Size-Dependent Plasticity in Twinned Metal Nanowires

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1. Introduction

Face-centered cubic (FCC) metal nanowires, such as gold nanowires, are basic building blocks for numerous applications of nanotechnology ranging, for example, from electronics to self-assembly and medicine [1,2]. Therefore, it is critically important to gain fundamental insight into their mechanical behavior at the nanometer scale, in order to build more robust nanoscale devices. In particular, past atomistic simulation studies have proved that coherent twin boundaries can be strong obstacle to crystal slip in nanoscale FCC metals [3-8]. However, meaningful results related to FCC metal nanowires can only be achieved if the influences of microstructure and sample size on crystal plasticity and fracture behavior are fully understood.

In this paper, particular focus is placed on the effects of nanoscale twins, which are commonly grown during synthesis in FCC metal nanowires [9-12], on the tensile plastic behavior and fracture of Au nanowires. Both tensile yield and fracture at room temperature in [111]-oriented Au nanowires were investigated using molecular dynamics (MD) simulations. The nanowires exhibited same diameter (12.3 nm), but different number of coherent (111) twin boundaries per unit length along the wire axis, from 0.12 to 0.71 nm^{-1}. Further details on the simulation procedure are provided in the next section. We show in Section 3 that the crystal plasticity and fracture behavior of Au nanowires strongly depends on the density of preexisting twin boundaries. The underlying mechanisms of plastic deformation and fracture in twinned gold nanowires at atomic scale are also addressed.

2. Simulation methods

Parallel MD simulations were performed using LAMMPS molecular dynamics simulator [13] with an embedded-atom-method (EAM) potential for gold developed by Grochola *et al.* [14]. This potential enables the prediction of realistic values for the stacking fault energy of gold ($\gamma_{SF}^{prediction}$ = 43.4 $mJ{\cdot}m^{-2}$) as compared to experimental data ($\gamma_{SF}^{experimental}$ ~ 32-46.4 $mJ{\cdot}m^{-2}$) [14]. The structure of the nanowires was considered to be perfectly cylindrical and oriented along the [111] crystallographic direction. A periodic boundary condition was imposed along the nanowire axis, while the nanowire was kept free in the other directions. The periodic length and diameter of each cylinder was fixed at 33.6 nm and 12.3

nm, respectively, for all nanowires. The models consisted of ~235,000 atoms. The simulations were carried out using a Verlet algorithm with a time step of 5 fs. Each model was relaxed before deformation for 20,000 steps (100 ps) under zero stress. The nanowires were deformed at a constant strain rate of 2.7×10^{7} s^{-1} in tension along the [111] axis using constant NVT integration. All the simulations were performed at 300K. The tensile stress was calculated by adding the local atomic stress along the loading direction over all atoms in the cylinder and dividing by the deformed cylinder volume [15]. To visualize the deformation in nanowires, atoms were colored according to their local crystal structure based on Ackland's formulation [16]. All FCC atoms and some surface atoms were omitted for clarity.

3. Results and discussion

3.1. Tensile behavior in single-crystal nanowire

The tensile behavior of a single-crystal Au nanowire is shown in Fig.1. The corresponding stress-strain curve (Fig. 1a) is characterized by a linear elastic regime up to a very high yield stress (3.1 GPa) followed by a sharp yield point and severe strain softening effect. This behavior is in good agreement with that observed in past atomistic simulations of deformation in FCC metal nanowires [14-16]. The yielding mechanism is here related to the surface nucleation of $1/6\langle 11\bar{1}\rangle\{112\}$ Shockley dislocations, as shown in Fig. 1b, followed by their propagation through the cross-section of the nanowire and escape at the crystal free boundary on the opposite side (Fig. 1c). This result is reminiscent of the mechanical behavior of micrometer-scale, defect-free Au whiskers, which were already tested in classic tensile experiments by Brenner [17] half a century ago. Similarly, in nanowires, not only the ultrahigh strength, but also the lack of strain hardening, is related to the absence of preexisting dislocations or internal defects, which are usually strong barriers to the glide of dislocations and promote Stage II hardening in conventional metals [18].

3.2. Tensile behavior in twinned nanowires

We found a marked difference in tensile behavior between single-crystal and twinned nanowires with corresponding diameters. Fig. 2a presents the typical stress-strain response of a nanowire consisting of several twin boundaries. This figure shows that, while the elastic modulus of a twinned nanowire (~130 GPa) is not different from that of single-crystal nanowires, its tensile response after yielding (Fig. 1a) is prone to more significant strain hardening. Fig. 2b reveals that the dislocation nucleation at yield point is site-specific and takes place at the intersection of twin boundaries with the free surface. Fig. 2c shows that all partial dislocations nucleated are blocked by twin boundaries until the maximum flow stress is reached, and can no longer escape the crystal freely, as opposed to single-crystal nanowires. Moreover, the peak stress occurs when the transmission of dislocations across twin boundaries is enabled as shown in Fig. 1d.

