Detwinning-induced reduction in ductility of twinned copper nanowires

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Detwinning is a unique deformation mechanism of nanotwinned metals with twin lamellae thickness down to a few nanometers. In this work we investigate the impact of detwinning mechanism on the tensile ductility of twinned Cu nanowires containing high density of parallel twin boundaries by means of molecular dynamics simulations. Simulation results show that the fracture strain of twinned Cu nanowires has a strong dependence on twin boundary spacing, resulting from the competition between individual deformation modes. Particularly for the twinned Cu nanowires containing the thinnest twin lamellae, the dominant detwinning mechanism leads to a significant reduction in the tensile ductility. It is found that detwinning originates from twin boundary migration, which is a result of the glide of lattice partial dislocations on the twin planes. This work advances our fundamental understanding of the twin boundary-related mechanical properties of twinned metallic nanowires.

Cu nanowires, twin boundary, uniaxial tension, detwinning, molecular dynamics

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Coherent twin boundary (TB) is a special kind of planar defects whose lattice structures exhibit mirror symmetry across the boundary. TB has drawn wide range of interest for its unique properties: it acts as effective obstacle to dislocation motion due to its low excess energy and thus strengthens materials, and has low electrical resistivity because of the coherent characteristic. Consequently, a superior combination of ultrahigh strength and high electrical conductivity was achieved in ultrafine-grained polycrystalline Cu by introducing high density of growth TBs [1,2]. Most importantly, unlike the conventional grain boundary (GB) strengthening which makes materials strong but brittle, the TB strengthening found in metallic materials is accompanied with no significant reduction in ductility, which thus provides novel possibilities to develop advanced functional nanostructures [3,4]. However, the role of TBs playing in

the ductility of metallic materials of extremely small dimensions, e.g. nanowires (NWs) with high surface to volume ratio, is distinctly different from their bulk counterparts, as the introduction of TBs does not always monotonically contribute to their ductility. Atomistic simulations have demonstrated that the introduction of fivefold growth TBs can compromise the ductility of metallic NWs significantly [5–7]. Sansoz et al. [8] found via atomistic simulations that the failure strain of Au NWs containing embedded TBs is significantly smaller than the single crystal one. More recent tensile experiment discovered the mechanical formed TBs-induced brittle-like fracture in sub-20 nm Au NWs [9]. Therefore, our fundamental understanding of the TBs-related ductility in metallic NWs is far from being completed.

The unique dislocation-TB interaction, as the central issue governing the mechanical properties of nanostructured materials containing TBs, has strong dependence on twin lamellae thickness. Both experiments and atomistic simula-

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tions have demonstrated that there exists a critical twin boundary spacing (TBS) below which softening occurs. The softening is ascribed to the transition in yielding mechanism from the slip transfer across TBs to the mobilization and multiplication of pre-existing dislocations or the nucleation and motion of partial dislocations parallel to twin planes [10,11]. The alternation of dominant deformation mechanism in softening regime accompanied with the transition in yielding mechanism is expected to have strong impact on the ductility of materials. Particularly for metallic NWs containing high density of TBs, the TB-associated mechanism such as TB migration and detwinning may play pronounced even dominant role in the plastic deformation, because the nucleation and motion of lattice dislocations are severely restricted. In this work, we perform molecular dynamics (MD) simulations to elucidate the fundamental deformation mechanisms operating in twinned Cu NWs containing high density of parallel TBs subjected to uniaxial tension. We further study the influence of TBS on the deformation behavior of the NWs. We find that the dominant detwinning mechanism leads to a significant reduction in the tensile ductility of twinned Cu NWs with the thinnest twin lamellae thickness.

1 Simulation method

Figure 1 shows that four [111]-oriented Cu NWs, as one

Figure 1 (Color online) Cross-sectional views of MD models of Cu NWs. (a) Single; (b) NW1; (c) NW19; (d) NW9. Atoms are colored according to calculated CNA values, as green for FCC atoms, blue for TB atoms, and gray for surface atoms.

single crystalline and three twinned, are considered in current work. The diameter and length of those NWs with circular cross-section are the same as 5.9 and 28.2 nm, respectively. The atomic interactions between approximately 65600 face-centered cubic (FCC) Cu atoms are described by the well-established EAM potential developed for Cu [12]. The three twinned Cu NWs have different twin lamellae thicknesses: NW1 and NW9 have monotonic TBS of 0.63 and 5.64 nm, respectively, and NW19 has gradient TBS at a range of 0.63–5.64 nm. Periodic boundary condition (PBC) is only applied along the [111] axial direction of the NWs, and the other directions are free. Note that, the applying of PBC along axial direction yields an infinite long length, which may result in the Rayleigh instability of NWs under high strain rate. The size-dependent deformation behavior of NWs with finite length can be found elsewhere [13,14].

