Effects of twin and stacking faults on the deformation behaviors of Al nanowires under tension loading*

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The effects of twin spacing and temperature on the deformation behavior of nanotwinned Al under tensile loading are investigated using a molecular dynamic (MD) simulation method. The result shows that the yield strength of nanotwinned Al decreases with the increase of twin spacing, which is related to the repulsive force between twin boundary and the dislocation. The result also shows that there is no strain-hardening at the yield point. On the contrary, the stress is raised by strain hardening in the plastic stage. In addition, we also investigate the effects of stacking fault thickness and temperature on the yield strength of the Al nanowire. The simulation results indicate that the stacking fault may strengthen the Al nanowire when the thickness of the stacking fault is below a critical value.

Keywords: molecular dynamic simulation, deformation twin, stacking fault

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1. Introduction

In the past decades, nanotechnology has been under rapid development and attracted more and more attention in the field of nanoscale materials. As an important nanostructure, metal nanowire (NW) has been a hot point of research, owing to its excellent mechanical and electronic properties.[1−4] Atomistic simulation studies have also shown that the elasticity and ultimate strength of face-centred cubic (fcc) metal NW can be significantly influenced by additional defects such as special surface defects and coherent twin-boundaries (CTBs).[5−7] Among the studies, the role of CTBs has received increasing attention in recent years for the plastic behavior in NW.[8−19] Understanding the physical mechanism associated with a particular deformation mode is conducible to the development of materials with improved strength and ductility. Deng and Sansoz[7] reported that there is a significant strain hardening in twinned gold NWs when nanowire diameter and twin spacing are balanced. They considered that the twin boundaries block the emission of nucleared dislocations, which leads to the hardening effect. However, Zhang and Huang[20] argued that whether twin-boundaries strengthen NWs or not depends on the necessary stress for dislocation nucleation, which in turn relies on surface morphology. Their results show that the CTB-induced strengthening effect disappears when the surface morphology of copper NWs is changed from square to circular. Li *et al.*[8] and Wei[21] have shown that the average flow stress increases with the decrease of twin spacing, reaches a maximum at a critical twin spacing, and then it drops progressively with the further decrease of twin spacing in Cu NWs. Guo and Xia[14] have reported that a transition from softening to strengthening results from the change in the dominant mechanism of plastic deformation as the twin spacing decreases in Au NWs. So far, the studies concerned with the deformation mechanisms of twinned fcc metals have focused mainly on Au[7] and Cu.[8,15,19,21] However, the relevant studies on Al are still limited despite its industrial importance. Here in this paper, we investigate the effect of twin spacing on the mechanical property of Al NWs, and discuss how the mechanical property of Al NWs with a square cross-section varies with twin spacing. The stacking fault energy (SFE) of Al and Al alloys were investigated very recently by using the first-principles method based on the density functional theory (DFT).[22,23] Nevertheless, the relevant studies concerning the effects of stacking faults on the yield strength of nanowires are still very rare. Many studies mentioned above show that introducing an ap-

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propriate number of coherent nanoscale twins into fcc metals, such Cu and Au, can obviously improve the mechanical properties of metals, and obtain ultrahigh yield strengths and flow stresses in metals. We here introduce a stacking fault into single-crystal Al to investigate whether this configuration could strengthen nanometals in the same way as nanoscale twins.

The rest of the present paper is organized as follows. In Section 2 we discuss the simulation method and models that we choose for our study. The results and discussion are shown in Section 3. Finally, the conclusions are drawn from the present study in Section 4.

2. Simulation model and method

Three types of microstructures in [111]-oriented Al NWs are simulated as shown in Fig. 1: single-crystalline square cross-sectional NWs (Fig. 1(a)), NWs with stacking faults (Fig. 1(b)), and twinned square NWs (Fig. 1(c)). The square cross-section of the NWs is 4.9 nm $\times$ 5.6 nm. The twin spacing and the stacking faults thickness are shown in Fig. 1, where the twin spacing varies from 0.701 nm to 7.010 nm and the thickness of stacking faults of NWs changes from 1.169 nm to 7.478 nm. For a perfect fcc metal, the stacking sequence of atoms in successive close-packed planes is ABCABCABCABC,[24−26] which is shown in Fig. 1(a). The slip of the first part $b1 = a/6[2\bar{1}\bar{1}]$ produces an intrinsic stacking fault as shown in Fig. 1(b), which is identical to the removing of a layer of A atoms, i.e., ABCABCABCABC BC. Further slip of the $b1$ part grows the twin nucleus into a two-layer, three-layer, and more-layer twin. Figure 1(c) shows a 15-layer twin CBACBACBACBACBA.[24−26] Periodic boundary conditions contribute to [111] axis and all other directions are kept free. The number of atoms in the computational models ranges from 4800 to 48000, depending on the thicknesses of the twin and stacking fault.

