Twin-size effects on the deformation of nanotwinned copper

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The strength and ductility of nanolayered materials are determined by a delicate balance between dislocation and interface motion under applied mechanical loading. We present here studies of dislocation and interface motion in single crystal and nanotwinned copper, utilizing molecular dynamics simulations. Motion of twin boundary interfaces themselves is dictated by the stress state at the interface, and is found to be maximum for applied shear loads parallel to the boundary. The mechanism of twin boundary migration is shown to be a result of Shockley partial nucleation and growth at twin interfaces. The stress state at twin boundaries is found to play a significant role in determining the deformation mode. While deformation twinning is found to be the dominant mode under tensile loading, shear loading is found to favor twin boundary migration. The influence of the twin lamella thickness on the deformation behavior of nanotwinned Cu is determined under constant applied strain rate and constant applied stress, and the conditions for dislocation confinement within nanotwins are determined. The stacking fault density and the number of nucleated dislocations are compared for different size lamellae of twin structures. The present simulations reveal the origins of strengthening caused by nanotwins as the restriction of dissociated dislocation loop motion in narrow channels. A critical twin thickness for the maximum strength in twinned copper is found to be around 4 nm.

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I. INTRODUCTION

Nanocrystalline materials manifest very fascinating properties, which can be exploited in a variety of structural and nonstructural applications. Such materials possess unique beneficial chemical, physical, and mechanical properties. An important problem concerning the microelectronics industry is the reliable operation of integrated circuits, where the lifetime is limited by the failure of interconnect wires in between submicron semiconducting chips. Future electronic and optoelectronic devices are expected to be even smaller, with nanowires connecting nanosize memory and information storage and retrieval nanostructures. Recently, high-purity Cu samples with nanoscale growth twins were synthesized using a pulsed electrodeposition technique from an electrolyte of $CuSO_4$.[1] Transmission electron microscopy observations indicated that the as-deposited Cu consisted of irregular-shaped grains with random orientations. Grain sizes were between 100 nm and 1 μm, with an average value of about 400 nm, and each grain contained a high density of growth twins of the 111/[112] type. Measurements of the lamella thickness along the [110] orientation showed a wide distribution ranging from several nanometers to about 150 nm, due to the fact that in this orientation, only $(\bar{1}11)$ and $(11\bar{1})$ twins are edge on, whereas (111) and $(11\bar{1})$ twins are inclined to the surface. Tensile tests of as-deposited Cu foils performed at ambient temperature showed extremely high strength.[1] Strength values were found to be at least one order of magnitude larger than those of the coarse-grained (grain size >100 μm) Cu samples.

The flow stress in nanolayered structures can approach $\sim 1/3$ of the theoretical shear strength of order $\mu/30$, where μ is the shear modulus.[2,3] The strengthening mechanism is understood to be the result of restricting the motion of dislocations from one layer to another.[4] Restricted motion of dislocations in nanolayered materials is a result of several factors discussed in recent literature.[4,5] Impedance to dislocation motion in nanolayered materials can result from the mismatch between two adjacent materials in a number of properties, such as elastic moduli (the Koehler effect), lattice parameter (coherency strain), stacking fault energy (SFE), and slip plane geometry.[6–8] Differences in the values of any one of these properties in the two materials would create an additional energy barrier to dislocation motion from one material to another across their common interface. Moreover, the structure of the interface itself plays a role in influencing the transmission of dislocations from one layer to an adjacent one. Misfit dislocations can interact with slip dislocations and obstruct their motion. Also, if the interface structure permits spreading of the dislocation core, an incoming dislocation may be absorbed and a higher level of stress would be required to nucleate an outgoing dislocation. The strength of multilayer materials is thus derived from the resistance of interfaces between layers to dislocation motion, as dislocations cross them from one layer to another. To design ultrastrong, yet ductile materials, one needs to understand the interplay between dislocations and interfaces. The "inverse Hall-Petch effect;" that is the decline in strength as the nanograin size gets smaller is evident in fcc systems; albeit the opposite behavior is observed for duplex fcc/bcc systems, as for example in the Cu-Cr and Cu-Nb cases.[2] This effect has been attributed to be a result of dislocation core structure and splitting into partials during the nucleation process from grain boundaries (GBs) in fcc crystals.[9] In fcc metals, the strongest grain size is that corresponding to the cross over between normal and inverse Hall-Petch regimes, and is equal to the splitting distance between the two partials at the applied stress.[10]