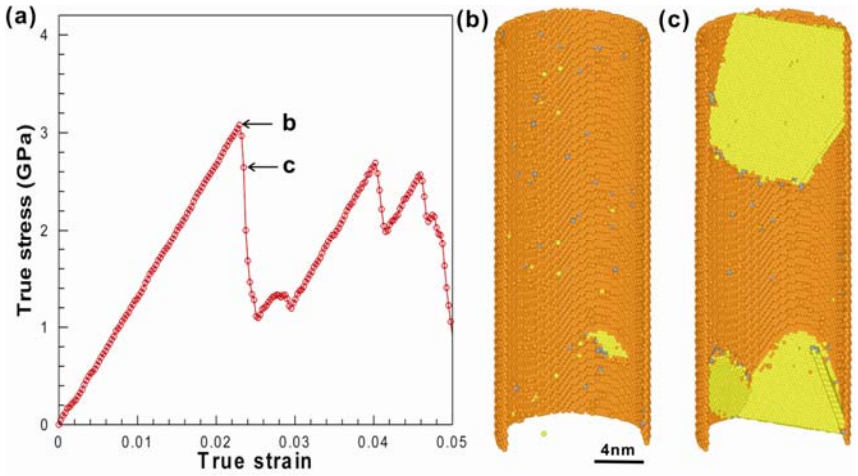

Fig. 1. Tensile behavior of a single-crystal, defect-free Au nanowire with a diameter of 12.3 nm from molecular dynamics simulation. (a) Simulated stress-strain curve. (b) Surface dislocation emission at yield point. (c) Propagation of $1/6\{11\bar{1}\}\langle 112\rangle$ partial dislocations followed by strong strain softening effects in the post-yielding stage. (b)-(c) Only non-FCC atoms and one half of the nanowire model are represented for clarity.

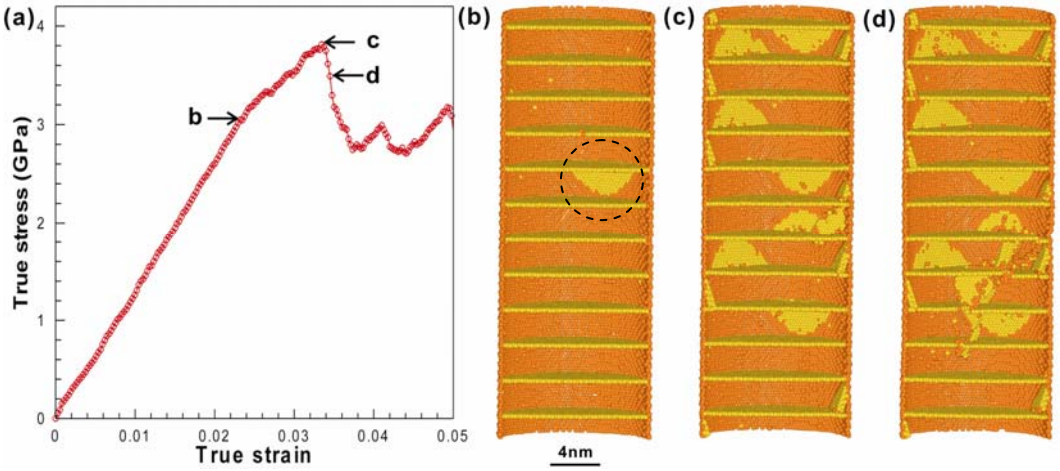

Fig. 2. Tensile behavior of a 12.3-nm-diameter Au nanowire with a number of twins per unit length equal to 0.36 nm^{-1} from molecular dynamics simulations. (a) Simulated stress-strain curve. (b) Site-specific dislocation emission (dashed circle) at yield point. (c) Multiple partial slip blockage in the strain hardening stage until maximum flow stress is reached. (d) Slip transmission of dislocations through coherent twin boundaries after peak stress. (b)-(d) Only non-FCC atoms and one half of the nanowire model are represented for clarity.

Since the dislocation nucleation process at yield point was found to be site-specific in twinned nanowires, we further investigated whether the critical resolved shear stress (CRSS) varies as a function of the number of twins per unit length. Fig. 3 reveals that there is a linear increase in CRSS measured at yield point as the twin boundary density increases or, inversely, the twin boundary spacing decreases. In comparison to the CRSS value obtained on the single-crystal nanowire, this figure allows us to conclude that introducing coherent twin boundaries during the growth of Au nanowires may have either detrimental or beneficial effects in terms of yield stress based on the twin size.