The selection of potential function is a key factor, which determinates the result accuracy in MD simulation. Here, the tight-binding potential developed by Cleri and Rosato[27] is used to describe the atomic interactions in these simulations. All the MD simulations are performed using the Verlet integration algorithm in time steps of 2 fs. Each of the models is equilibrated for 30 ps in the canonical ensemble (namely, number of atoms, volume, and temperature conservation) using a Nosé–Hoover thermostat.[28] The NWs are deformed by stretching the simulation box along the [111] direction, where the tensile strain is 0.001. The common neighbour analysis (CNA)[29] is used to detect the microstructure of the nanotwinned NWs, which can distinguish the local crystal structure of atoms by obtaining information about the relation between neighbours and atom pairs. This is implemented by using the Open Visualization Tool (OVITO).[30]

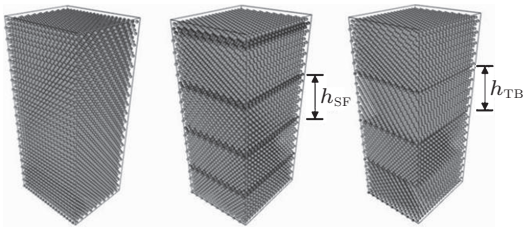


Fig. 1. Atomistic models for [111]-oriented Al NWs with three different microstructures, (a) single-crystalline square cross-section NW, (b) NWs with stacking faults and constant stacking fault thickness h_{SF}, and (c) coherent twin boundaries and constant twin spacing h_{TB}. The hexagonal close-packed (hcp) atoms are light-colored and the fcc atoms are darker colored.

3. Results and discussion

3.1. Effect of twin on mechanical behavior

Figure 2 shows the typical stress–strain curves of twinned Al NWs under tensile loading. The stress used to describe the stress–strain relation is computed by the Virial scheme, which is commonly used in atomistic simulations.[14] It can be seen from Fig. 2 that in all cases, the stress increases linearly with strain up to a peak value (at this point, the stress is defined as yield strength), before and after which the stress stage is called elastic stage and plastic stage, respectively. The Young's modulus derived from the stress–strain relationship at a small tensile strain level in the linear elastic regime is about 83.33 GPa. The flow stress gradually decreases to a steady-state level and fluctuates around the steady value with the increase of strain in plastic stage. The nearly constant flow stress is related to the nucleation and propagation of dislocations in nanotwinned Al as shown in Fig. 3. A key result found in our simulation is that there is no strain-hardening in nanotwinned Al at the initial yield point. That is different from the strain-hardening effect at the yield point in Au NWs.[31] Figure 3 shows the deformation structures of the nanotwinned Al at yield point. It can be seen from Fig. 3 that the partial dislocations are able to penetrate into the CTB

without being blocked, which causes a sharp and substantial drop in the yield stress immediately after the initial yield point. Under tensile loading, the dislocations are emitted, accompanied by the nucleation and propagation of a partial dislocation through a {111} plane. At the same time, some stacking fault steps occur around the CTB on the other side. This may explain why there is no strain-hardening effect in nanotwinned Al, which occurs only when the CTBs are able to block the leading partial dislocations emitted at the initial yield point.

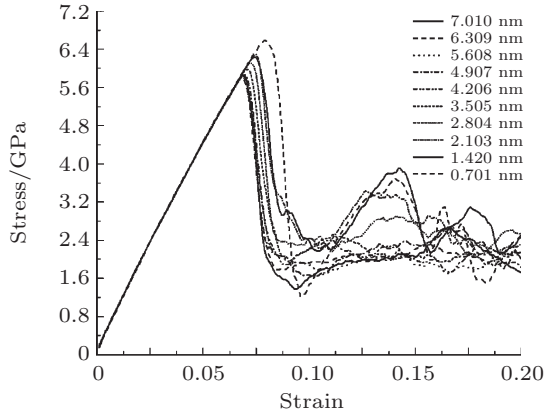


Fig. 2. Stress–strain curves of nanotwinned Al with different twin spacings under tension loading at 10 K.

