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Layer thickness dependent tensile deformation mechanisms in sub-10 nm multilayer nanowires

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Using molecular dynamics simulations, the tensile deformation behavior for two types of sub-10 nm multilayer nanowires (NWs) have been investigated. For the structure with interfaces perpendicular to the wire axis, the deformation mechanism is changed from interface crossing by dislocations to interface rotation as the layer thickness is decreasing, causing a significant reduction in yield strength. However, the deformation mechanisms are all accommodated through interface crossing by dislocations regardless of layer thickness for the structure with interfaces parallel to the wire axis. Moreover, the yield strengths in the second structure are found to be controlled by two competing mechanisms: the interface strengthening by increased repulsive force and interface softening by increased dislocation source sites. The sudden stress drop after yielding point in NWs could be explained by the dislocation source-limited hardening mechanism: the more atomic fraction of newly formed stacking faults (SF) after stress drop, the larger normalized stress drop and the larger uniform tensile elongation. For the second structure, the larger total tensile elongation for larger layer thickness could be related to the twinning induced plasticity at the necking position. These findings should have implications for designing functionalized structures and devices in nanoelectromechanical systems. © 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4730337>]

I. INTRODUCTION

The continuing trend of miniaturization in many modern technological applications, such as sensors, actuators, and electronic devices, has led to a strong demand for understanding the size-dependent deformation and fracture behaviors in one-dimensional (1D) metallic nanostructures.^{1–4} Recent experiments and simulations on 1D nanostructures, such as nanopillars and nanowires (NWs), have revealed the phenomenon so called “smaller being stronger”—the strength of structures tends to rise up as their sample size decreases without the presence of strain gradients.^{3–24} In the micron and sub-micron length scale, a conceptual framework of “dislocation starvation”^{6,7,12,16} was proposed to be responsible for the apparent size-dependent behavior. Unlike bulk samples, gliding dislocations in 1D sub-micron structures can travel only very small distances before annihilating at free surfaces, thereby reducing the overall dislocation multiplication rate. Such processes would lead to a dislocation-starved state requiring very high stresses to nucleate new mobile dislocations. When the sample size is further reduced to tens of nanometers or below, the possibility of defects and flaws is dramatically decreased inside the sample, so surface dominated plasticity (surface nucleated short-lived dislocation) has been found to play a more critical role in controlling deformation and subsequent fracture behaviors.^{5,13,22,23} Bi-metal multilayer NWs have attracted

much more attention in recent years because of their potential applications for functionalizing purposes in nanoelectromechanical systems (NEMS).^{25–30} The sample size and layer thickness may exert significant influence on the mechanical, electrical, optical, and magnetic properties in multilayer NWs, especially when both length scales reach tens of nanometers or below. Unlike in the bulk multilayer systems, where strengthening is arising only from interface,^{31–34} both free surface and interface are expected to compete in controlling the plastic deformation in multilayer NWs. When both of the two characteristic length scales (sample size and layer thickness) reach tens of nanometers or below, two intriguing issues worth of comprehensive study are (1) What are the dominant plastic deformation mechanisms in such NWs? (2) How the layer thickness affects the dominant plastic deformation mechanisms in such NWs?

In this regard, atomistic simulation has been used to investigate uniaxial tensile deformation in two types of sub-10 nm Cu-Ag multilayer NWs in the present study [see Fig. 1 for illustration]. The first structure is a composite NW formed by alternating nano-layers of Ag and Cu with interfaces perpendicular to the wire axis, while the second structure has interfaces parallel to the wire axis. As suggested by the experimental results for the textured Cu-Ag multilayer systems,^{31,32} the simulated interface plane in the NWs is {111}Cu/{111}Ag and the layer thickness could be less than 1 nm. To circumvent the complexity of highly disordered surface structures in cylindrical samples, NWs with rectangular cross sections were considered in the present simulations. In order to study the layer thickness effect on

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FIG. 1. Schematic of tensile deformation for bi-metal multilayer nanowires: (a) Structure with interfaces perpendicular to the wire axis; (b) structure with interfaces parallel to the wire axis.

the deformation mechanisms, we fixed the lateral dimension of NWs to be approximately 6 nm and the modulation ratio (defined as the ratio of Cu layer thickness to Ag layer thickness) to be approximately 1, and varied the layer thickness from 0.68 to 10.93 nm.