Prior to uniaxial tension, the as-created NWs are subjected to following relaxation procedures to reach their equilibrium configurations: the atoms are first relaxed to their local minimum energy configurations, followed by dynamic relaxation at 30 K under 0 bar using the Nose-Hoover thermostat for 150 ps in the isothermal-isobaric NPT ensemble. After the completion of relaxation, uniaxial tension of Cu NWs is performed in the canonical NVT ensemble at 30 K by straining the simulation box along [111] axial direction with constant strain rate of $5 \times 10^7 \text{ s}^{-1}$. The common neighbor analysis (CNA) is adopted to identify defects generated in the NWs during deformation process, and the difference between intrinsic stacking fault (ISF) and TB is further distinguished [15,16]. The coloring scheme is: green stands for FCC atoms, red for ISF atoms, blue for TB atoms, and gray for Other atoms including free surface and dislocation cores. All the MD simulations are performed by using the LAMMPS code with a time step of 1 fs [17]. And the OVITO is utilized to visualize MD data and generate MD snapshots [18].

2 Results and discussion

Figure 2 plots the stress-strain curves of the four Cu NWs subjected to uniaxial tension. The elastic deformation behaviors of all the NWs are approximately the same, as the stress increases linearly with the same slope until the strain reaches its elastic limit. It indicates that the Young's modulus of Cu NWs is not influenced by the introduction of aligned TBs, which agrees well with previous observations [13]. The calculated Young's modulus of the [111]-oriented Cu NWs is 161 GPa. The yield stress and associated elastic strain limit are approximately the same for all the NWs, indicating there is no obvious strengthening effect of TBs in the NWs. It should be noted that our observation is of considerable difference from the strengthening effect of TBs reported by previous studies [19,20]. This discrepancy may be related to the low temperature of 30 K and the Foiles

Figure 2 Stress-strain curves of uniaxial tension of Cu NWs. The inset shows the fracture strains of simulated NWs.

EAM potential utilized in current work. The temperature-dependent mechanical properties of NWs have been widely reported [21,22]. Furthermore, recent experimental study also suggested that the strengthening effect of TBs depends strongly on temperature [23].

It is seen from Figure 2 that the slope of dramatically decreased stress after the yield point, caused by the initiation of plasticity, is also the same for each NWs. However, there is dramatic difference in the yielding mechanism of Cu NWs with different twin thicknesses. The incipient plasticity of single crystal and twinned NWs with large TBS, i.e. NW19 and NW9, is governed by the nucleation of lattice partial dislocations from free surface and subsequent glide. In contrast, the yielding of NW1 is dominated by the nucleation of twinning partials from perfect TBs, which is also seen in indentation test [24]. Figure 2 demonstrates that the stress-strain curves show significant deviations after the precipitous drop of stresses. In particular, the inset of Figure 2 shows that there is distinct difference in the fracture strain

of Cu NWs containing different internal microstructures. It is seen that the single crystalline Cu NWs possesses larger fracture strain than twinned ones, indicating that the tensile ductility of twinned Cu NWs is compromised by the presence of TBs due to the plastic localization [8]. While the lower and upper bounds of the TBS of NW19 correspond to the TBS of NW1 and NW9, respectively, it is interesting to note that the fracture strain of NW19 with gradient TBS is also intermediate among twinned Cu NWs. Thus, Figure 2 clearly demonstrates the twin lamellae thickness dependence of the tensile ductility of twinned Cu NWs: the smaller the TBS, the lower the tensile ductility.

To reveal the origin of the twin lamellae thickness-dependent tensile ductility in twinned Cu NWs shown in Figure 2, the deformation mechanisms of Cu NWs are investigated by statistically analyzing the evolutions of atoms in different lattice structures. Figure 3(a) and (b) shows the variations in the reduced numbers of FCC atoms and Other atoms upon strain, respectively. The reduced number is calculated by subtracting the base number before deformation using the measured number. For single crystalline Cu NWs and twinned ones with large TBS, i.e. NW19 and NW9, the number of FCC atoms decreases accompanied with increasing Other atoms prior to fracture, demonstrating that dislocation activity is the major plastic deformation mode as the change in Other atoms is mainly contributed by nucleation and motion of lattice dislocations. However, the strong fluctuations in their evolutions of FCC atoms suggest that there is another deformation mode of deformation twinning also playing role in the plastic deformation. Dynamic analysis of instantaneous defect evolutions reveals that the newly formed mechanical TB is originated from the dissociation of lattice partial dislocations, which consequently results in an increase of FCC atoms [25].