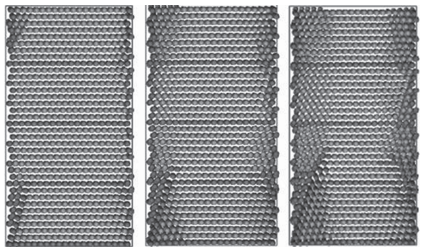


Fig. 3. Transmission of a twinning partial dislocation through the CTB in an NW with a square cross-section. The darker atoms inside, and the light-colored atoms and darker colored atoms along the edge present the hcp, fcc, and non-structured atoms, respectively.

Another interesting aspect of our study is that during the plastic deformation in the square Al NWs, there is a noticeable rise of the stress as the stress continues to increase after the yield point. This conspicuous rise can be seen as a strain-hardening, which exists only when the twin spacing is relatively small. It is found in Fig. 2 that for smaller twin spacing, for example, spacing less than 2.804 nm, a conspicuous strain-hardening can be seen as the strain increases to 0.125. That may be attributed to the CTB blocking the emission of the subsequent dislocations. In order to search for more details of the deformation mechanism of nanotwinned Al, we examine the dislocation dynamics and we will give a theoretical explanation of this phenomenon in the following text.

Figure 4 shows the variations of the calculated yield strength in nanotwinned Al with twin spacing at three different temperatures. The simulation results indicate that the yield strength increases as twin spacing decreases from 7.010 nm to 0.701 nm, which is well in consistence with the previous conclusion obtained from nanotwinned Cu by Zhang and Huang.[20] It can be also seen from Fig. 4 that the effect of temperature on the yield strength of Al NWs is obvious. Figure 4 shows that the yield strength varies from 5.311 GPa to 6.228 GPa with twin spacing decreasing from 2.103 nm to 0.701 nm, which corresponds to a 17.266% increase in strength at 100 K. However, the yield strength increases from 4.744 GPa to 5.287 GPa with twin spacing decreasing from 7.010 nm to 2.804 nm, corresponding to an increase of 11.446% at 100 K. Likewise, a 21.840% increase can be obtained when the twin spacing decreases from 2.103 nm to 0.701 nm and a 10.631% increase in strength can be obtained with twin spacing decreasing from 7.010 nm to 2.804 nm at 10 K. To put it another way, for smaller twin spacing, the strength of nanotwinned Al is strongly dependent on twin spacing. Atomic configurations of the nanotwinned Al with twin spacings of 2.103, 3.505, and 7.010 nm subjected to tension loading at various strains are shown in Figs. 5(a)–5(f), respectively. It can be seen from Figs. 5(a), 5(c), and 5(e) that the leading dislocations are emitted from the sharp edges where the atoms have the largest vibration amplitude at the yield point. It is well known that CTBs may serve as barriers, which hinder the nucleation and glide of dislocations in NWs. The configuration force resulting from the mismatch of material properties across the twin-boundary can describe the

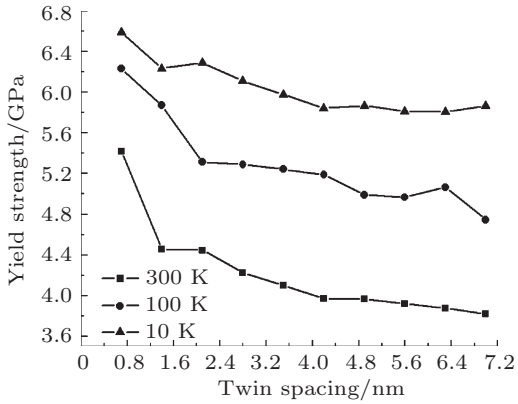


Fig. 4. Variations of yield strength of nanotwinned Al with twin spacing at three different temperatures.

interaction between the dislocations and CTBs.[14] The twin boundaries can exert a repulsive force on the dislocations that move towards them. This repulsive force will be helpful for hindering the nucleation and glide of dislocations in nanometals and will be inducible to the increasing of the initial yield strength of twinned nanometals. This may contribute to explaining why the yield strength increases as twin spacing decreases.