II. SIMULATION METHODS

Schematic of uniaxial tensile deformation for two types of sub-10 nm Cu-Ag multilayer NWs is shown in Fig. 1. In the first structure, the dimensions for the NWs were kept to be $6 \times 6 \times 42.5$ nm, and four different layer thicknesses $\lambda/2 = 0.68, 1.37, 5.46, 10.93$ nm were investigated (where λ is the modulation period). In the second structure, the dimensions for the NWs were kept to be $6.5 \times 6.5 \times 38.1$ nm, and three different layer thicknesses $\lambda/2 = 0.68, 1.70, 3.40$ nm were simulated. It should be noted that the lateral dimensions of NWs used in the present study are much larger than those of NWs (which typically have

diameters less than 3 nm) showing pseudoelasticity induced by crystal reorientation or phase transformation.^{27–30,35–41}

MD simulations reported in this work were performed using large-scale atomic/molecular massively parallel simulator (LAMMPS) developed by Plimpton and co-workers.⁴² The Cu-Ag system is simulated using embedded atom method potentials developed by Williams *et al.*⁴³ The calculated intrinsic stacking fault (SF) energies based on the potential are 44.4 and 17.8 mJ/m² for Cu and Ag, respectively, which are consistent with the experimental data.⁴³ The calculated unstable stacking fault energy based on the potential are 158 and 115 mJ/m² for Cu and Ag, respectively, which are consistent with either the tight-binding approximation or the *ab initio* calculation.⁴³ The surface energies based on the potential are 1472, 1330, and 1231 mJ/m² for (110), (100), and (111) surfaces in Cu, respectively, while the corresponding surface energies are 1017, 940, and 862 mJ/m² for (110), (100), and (111) surfaces in Ag, respectively.⁴³ Those values may be slightly underestimated compared to those of experimental data, but it is a common feature of embedded atom model (EAM) potentials. Although the interface energy from the potential⁴³ is not provided, the value should be similar to those of stacking fault energies and much smaller than those of surface energies. The Cu-Ag cross-interaction function in the potential is also fit to first-principles data, and the calculated Cu-Ag phase diagram is in satisfactory quantitative agreement with experiment.⁴³ Periodic boundary conditions were imposed along the wire axis to mimic infinitely long wires, while the NW was kept free in all other directions. A constant time step of 2 fs was used. Before tensile loading, the NWs were first subjected to energy minimization by the conjugate gradient method, then gradually heated up to the desired temperature in a step-wise fashion, and finally relaxed in the Nose/Hoover isobaric-isothermal ensemble (constant number of particles, pressure, temperature, NPT) under both the pressure 0 bar and the desired temperature (300 K) for 50 ps. The NWs were then deformed in tension by straining the simulation box at a constant strain rate of 5×10^8 s⁻¹ along the wire axis with canonical ensemble (constant number of particles, volume, temperature, NVT) at 300 K. The local atomic arrangement of the deformed configuration was then visualized using a common neighbor analysis algorithm.⁴⁴

The stresses reported in this work were calculated based on the Virial theorem,⁴⁵ which is equivalent to the Cauchy stress in the average sense,

$$\sigma^{\alpha\beta} = \frac{1}{V} \left(\sum_{i=1}^N m_i v_i^\alpha v_i^\beta + \frac{1}{2} \sum_{i \neq j}^N r_{ij}^\beta F_{ij}^\alpha \right), \quad (1)$$

where V is the volume of the sample, m_i is the atomic mass, v_i^α is the α component of the velocity vector at atom i , r_{ij}^β is the β component of the vector that joins atom i and j , and F_{ij}^α is the α component of the force that atom i exerts on atom j . Stress calculations have been done replacing V at each instant by its initial value. This gives what is known as engineering stress. Accordingly, we have used the increment in length divided by the initial length to calculate engineering strain.