In contrast to the decreasing FCC atoms in single crystalline Cu NWs and twinned ones with large TBS, Figure 3 shows that the number of FCC atoms in NW1 with the

Figure 3 Evolutions of atoms in different lattice structures during the tension process. (a) Reduced number of FCC atoms; (b) reduced number of Other atoms; (c) reduced number of HCP atoms. The reduced number is calculated by subtracting the base number before deformation using the measured number.

smallest TBS increases during plastic deformation, accompanied with simultaneously increase in the Other atoms. Since the increment of Other atoms in the NW1 is the smallest and there is no reduction in FCC atoms, it suggests that the dislocation density in NW1 is minor and dislocation activity cannot be the dominant deformation mechanism. To reveal the deformation mechanisms of NW1, Figure 3(c) further presents the evolutions of HCP atoms in twinned NWs upon strain. It is seen that during plastic deformation the number of HCP atoms in the twinned NWs with large TBS increases with strong fluctuations, which are resulted from the dissociation of lattice partial dislocations into mechanical TBs. However, the number of HCP atoms in NW1 decreases slightly. The decrease of HCP atoms can be caused by detwinning, i.e., disappearance of TBs, in addition to the formation of mechanical TBs. However, deformation twinning cannot be the dominant plastic deformation mode of NW1 with TBS of 0.63 nm, which is the minimum period of stacking sequence of ABC in [111] crystallographic orientation of Cu lattice. Thus, it reveals that the plastic deformation of NW1 is dominated by detwinning.

Figure 4 presents cross-sectional views of Cu NWs at their fracture points, which shows that there is a neck region formed accompanied with failure in each NWs. Furthermore, the length of neck region is larger in NWs with larger fracture strain. Figure 4 also demonstrates that the failure position of NWs varies significantly upon internal microstructure. Previous atomistic simulations suggested that the failure position of NWs under nano-stretching strongly depends on the NWs length, and follows a statistical distribution [13,26]. Figure 4(a) shows that there is no TB observed in the neck region of NW1, and dislocation activity in the NWs is severely restricted by TBs. Furthermore, the TBs near the neck region of NW1 undergo significant TB migration, as evidenced by their increased TBS. The occurrence of significant TB migration and subsequent detwinning in NW1 provides increased space to accommodate nucleation and subsequent glide of lattice dislocations. Correspondingly, the number of FCC atoms in NW1 first increases

dramatically caused by detwinning, followed by minor decrease due to the emergence of dislocation activity, as shown in Figure 3(a). In contrast to glide of lattice partial dislocations parallel to twin planes in bulk nanotwinned Cu with small TBS, Figure 4 shows that lattice dislocations are mainly inclined to TBs for all the twinned Cu NWs. Figure 4(a) and (b) shows that lattice partials nucleate from TBs that lose their coherency due to dislocation-TB interaction. However, TB migration is not pronounced in twinned Cu NWs with large TBS, the plastic deformation of which is dominated by dislocation activity. Figures 3 and 4 jointly demonstrate that dislocation activity has strong dependence on twin lamellae thickness: the larger the TBS, the higher the dislocation density, and the higher the tensile ductility.

To probe the mechanism of dominant detwinning in NW1 with the thinnest twin lamellae thickness, the instantaneous deformation structures prior to the occurrence of fracture are analyzed. Figure 5(a) shows that the plasticity of NW1 is governed by the nucleation of twinning partials and resulting TBs losing coherency, accompanied with the nucleation and subsequent glide of lattice partials parallel to twin planes. The glide of lattice partials on twin planes leads to shrinking of TBs and formation of three HCP-coordinated layers. Figure 5(b) shows the widening of twin lamellae thickness in the neck region due to TB migration, and complete annihilation of lattice partials is also observed. Upon further loading, TBS is significantly increased to provide additional space to accommodate dislocation activity. Figure 5(c) shows that a leading partial nucleates from the surface of neck region and intersects with TB. Consequently, TB migration and detwinning triggered by the dislocation-TB interaction occur again. The thickness of twin lamellae containing leading and trailing partials shown in Figure 5(d) is 3.75 nm, increased by a factor of 6 in comparison with the original value of 0.63 nm. Figure 5 reveals that TB migration and subsequent detwinning are originated from the nucleation and subsequent glide of lattice partial dislocations parallel to the twin planes, which is in good agreement with recent experimental studies and atomistic simulations [11,27–29].

Figure 4 Cross-sectional views of Cu NWs at fracture strain. (a) NW1; (b) NW19; (c) NW9; (d) single. Atoms are colored according to CNA values.

Figure 5 Instantaneous deformation structures of NW1 during detwinning process. Strain of (a) 0.084; (b) 0.144; (c) 0.16; (d) 0.176.

3 Summary

In summary, we perform MD simulations to investigate the uniaxial tension of twinned Cu NWs containing high density of parallel TBs. Simulation results reveal that the plastic deformation modes of Cu NWs include dislocation activity, deformation twinning, TB migration and detwinning. Furthermore, twin lamellae thickness has strong influence on the competition between individual deformation modes, which in turn affects the tensile ductility of Cu NWs: the smaller the TBS, the smaller the fracture strain. In particular for the smallest TBS of 0.63 nm, the dominant detwinning mechanism leads to a significant reduction in the tensile ductility of the twinned NWs. It reveals that TB migration and subsequent detwinning originate from the nucleation and glide of lattice partial dislocations parallel to the twin planes.

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