Two of the most common and important modes of plastic deformation in fcc metals at low temperatures are slip and deformation twinning. Slip is propagated through disloca-

tions while deformation twinning occurs when a region of crystal is transformed by the external loading into its twin (mirror) counterpart. Experimental observations have shown that a low intrinsic stacking fault energy is correlated with a higher tendency to twinning in fcc metals. It has also been suggested that the SFE of the metal will have to be less than some critical value for a metal to exhibit deformation twinning. Twins prefer to nucleate at grain boundaries to reduce the grain-boundary energies by means of the twinning-induced orientation change. The formation of twins depends strongly on the ratio of the twin boundary energy, γ_{TB}, to the GB energy, γ_{GB}, $\alpha = \gamma_{TB}/\gamma_{GB}$. Large twin density may be obtained in metals with smaller α values. Another important microstructural parameter influence deformation twinning is the grain size in the metal. It has been reported that increasing the average grain size results in a lower twin nucleation stress for a given metal.

Twin boundaries are very special interfaces between parts of the same material that are oriented in different directions. Since Cu is elastically anisotropic, the elastic compliance tensor, when described in a common coordinate system, results in anisotropic elastic fields for dislocations as they cross from one twin lamella into a neighboring one.[5] Thus, not all of the factors mentioned above would be operating during dislocation motion in twinned structures, and only dislocation nucleation, confinement transmission would be of main importance. Because of the special structure of coherent twin boundary interfaces, they may themselves move if an external stress is applied, thus creating competitive modes of deformation in nanotwinned structures. Utilizing a high-pressure torsion technique, Liao *et al.*[11] performed an experimental study of the deformation mechanisms of nanostructured copper. Dislocations were found to form under high-pressure torsion into elongated nanodomains. Further deformation was observed to take place mainly through partial dislocation emission from nanodomain boundaries, resulting in high density of nanotwins and stacking faults. Recent molecular dynamics (MD) simulations by Cao and Wei[12] indicated that twin boundaries formed under tension, and that they provide obstacles to dislocation motion, thus increasing the strength of nanotwinned Cu. Moreover, it was shown that thinner twin lamella resulted in increased strength. Using atomistic reaction pathway analysis, Zhu *et al.*[13] demonstrated that slip transfer of dislocations, mediated by twin boundaries is the rate-controlling mechanism of plastic flow in nanostructured metals. The high ductility of nanotwinned copper was attributed to the hardening of twin boundaries as they lose coherency at high strains.

The objective of the present research is to develop a mechanistic understanding of the deformation modes operating in nanotwinned copper, and to determine the key factors that influence the mechanics of ultrastrong nanolayered structures. Of primary interest here is the influence of the twin lamella length scale on the strength and ductility of nanotwinned copper. To reach this objective, we will analyze dislocation motion in nanotwinned structures, the interaction of dislocations with interfaces, and the conditions for their confinement and transmission. On the basis of dislocation and twin boundary behavior, we will investigate the dependence of strength and ductility on the size of nanotwin lamella. In Sec. II, we give a brief description of the computational model utilized for MD simulations in this study. This is followed in Sec. III by analysis of simulation results for the influence of the stress state (tension and compression) on the deformation behavior of copper, on twin boundary migration (TBM), and on the initiation of various deformation modes. In Sec. IV, we investigate the effects of the twin lamella size in a layered twinned copper structure on its plastic deformation at this nanoscale. Finally, we present a summary of this study and its conclusions in Sec. V.

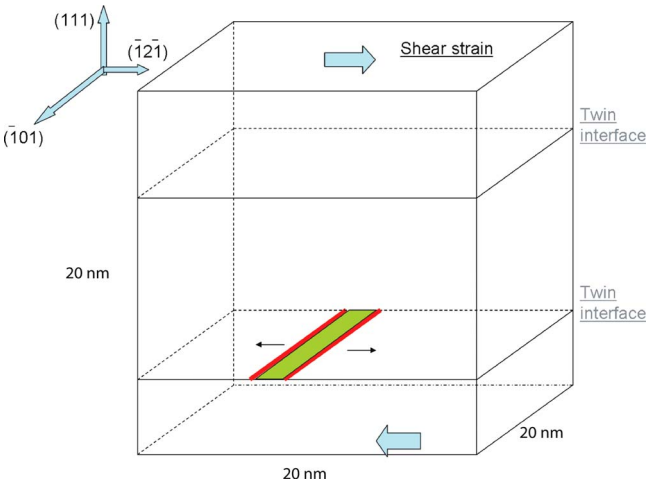

FIG. 1. (Color online) Schematic for the computational box used in MD simulations of the Cu twin structure.