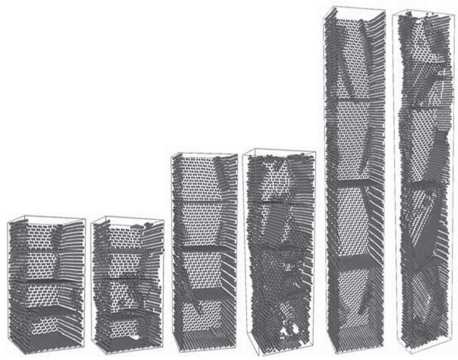


Fig. 5. Images of atomic-scale deformation with different twin spacings at 10 K, showing (a) deformation of NW at yield point with twin spacing = 2.103 nm, (b) deformation at strain-hardening point with twin spacing = 2.103 nm, (c) deformation of NW at yield point with twin spacing = 3.505 nm, (d) deformation of NW at plastic stage (no strain-hardening point) with twin spacing = 3.505 nm, (e) deformation of NW at yield point with twin spacing = 7.010 nm, and (f) deformation of NW at plastic stage (no strain-hardening point) with twin spacing = 7.010 nm. The darker and light-colored atoms represent the hcp, non-structured atoms, respectively.

Figures 5(b), 5(d), and 5(f) show the deformation images of nanotwinned Al in plastic stage with the twin spacings of 2.013, 3.505, and 7.010 nm, respectively. It is observed from Fig. 5(b) that when the strain is 0.135, corresponding to the second strain-hardening with a twin spacing of 2.013 nm, the CTBs hinder the emission of the dislocations. However, the dislocations are able to transmit through the CTBs without being blocked when the twin spacing is larger than 2.804 nm, for example 3.505 nm, and 7.010 nm in Figs. 5(d) and 5(f). That is to say, strain-hardening is enabled in NWs when the stress for dislocation emission from the parent grain becomes smaller than the maximum stress for the resistance of CTBs to dislocation glide. This result is in agreement with previous simulation result in the square Ag NW.[31] Furthermore, dislocation starvation is also a reason for this second hardening.[32,33] The local analysis may contribute to the explanation of strain-hardening in the plastic stage after the yield point in Fig. 2.

We can also find from Fig. 4 that the yield strength of nanotwinned Al increases with the decrease of temperature regardless of twin spacing. The reasons are as follows: for lower temperature, the internal thermal motion of the Al atoms is weak and a large number of atoms vibrate around their equilibrium position; but at higher temperature, a large number of atoms can gain sufficient energy to overcome the activation energy barrier,[34] and then they escape from their equilibrium positions, therefore the initial configuration is rearranged.

3.2. Effect of stacking faults on mechanical behavior

The above results and analyses suggest that introducing nanoscale twins into Al NWs is useful for obtaining stronger mechanical properties for materials. Here, we introduce stacking fault into single-crystal Al so as to investigate whether this configuration could strengthen nanometal similar to the case of nanoscale twins. We have given the structural form of Al NW with a stacking fault (Fig. 1(b)) and the schematic of fault generation for nanofilms with the projection of $\langle 111 \rangle$ planes in Section 2. The variation of yield strength of Al NWs with stacking fault thickness h_{SF} at $T = 300$ K is shown in Fig. 6. It can be observed from Fig. 6 that the yield strength of nanoscale Al increases from 3.553 GPa to 4.563 GPa as the thickness of the stacking fault decreases from 7.478 nm to 1.169 nm. That is to say, there is a strengthening effect of NWs containing stacking faults with h_{SF} decreasing. Especially, when the h_{SF} decreases to 2.015 nm, the yield strength of Al NWs with stacking faults is larger than that of single-crystal Al at 300 K. In order to characterize the influence of the thickness of stacking faults on yielding mechanisms, the atomic configurations of Al NWs with different stacking fault thicknesses subjected to tension loading are presented in Fig. 7. It can be clearly seen from Figs. 7(a), 7(c), and 7(e) that the nucleation mainly occurs at the stacking fault boundary at the yield point, which is similar to the deformation mechanism in the twin boundary. The stacking fault boundary hinders the nucleation of dislocations and may act as a repulsive force on the dislocations moving towards it. At the same time, the magnitude of the repulsive force drops as h_{SF} increases, which may result in the nucleation of dislocations at a lower stress level. This is the main reason why there exists a strengthening effect with h_{SF} decreasing. It should be noted that the deformation mechanism related to strain-hardening after the yield

point is quite different from that of twin. In twinned Al NWs, the CTBs block the emission of the subsequent dislocations when the twin spacing is relatively small after the yield point. However, the boundaries of the stacking fault gradually disappear with the increase of tension loading regardless of the h_{SF}. So this blockage of stacking fault boundary to the dislocations does not work. Yet the dislocations glide on the plan, which leads to the rise of the flow stress after the yield point in plastic stage as shown in Figs. 7(b), 7(d), and 7(f).

