gold NWs: dislocation source number vs. repulsive force, which leads to a transition from softening to strengthening, depending on the dominant mechanism of plastic deformation. Furthermore, studies on transmission of dislocation through TB revealed that TB exerts a repulsive force against the lattice dislocation approaching them [17], and serves as strong barrier to slip. In addition, Song et al. [18] have shown that the yield strength of material can be associated with the dislocation storage ability and the repulsive force between TBs and dislocation. Lu

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et al. [19] indicated that there exists a critical TB spacing revealing the maximum strength in nanotwinned copper. Compared with TB, stacking fault (SF), as one another kind of defects in nanocrystal, seems to draw much lower attention on mechanical properties. Very recently, the SF energy of copper under volumetric, longitudinal, and shear strains are investigated by using the first-principles method based on the density functional theory [20]. However, the relative studies concerning the effects of SF on the deformation behaviors of NWs are still very rare [21,22]. As mentioned above, many studies indicate that introducing appropriate size coherent nanoscale twins within FCC metals can obviously improve the mechanical properties of metals, and obtain ultrahigh strength in metals. According to the strengthening mechanism of TB, it still remains unknown that whether the SF would strengthen the FCC metals in a similar way. Here, we investigate the effect of TB spacing and SF spacing on the tensile deformation behavior of crystalline copper using our MD simulation codes. In addition, the mechanical properties of crystalline copper containing parallel alternate TB and SF are also investigated to reveal the interaction of TB and SF. The general conclusions derived from this study may provide a guideline for the design of high-performance copper.

The rest of the paper is organized as follows: the description of the simulation method will be offered in Section 2. And Section 3 provides the discussion to the results of the simulation. The concluding remarks via the simulation results will be given in Section 4.

2. Simulation model and methodology

The initial configuration used in the present study is completed by a two-step process: (1) create such a unit cell which is bonding the two single copper crystals according to a certain TB or SF orientational relationship; and (2) repeat the coherent TB unit cell, SF unit cell and the alternate TB and SF unit cell for twice along the tension direction. The *X*, *Y* and *Z* directions of the specimens are along the $\langle\bar{1}, 1, 0\rangle$, $\langle 1, 1, \bar{2}\rangle$ and $\langle 1, 1, 1\rangle$, respectively, and *Z* is the tensile loading direction, as shown in Fig. 1. The dimensional sizes of the simulation system in the *X*- and *Y*-directions are 5.7 and 5.8 nm, respectively. The *Z*-direction dimensions for nanotwinned specimens range from 10.8 to 60.9 nm, depending on the TB spacing of nanotwinned copper. For the specimens with SF, the *Z*-direction dimensions range from 6.6 to 61.7 nm, and for copper containing alternate TB and SF, the *Z*-direction range from 11.7 to 61.4 nm, respectively. A standard $(1, 1, 1)$ plane placed without any displacement along the *Z*-direction is denoted as "A", a shift along the *Z*-direction of the plane "A" by a distance $\sqrt{3}a/3$ (α is the lattice constant of copper) is denoted as "B", and a plane with a displacement of $2\sqrt{3}a/3$ along the *Z*-direction is denoted as "C". A perfect single crystal of copper has a plane stacking sequence of ...ABCABCABC... along the *Z*-direction and a single crystal of copper with two TBs has the sequence ...$AB\bar{C}BACBA\bar{C}ABC$..., in which the bold overlined "$\bar{C}$" represents the TB. According to the definition of SF, we can reasonably construct stacking sequence of atoms in our simulation: ...ABC<u>AC</u>ABC... in which the bold underlined "<u>AC</u>" represents the SF. The periodic condition is applied to *Z*-direction while the other two keep free.

The selection of potential function is a key factor, which determinates the results' accuracy in MD simulation. Here, the embedded atom method (EAM) potential developed by Mishin et al. [23] is used to describe the atomic interactions in these simulations. All the MD simulations are performed using the Verlet integration algorithm with the time step of 3 fs. Each model is firstly relaxed prior to deformation for 10,000 steps (30 ps) under the pressure zero pressure (using constant NPT ensemble) to reach the equilibrium state. Then the copper NW is deformed in tensile loading by uniformly adjusting the *Z*-coordinate of each atom according to the applied strain rate of 8.3×10^8 s^{-1} with NVT ensemble at 0.01 K. The common neighbor analysis (CNA) [24] is used to detect the microstructure of the nanocrystal NWs, which can distinguish the local crystal structure of atoms by obtaining information about the relationship between neighbors and atom pairs. This is implemented by using the open visualization tool (OVITO) [25]. It is achievable to analyze and classify the environment of each atom to identify the various deformation mechanisms during tension loading. Here, the FCC, hexagonal close-packed (HCP) and non-structured atoms are colored yellow, red and cyan, respectively.

3. Results and discussion

3.1. Effect of coherent twin boundary on the mechanical behavior of copper

In the first stage, we investigate the effect of TB spacing on the deformation behavior of the copper NWs. Fig. 2 shows the typical stress–strain curves of nanotwinned copper NWs with various TB

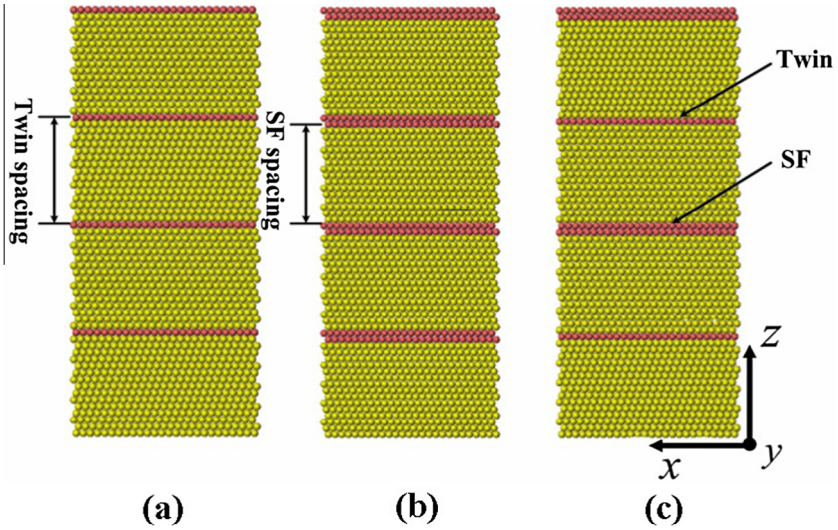

Fig. 1. Atomistic schematic for copper NWs with three different selected structures. (a) NW with coherent TBs, (b) NW with SF, and (c) NW with alternate TB and SF.