II. COMPUTATIONAL MODEL

Interactions between copper atoms in the present MD simulations are represented by the embedded-atom method (EAM) Mishin potential,[14] and all simulations were performed with the XMD computer code.[15] The potential developed for copper in Ref. 14, and used in this work, shows excellent agreement between *ab initio*, tight binding, and EAM results for the energies and stability of several nonequilibrium structures of Cu, as well as for the stacking fault energy of copper (reported to be 44.4 mJ/m^2), compared to the experimental value measured by Carter and Ray[16] of 45 mJ/m^2. In addition, the potential reproduces the defect and elastic properties of copper to within less than 1% in many cases.[14] MD simulations were performed in the canonical constant number of particles, volume and temperature (NVT) ensemble, using a constant-temperature Nosé-Hoover-type thermostat. To investigate the detailed mechanism of twin boundary migration, we set up typical simulation boxes as shown in Fig. 1. The x, y, and z axes of the simulation cells were selected as $[110]$, $[1\bar{1}\bar{1}]$, and $[1\bar{1}2]$, respectively. Typical box dimensions are 20 nm along all the x, y, and z directions, containing 0.5 million atoms. Both perfect and twinned crystals were simulated. In the case of twinned crystals, two twin interfaces are situated on the y plane, which divide the box into three layers along the y direction. Periodic boundary conditions were applied along the z direction, and free-surface boundary conditions were

applied along the x direction. Uniform shear strains on the $(1\bar{1}\bar{1})$ plane along the [110] direction or tensile strains on the $(1\bar{1}\bar{1})$ plane along the $(1\bar{1}\bar{1})$ direction were applied in various simulations. Simulations were conducted in two stages: the system was first elastically preloaded up to 6.9% uniform shear strain, relaxed by MD for 0.25 ns, and then constant strain rates in the range of 5×10^{7} to 5×10^{9} s^{-1} were applied to the top and bottom boundary layers of atoms. Those top and bottom boundary layers were fixed after each shearing step, while the atoms in the cells were allowed to relax. By applying a constant velocity to the upper fixed region while holding the lower region motionless, an external shear stress parallel to the twin boundary can be introduced. MD simulations were conducted at a temperature of 300 K.

To identify atoms in defect configurations, the centrosymmetry method is generally used.[17] The method is based on a space group, which contains an inversion center as one of its symmetry elements. In a perfect crystal, for every atom at (x,y,z) in the unit cell there is an equivalent atom at $(-x,-y,-z)$. Since this method does not differentiate between twin interfaces and dislocations, we developed a new algorithm to identify atoms on twin boundaries. The approach is to combine the nearest neighbor and the centrosymmetry techniques to identify and classify defect atoms in dislocation cores, on surfaces and on twin interfaces. An atom at a hcp position (such as a twin interface), does not have the centrosymmetry property, but the vector sum to its 12 nearest neighbors is zero. In the present algorithm, we first check if an atom has 12 nearest neighbors within a cutoff distance. If this condition is not satisfied, the atom is marked off as a surface atom, in a void, or in a dislocation core. For all remaining atoms, all 12 neighbor vectors are summed, and if the sum does not fall within a certain tolerance, the atom is considered to be in a distorted position. The centrosymmetry method is finally used to check if the surrounding crystal structure to an atom is a perfect fcc lattice structure.

III. DEFORMATION MODES OF NANOTWINNED COPPER

We investigate here the various possible modes of deformation in nanostructured copper, and the influence of the stress state and strain rate on the competition between these deformation modes. There are four possible plastic (irreversible) deformation mechanisms, depending on the conditions of deformation, such as the state of stress and applied strain rate:

(1) *Stacking fault extension*: One Shockley partial dislocation extends across an entire grain, leaving a stacking fault behind.

(2) *Dislocation motion*: Plastic deformation is achieved by the irreversible motion of a leading and a trailing partial dislocation on the same slip plane, leaving no dislocation debris behind, but resulting in a shear displacement on the glide plane.