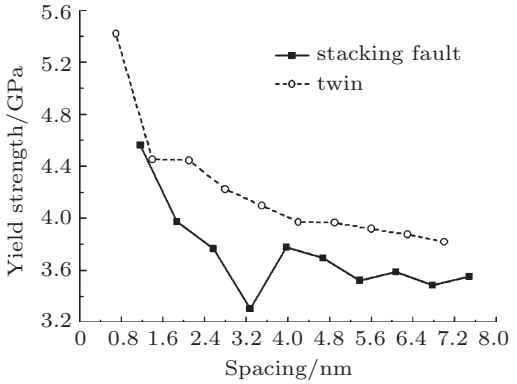


Fig. 6. Variations of yield strength of Al nanowires with defect spacing at 300 K.

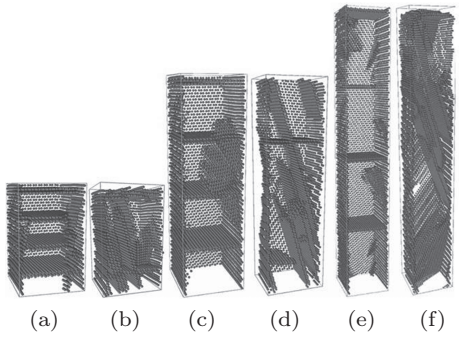


Fig. 7. Deformation mechanisms of NWs with different values of h_{SF}, showing (a) deformation at yield point with h_{SF} = 1.870 nm, (b) deformation in plastic stage after yield point with h_{SF} = 1.870 nm, (c) deformation at yield point with h_{SF} = 3.973 nm, (d) deformation in plastic stage after yield point with h_{SF} = 3.973 nm, (e) deformation at yield point with h_{SF} = 7.478 nm, and (f) deformation in plastic stage after yield point with h_{SF} = 7.478 nm. The darker and light-colored atoms represent the hcp, non-structured atoms, respectively.

To compare the strengthening effects of twin and stacking fault, Fig. 8 shows the stress–strain curves of nanowires with a thickness of the stacking fault (or twin) spacing about 4.0 nm in 300 K. It can be seen from Fig. 8 that the yield strength in twin-nanowires is higher than that of nanowires with stacking faults, and the flow stress of the former is bigger than that of the latter. Figure 6 shows the calculated yield strength varying with stacking fault (or twin) spacing increasing from 0.701 nm to 7.478 nm at 300 K. We can clearly see from Fig. 6 that on the condition that twins and stacking faults have the same densities (namely with the same defect thickness), the yield strength of twin nanowires is higher than that of stacking fault nanowires. The comparison of results between two models indicates that the introduction of nanotwins into nanocrystalline Al is a more effective way to improve the strength, which may be attributed to the different deformation mechanisms. The general conclusions drawn from this work may provide a guideline for the design of high performance nanopolycrystal Al.

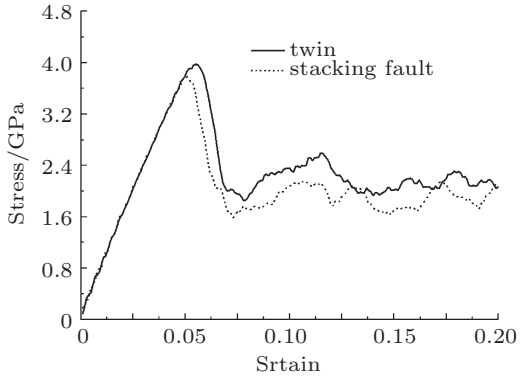


Fig. 8. Stress–strain curves of nanowires with the thickness of the defects spacing near 4.0 nm.

4. Conclusion

The effect of twin spacing on the mechanical characteristics of nanotwinned Al is investigated by MD simulation at three different temperatures. The results indicate that the yield strength of nanotwinned Al NWs increases as the twin spacing decreases. This may be due to the fact that a repulsive force resulting from the CTBs on the dislocations moving towards them decreases with the increase of the twin spacing. We also find that there is no strain-hardening at the yield point due to the dislocations transmitting through the CTB without being blocked. However, a strain-hardening exists after the yield point, owing to the CTBs hindering the emission of dislocations in NWs when the twin thickness is smaller than 2.804 nm. The results also show that the yield strength of nanotwinned Al increases with temperature decreasing regardless of twin spacing. In addition, the effect of stacking faults on yield strength of Al NWs is also investigated in the present work. The study demonstrates that this atomistic configuration

may exert a strengthening effect with stacking fault thickness decreasing. However, the strain-hardening after the yield point is related to the glide of the dislocations, which is different from the deformation mechanism in the twin.

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