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Mechanical behaviors of single crystalline and fivefold twinned Ag nanowires under compression

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ABSTRACT

The mechanical behaviors of fivefold twinned (FT) Ag nanowires under compression are investigated by molecular dynamics simulations. As a comparison, the single crystalline (SC) nanowires are also investigated. The fivefold twin boundary strengthens not only the tensile yield strength but also the compressive yield strength, suggesting the initial stress distribution is not the main factor behind the strengthening. The modulus-based explanation is also found invalid since similar modulus is observed between these two types of nanowires. In contrast to "dislocation starvation" state observed in SC nanowires under compression, the addition of fivefold twin boundary into nanowires leads to complex dislocation–dislocation and dislocation–twin interactions, contributing to increased dislocation density. While extend dislocation slip dominates the plastic deformation in SC nanowires, generation of {001}⟨110⟩ Lomer dislocations and their subsequent cross-slip are found to be the dominant deformation mechanisms in FT Ag nanowires under compression. Effects of boundary condition and sample geometry on plastic deformation behaviors are also investigated.

1. Introduction

In past decade, there has been a great deal of interest in exploring the plastic deformation characteristics of materials at the sub-micron scale. Uchic et al. [1] introduce a new approach to investigate the mechanical behavior of micron-scale single crystals (SC), fabricated by a focused ion beam (FIB), by uniaxial compression test in 2004. This technique opens up a era of mechanically test on various nanopillars [2–5]. The mechanical behavior of these nanopillars beyond the elastic regime is proved to be different from that of bulk materials. Experiments and Molecular dynamic (MD) simulations have demonstrated that yield in metal nanowires (NWs) is dictated by nucleation of Shockley partial dislocations from free surface [6–9]. Furthermore, since the confined volume, dislocations are likely to leave the small crystals before they have a chance to multiply, leading to "dislocation starvation" state. Plastic deformation thus requires nucleation of fresh dislocations from free surface at high stress, which results in the ubiquitously observed size effect of "the smaller, the stronger" and the emergence of intermittent discrete strain bursts [2,10].

Microstructure has a significant effect on the mechanical properties and mechanical behaviors of materials. Among which, the role of nanoscale twins on mechanical strength and plastic deformation in nanomaterials has became a focus of research over last few years [11–25]. Ultrafine-grained copper containing layered growth nanotwins exhibits an unusual combination of ultrahigh yield strength and high ductility [11,12]. By modification of the twin boundary spacing, the mechanical properties can be further optimized [13,14]. The coherent twin boundaries can also significantly influence the limit of elasticity, ultimate strength, rate sensitively, activation volume, work hardening and fracture toughness of FCC metal NWs [15–22]. MD simulations are performed to obtain an atomically resolved observation of plastic deformation mechanisms to understand the role of twin boundary in real materials. The results show twin boundary not only acts as sources of dislocation nucleation [14,23] bust also acts as obstacle for dislocations glide and slip transfer [14–16]. The dislocation-twin reactions are also investigated. The results show a dislocation with burgers vector of 1/2⟨110⟩ can nucleate and glide on a {100} plane instead of conventional {111} planes when a perfect dislocation transmits across twin boundary [24]. Recent study also shows the twin boundary can act as cleavage plane, resulting in ductile-to-brittle transition [25,26].

While a large number of studies have been conducted to investigate the mechanical behaviors of periodically twinned ⟨111⟩ NWs, knowledge about the role of fivefold twin boundary on mechanical behavior is still limited [27–33]. Notably, the technique of synthesizing FT NWs has been greatly improved [34,35].

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Since the orientation of twin boundary with respect to loading axis is found to have significant effect on the mechanical behaviors [18], the deformation behaviors of FT NWs are expected to be quite different. Some novel deformation behaviors have been observed in FT NWs under tension. For example, Wu et al. [36] find the quinquefoliolate flower pattern distribution of initial stress has a significant effect on subsequent mechanical behaviors of FT NWs. By combining experiments and MD simulations, Filleter et al. [37] find surface nucleation of stacking fault decahedrons (SFD) in multiple plastic zones distributed along the axis is the governing deformation mechanism in FT Ag NW under tension. Recently, Jiang et al. claims formation of quasi-icosahedral structures in necking region could also be a possible mode for plastic deformation in FT NWs under tension [38]. However most atomistic calculations have been performed considering axial tensile loading, while comparably few results exist for compression tests [32]. It is well known that the deformation behaviors of NWs under tension and compression are quite different. For example, the ⟨1 1 0⟩ Au NWs are found to deform by dislocation slip under compression and by twinning under tension [39]. The periodically twinned ⟨1 1 1⟩ NWs also display different deformation behaviors under tension and compression [40]. Therefore, it is of great interest to investigate the plasticity of FTNW under compression, which will greatly enrich our knowledge about the twin-mediated plasticity.