III. RESULTS AND DISCUSSIONS

The engineering stress-engineering strain curves for the first structure and the second structure are shown in Figs. 2(a) and 2(b), respectively. In Fig. 2(b), the stress-strain curves for single crystal Ag and Cu nanowires with the same orientation and sample size as the second structure are also shown. The yield stress versus the inverse square root of layer thickness $((\lambda/2)^{-1/2})$ for both structures are plotted in Fig. 2(c). In Fig. 2(c), the stress level calculated by rule of mixed (mixed by the yield stresses of single crystal Ag and Cu nanowires with volume percentages) is also shown for the second structure. For the first structure, the results in the Fig. 2(c) indicate that when the sample size and modulation ratio are fixed, the yield stress decreases slightly as the layer thickness is reduced from 10.93 to 5.46 nm, while there is a dramatic reduction for the yield stress as the layer thickness is further reduced from 5.46 to 1.37 nm.

In order to understand the underlying mechanisms for the dramatically reduction of yield stress when the layer thickness is reduced from 5.46 to 1.37 nm in the first structure, close inspections of the deformation snapshots showing onset of plasticity have been done for the first structure with these two layer thicknesses. Fig. 3(a) shows the corresponding results for the large layer thickness ($\lambda/2 = 5.46$ nm). The lattice mismatch between FCC Cu and FCC Ag is about 13.1%. Due to this large mismatch of lattice parameters, misfit dislocation networks are formed at the interface as shown in Fig. 3(a), which makes the interface to be so-called semi-coherent interface.³² When the NW is deformed to 3.65%, the stress in the NW reaches the maximum, and the first $1/6\{111\}\langle 112\rangle$ leading partial dislocation is nucleated from the ledge of free surface in Ag layer as indicated by black arrow, with SF left behind. When the NW is deformed to 3.7%, the partial dislocation propagates on the primary $\{111\}$ slip plane and reaches the interface 1. When the NW is deformed to 3.8%, the partial dislocation cuts through the interface 1 (interface crossing by dislocation interactions) due to the high yield stress and continues to propagate in Cu layer. When the NW is further deformed to 4.0%, the leading partial cuts through the interface 2 and finally is absorbed by the opposite free surfaces, another partial dislocation in different slip system is nucleated from the interface 2 and propagates to the free surfaces at the same time. Fig. 3(b) shows the corresponding results for the small layer thickness ($\lambda/2 = 1.37$ nm). When the layer thickness is such small, the deformation mechanisms for onset of plasticity are totally different, and the plastic deformation is accommodated by interface rotation and shear offset induced by interface rotation instead of dislocation nucleation from free surface and interface crossing. The dramatic drop of yield stress observed in Fig. 2(c) is most likely due to this change in the dominant plastic deformation mechanisms.

The plastic deformation mechanisms for the second structure with all layer thicknesses ($\lambda/2 = 0.68, 1.70, 3.40$ nm) are all accommodated by dislocation nucleation from free surface and interface crossing (the corresponding deformation snapshots are not shown here for spacing saving purpose). However, the yield stress still decreases slightly

FIG. 2. (a) Engineering stress strain curves for the structure with interfaces perpendicular to the wire axis; (b) Engineering stress strain curves for the structure with interfaces parallel to the wire axis (the apparent necking starting points are marked by solid circle point for the multilayer NWs); (c) the yield stress versus the inverse square root of layer thickness $((\lambda/2)^{-1/2})$ for both structures.

FIG. 3. Mechanisms for onset of plasticity for the first structure with layer thickness of: (a) $\lambda/2 = 5.46$ nm; (b) $\lambda/2 = 1.37$ nm. Color coding: hcp for Ag (pink); free surface, dislocation core, and other atoms for Ag (grey); hcp for Cu (red); free surface, dislocation core, and other atoms for Cu (green); perfect fcc atoms for both Ag and Cu (black). Perfect fcc atoms are not shown in this figure, and front two free surface atoms are not shown for clarity for Fig. 3(a). The same color coding is used in all figures of present study.