(3) *Mechanical twinning*: The leading and trailing partials on two adjacent (111)-planes nucleate an extrinsic stacking fault, three-layers thick. This nanotwin structure is the precursor for deformation twinning.

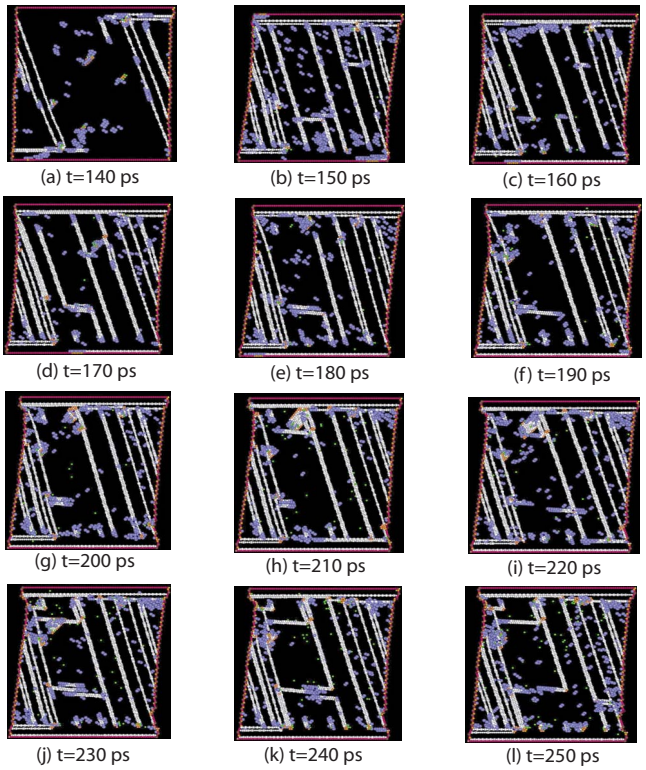

FIG. 2. (Color online) Time sequence of atoms in defect positions in a copper single crystal subjected to a high tensile strain rate of 5×10^{8} s^{-1}.

(4) *Twin boundary migration*: TBM takes place via the emission of a partial on a (111)-plane adjacent to the TB. This is a reversible form of deformation since twins can migrate back and forth if the stress is reversed.

It is noted that while existing twins can migrate under applied stress, mechanical twinning is the combined nucleation and growth of twins from a perfect lattice. Twin boundary migration does not involve the nucleation of new twins, and may not be strictly associated with growth of existing twins by thickening the twin width.

A. Effects of stress state

The interaction of an applied tensile or shear load with a copper nanocrystal is expected to result in a variety of deformation modes and atomic structures because of the near perfect symmetry of twinned crystals across twin boundaries. While shear on a plane that is parallel to the twin boundary may result in twin boundary migration, a substantial tensile stress across the boundary may partially destroy the boundary itself. Figure 2 displays snap shots of a time sequence for the positions of atoms in defect configurations for a single copper crystal under a high tensile-shear strain rate of 5×10^{8} s^{-1}. White atoms in the figures mark those in hcp positions (twin boundaries or stacking faults), while red (dark) atoms have less than 12 nearest neighbors, and blue (dark) atoms have more than 12 nearest neighbors (e.g., atoms around dislocation cores). Atoms in perfect positions are not shown for clarity. On the other hand, Fig. 3 shows the