2. Simulation methods

Large-scale MD simulations of uniaxial compression tests are performed on ⟨1 1 0⟩ SC and FT Ag NWs using LAMMPS code [41] with time step of 2 fs. The interaction is described by the embed atom method (EAM) potential developed for Ag [42]. The cross-sectional geometries of models considered in this work are displayed in Fig. 1. Each model has diameter of about 20 nm and initial length of about 40 nm. Here the diameter is defined for the circumscribed circle of the pentagonal cross section. Two kind of boundary conditions, viz periodic boundary condition and free boundary condition [6–8,32], are applied along the axial direction respectively, while the other two directions are kept free.

Prior to loading, all samples are relaxed by conjugate gradient energy minimization followed by NVT relaxation for NWs with free boundary condition and by NPT relaxation for NWs with periodic boundary condition at 0.1 K for 20 ps to obtain equilibrated configurations. Compression is performed by imposing displacement to atoms along the long axial direction that varies linearly from zero at bottom to a maximum value at the top layer for NWs with free boundary condition [6,7] and by homogeneously re-scaling the coordinates of all atoms for NWs with periodic boundary condition [8,32]. Regardless of load methods, the samples are relaxed between each increment of strain for 20 ps in NVT ensemble at 0.1 K. The resulting strain is about 5.0×10^7 s^{-1}. The atomic stress is computed by the virial scheme [43]. The local atomic shear strain [44] and central symmetry parameter (CSP) [45] are utilized to analyze the defect structures. Images in this paper are created using OVITO package [46].

3. Results and discussion

3.1. Initial stress distribution

It is well known that surface tensile stress induces intrinsic compressive stress at the interior of metal NWs during relaxation, which has a significant effect on the yield behaviors of NWs [17,47]. Diao et al. [47] propose that the ubiquitously observed size effect on yield stress mainly results from the size dependent intrinsic compressive stress in metal NWs. Therefore, it is necessary to investigate the initial stress distribution in relaxed NWs. Fig. 2 shows the initial stress distribution over the cross-sections of SC and FT Ag NWs after NVT relaxation at 0.1 K (similar results are also found in the case of NPT relaxation). As can be seen from Fig. 2a3 and b3, the initial distribution of Von Mises stress and axial stress over the cross-section of SC Ag NW is quite uniform. Although it is widely recognized that fivefold twin boundary significantly alters the distribution of intrinsic stress, the detail of the distribution of intrinsic stress in FT NW is still controversial [48]. A recent study by Wu et al. [37] shows a quinquefoliolate flower pattern distribution of stress in equilibrated FT Fe NWs, whereas similar distribution is barely observed in other metals, such as Cu [27], Pt [30], Ag [48]. Our current results show the quinquefoliolate flower pattern distribution of Von Mises stress with a local maximum distributing in the shape of five leaflets running along the twin boundaries indeed exists in relaxed FT Ag NWs (see Fig. 2a2). Moreover, in addition to circular FT NW reported by Wu et al. [37], the pentagonal FT NW also displays analogous distribution (see Fig. 2a1). For completeness, we also investigate the effect of temperature on the initial distribution of stress in equilibrated FT NWs by performing relaxation at 300 K, analogous distribution of initial stress still can be observed. This result refutes the speculation by Sun et al. [48] that the reason why they have not observed the specific distribution of initial stress is because the different temperature used in their simulations. A possible reason behind these different observations may be the inappropriate image rendering method by some researchers. In order to distinguish the specific distribution, the stress range of color legend has to be carefully adjusted, therefore the precise magnitude of maximum stress and minimum stress cannot be read out directly from Fig. 2. Anyway, one still can find out the core of FT NW is highly compressed area and considerable tensile area exists in the vicinity of free surface (see Fig. 2b). Furthermore,the axial stress in the core is considerable higher in FT NW than in SC NW.

3.2. Mechanical properties

The typical compressive stress–strain curves of the three samples are shown in Fig. 3. Under loading, all samples first undergo

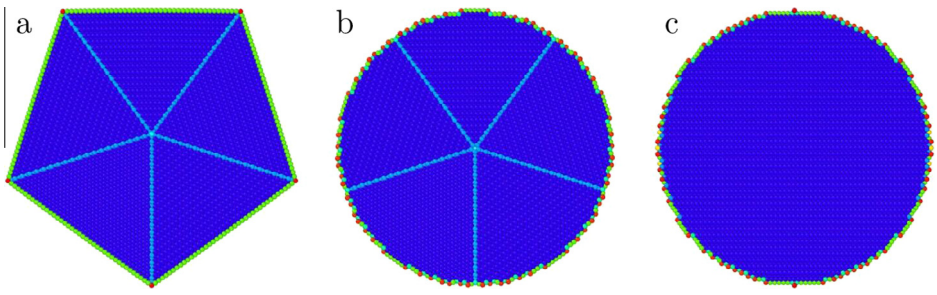

Fig. 1. The cross-sectional geometries and microstructures of models considered in this work. Atoms are colored according to CSP. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)