with the reducing layer thickness without change of deformation mechanisms [(see Fig. 2(c)]. Moreover, the yield stress is found to be higher than that calculated by rule of mixed when layer thickness is large ($\lambda/2 = 1.70, 3.40$ nm), while the yield stress is lower than that calculated by rule of mixed when layer thickness is smaller ($\lambda/2 = 0.68$ nm). As suggested in the literatures,^{46–48} the dislocation nucleation rate is used to measure the ease of dislocation nucleation and control the onset of plasticity in NWs. According to the Arrhenius law, the nucleation rate can be written as: $p = Np_0 \exp(-\frac{\Delta E}{k_B T})$, where p_0 is the attempt frequency, N is the number of dislocation nucleation source sites, ΔE is the activation free energy for thermally activated dislocation processes, k_B and T are the Boltzmann constant and absolute temperature, respectively. In our case, the activation energy

can be written as $\Delta E = E_d + E_\varepsilon + E_\gamma + E_{interface}$, where $E_d, E_\varepsilon, E_\gamma$, and $E_{interface}$ represent the self-energy of the dislocation, the strain energy relieved by the dislocation, the stacking fault energy, and the repulsive interaction energy due to the interface, respectively.⁴⁹ So, in multilayer NWs, the nucleation rate can be finally written as $p = Np_0 \exp(-\frac{E_d + E_\varepsilon + E_\gamma + E_{interface}}{k_B T})$. Based on this equation, it apparently shows that there are two competing mechanisms which control the onset of plasticity in the second structure: (1) the interface strengthening—interface is a generator of the repulsive force which acts against the nucleation of dislocations (more interfaces provide larger $E_{interface}$); (2) the interface softening—interfaces themselves serve as source of dislocation nucleation, more interfaces provide more heterogeneous structural sites on the surface and/or free surface/interface junctions to allow the nucleation of dislocations more easily (more interfaces give larger N).^{7,32,48} So the first strengthening mechanism could be used to explain why the yield stress is higher than that calculated by rule of mixed when the layer thickness is large ($\lambda/2 = 1.70, 3.40$ nm). While the slightly softening trend with decreasing layer thickness could be due to the second mechanism.

Besides the size dependent high yield stress observed in NWs, recent experiments⁵⁰ and numerical simulations^{5,8,15,51–54} have identified a sudden large stress drop at the yield point. Our simulation results also show this abnormal stress drop after yield point, and the normalized stress drop at yield point in the second structure is increasing with increasing layer thickness, as shown in Fig. 2(b). This abnormal stress drop may be explained by the dislocation source-limited hardening mechanism.^{5,55,56} Before yielding, a high stress is needed to nucleate dislocations from free surface and/or free surface/interface junctions because of limited dislocation sources. However, once the SF and other defects are introduced inside the NWs after yielding, the stress decreases abruptly due to the

FIG. 4. The normalized stress drop at the yielding point and the tensile elongation versus the atomic fraction of newly formed SF after stress drop.

FIG. 5. Deformation and failure processes for (a) the first structure with layer thickness $\lambda/2 = 5.46$ nm; (b) the first structure with layer thickness $\lambda/2 = 1.37$ nm; (c) the second structure with layer thickness $\lambda/2 = 0.68$ nm.

increased dislocation sources. The more SF and other defects introduced inside the NWs, the larger stress drop after yield point. We plotted the curve with the normalized stress drop at yield point against the atomic fraction of newly formed SF after stress drop for the second structure in Fig. 4. The uniform and total plastic elongations versus

the atomic fraction of newly formed SF after stress drop are also plotted in Fig. 4. The results indicate that the atomic fraction of newly formed SF is closely related to the magnitude of stress drop and the uniform tensile elongation: the more atomic fraction of newly formed SF, the larger normalized stress drop, and the larger uniform tensile elongation.