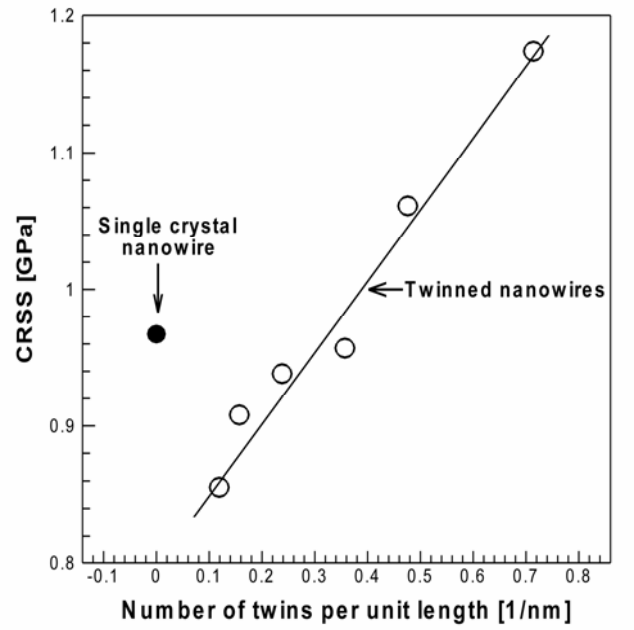

Fig. 3. Linear dependence of the critical resolved shear stress (CRSS) at yield point on the number of preexisting twins per unit length in Au nanowires with a diameter of 12.3 nm. The CRSS value for a single-crystal nanowire with corresponding diameter is shown for comparison.

Another consequence related to the change in slip activity and yield mechanisms between single-crystal and twinned nanowires, is noticeable in the plastic flow and fracture behavior as twins are added to nanowires. For example, we compare in Fig. 4 the deformation at failure of a nanowire with twin boundary spacing of 4.2 nm, to that for a single-crystal nanowire with same initial diameter. While failure in both types of nanowire occurred by necking, the plastic deformation was found to be more homogeneously distributed through the wire length in the single-crystal nanowire (Fig. 4a), as opposed to the twinned one (Fig. 4b). As such, the plastic localization caused the failure strain to be much smaller in the latter ($\varepsilon = 62\%$) than in the former ($\varepsilon = 89\%$).

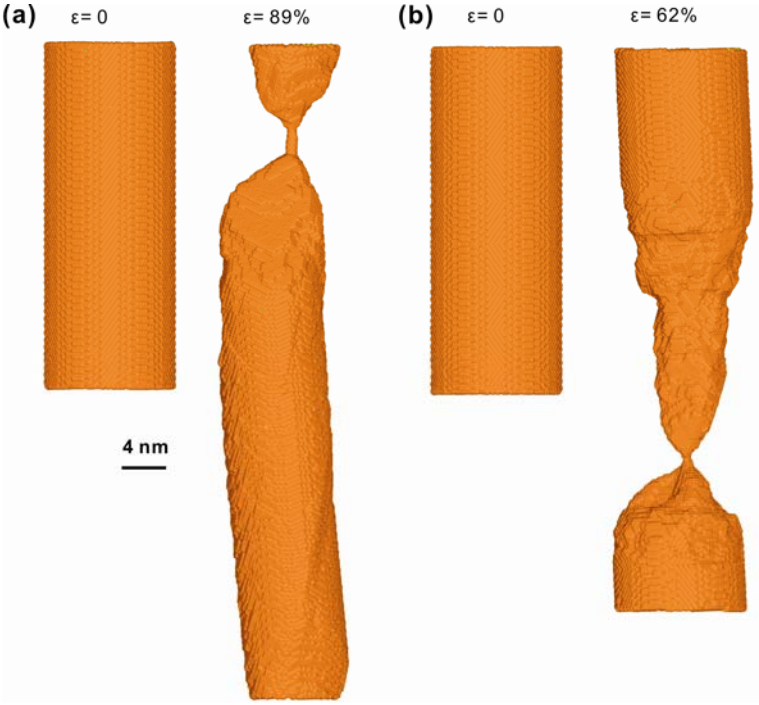

Fig. 4. Simulated fracture of Au nanowires of 12.3 nm in diameter. (a) Single-crystal, defect-free nanowire. (b) Twinned nanowire with 4.2 nm-twin boundary spacing. The loading direction is vertical for all nanowires.

4. Conclusion

MD simulations have been performed to investigate the difference in tensile deformation and fracture behavior between single-crystal and twinned gold nanowires with same initial diameters. The results presented in this study show clear evidence of significant size effects on the yield stress as a function of the number of twins per unit length in gold nanowires. These size effects can be interpreted by the fact that dislocation nucleation is site-specific in twinned nanowires. Furthermore, post-yielding plastic deformation and fracture mechanisms appear to be strongly influenced by the introduction of coherent twin boundary in gold nanowires. Further studies by the authors are currently underway to characterize the effects of nanowire diameter on yielding phenomena and crystal plasticity in twinned gold nanowires.

5. References

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