Fig. 5(a) shows the detailed failure processes for the first structure with large layer thickness ($\lambda/2 = 5.46$ nm) during tensile loading. The necking instability sets in at the Ag/Cu interface when the NW is deformed to 8%, causing limited uniform elongation. As we mentioned before, interfaces themselves serve as sources of dislocation nucleation, providing heterogeneous structural sites to nucleate dislocations more easily. So, it is not surprising to observe necking initiation accommodated by dislocation slip at the interface. This

FIG. 6. Formation processes of deformation twins at the position close to the necking point: (a) for the first structure with the layer thickness $\lambda/2 = 5.46$ nm; (b) for the second structure with layer thickness $\lambda/2 = 3.40$ nm. Only perfect fcc atoms and hcp atoms are shown in this figure for clarity.

strain localization leads to a final rupture in the weaker Ag layer, but at a position close to the interface. Fig. 5(b) shows the detailed failure processes for the first structure with small layer thickness ($\lambda/2 = 1.37$ nm) during tensile loading. In contrast, onset of plasticity is accommodated by interface rotation when the layer thickness is small. As a result, shear offset is introduced at the interface during stretching. With increasing strain, shear offset is exacerbated, localized at some specific interfaces, which finally leads to shear failure at one of interfaces. Fig. 5(c) shows the detailed failure processes for the second structure with small layer thickness ($\lambda/2 = 0.68$ nm) during tensile loading (the failure processes for larger thicknesses are not shown here because they have similar deformation and fracture processes). The failure of the second structure is fulfilled by the stable growth of shear offset and subsequently necking at the shear offset position. The growth of shear offset is accommodated by continuing dislocation nucleation from free surface and subsequently slip in two major slip planes. As a result, the dislocation slip leads to local area reduction and necking. The NW is eventually fractured at the necking position.

In order to understand the post necking deformation process, close inspections of the deformation snapshots at the position close to the necking point have been done for the first structure with larger layer thickness ($\lambda/2 = 5.46, 10.93$ nm) and the second structure with all layer thickness ($\lambda/2 = 0.68, 1.70, 3.40$ nm). For the first structure, deformation twins (DTs) are observed for all layer thickness when the fracture process is accommodated by necking ($\lambda/2 = 5.46, 10.93$ nm). However, DTs are only observed for the second structure when the layer thickness is large ($\lambda/2 = 3.40$ nm). Here, we only present the deformation snapshots with the formation processes of DTs for the first structure with layer thickness of 5.46 nm and the second structure with the layer thickness of 3.40 nm, as shown in Figs. 6(a) and 6(b), respectively. For the second structure, it is found that the total plastic elongation for large layer thickness ($\lambda/2 = 3.40$ nm) is much higher compared to those of smaller layer thickness ($\lambda/2 = 1.70, 0.68$ nm), as shown in Fig. 4. This could be related to the twinning induced plasticity at the necking position.⁵⁷

IV. CONCLUSION REMARKS

In summary, the tensile deformation behaviors for two types of sub-10 nm multilayer NWs have been investigated by using molecular dynamics simulations. For the structure with interfaces perpendicular to the wire axis, a change in the deformation mechanism from interface crossing by dislocations to interface rotation is observed with reducing layer thickness. The yielding stress associated with interface rotation is found to be much smaller compared to the case of interface crossing by dislocations. However, the deformation mechanisms are all accommodated through interface crossing by dislocations regardless of layer thickness for the structure with interfaces parallel to the wire axis. The yield stress still decreases slightly with the reducing layer thickness without change of deformation mechanisms for the second structure. Moreover, the stress level calculated by rule of mixed is found to be lower than the yield stress for large

layer thickness, while higher than that for small layer thickness. These results could be rationalized by two competing mechanisms which control the onset of plasticity in the second structure: interface strengthening by increased repulsive force and interface softening by increased dislocation source sites. The large stress drop after yielding in NWs could be explained by the dislocation source-limited hardening mechanism. The simulation results also indicate that the atomic fraction of newly formed SF in the second structure is increasing with increasing layer thickness and is closely related to the magnitude of stress drop and the uniform tensile elongation: the more atomic fraction of newly formed SF after yielding, the larger normalized stress drop and the larger uniform tensile elongation. For the second structure, the larger total tensile elongation for larger layer thickness could be related to the twinning induced plasticity at the necking position. These findings suggest that layer thickness control remains critical in 1D multilayered nanostructure to ensure the desired strength and ductility.

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