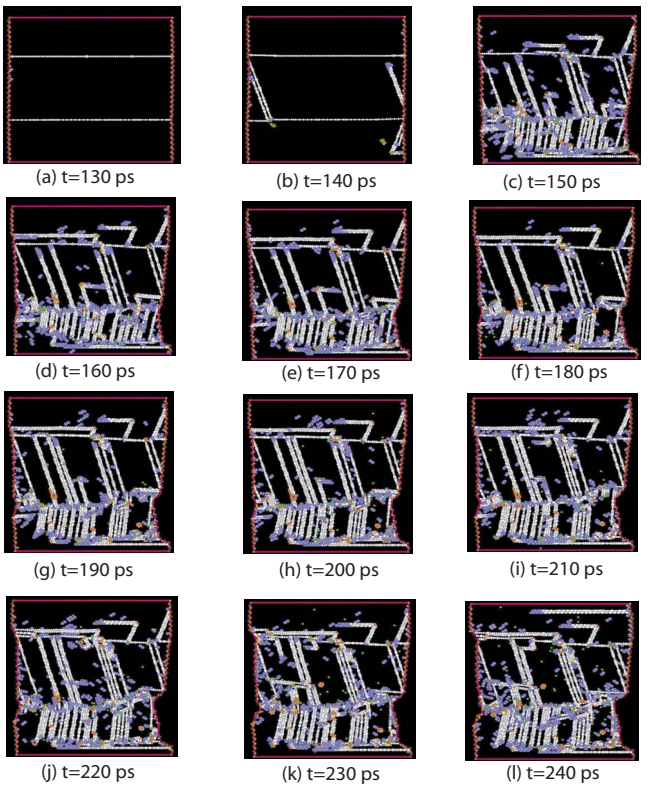

FIG. 3. (Color online) Time sequence of atoms in defect positions in a three-layer twinned copper crystal subjected to a high tensile strain rate of 5×10^8 s^{-1}.

defect atomic configurations a three-layer twinned copper crystal subjected to a high tensile strain rate of 5×10^8 s^{-1}. It is clear that in single crystals, the dominant mode of deformation under tension is mechanical twinning. The deformation mode of twinned nanocrystals is still mainly by the MT mechanism, as shown in Fig. 3, although pre-existing twin boundaries obstruct the extension of nucleated nanotwins. It is also observed that pre-existing twin boundaries undergo substantial destruction under tensile loading as a result of their interaction with nucleated deformation twins.

The influence of the applied stress state and the initial structure of the copper nanocrystal on the nucleation of deformation twins is shown in Fig. 4, where the density of twinned planes is displayed as a function of time at a strain rate of 5×10^8 s^{-1}. It is interesting to note that tensile loading results in a substantially larger density of deformation twins ($\sim$25–30%), as compared to shear loading ($<$10%). A slightly larger density of deformation twins is achieved in single copper crystals, as compared to twinned crystals. Pure shear loading of twinned copper crystals produces no additional mechanical twins, as shown in Fig. 4 (dotted-dashed line). When there are no original twin interfaces, as is the case for a single nanocrystal, dislocations are nucleated from surfaces and glide on (111) planes. A leading Shockley partial dislocation of a Burgers vector $\frac{1}{6}[112]$ is first nucleated from the surface, followed by the formation of a pair of twin interfaces on adjacent planes. Thus, a nucleus of a nanotwin is formed at the end of this process. The stress-strain curves for single and nanotwinned crystals, shown in Fig. 5, indicate that the deformation process starts in an elastic manner up to a strain of about 7%. Beyond this level of strain, dislocations are nucleated giving rise to plastic deformation via dislocation motion and nanotwin formation.

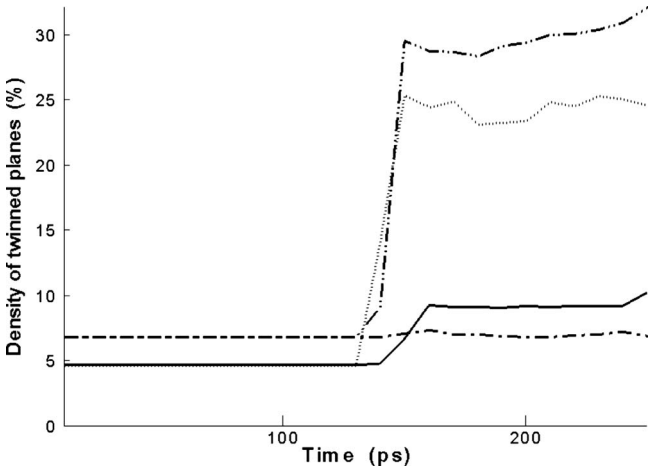

FIG. 4. The density of twinned planes as a function of time at a strain rate of 5×10^8 s^{-1}. (a) Dotted line: single crystal in tension, (b) dashed dotted line: three-layer twinned copper crystal in tension, (c) solid line: single crystal under shear, (d) dashed dotted line: three-layer twinned copper in shear.

Two types of atomic displacements are generally possible at a twin boundary: (1) shear for atoms lying on basic lattice points, and (2) shuffling of atoms at points described by the basis.[18,19] As we can see from Fig. 6, twin interfaces migrate under an applied shear strain that is parallel to the twin interface. It is found that shuffled atoms first appear in the near vicinity of the surface, where their position is still elastic but far from equilibrium. Their motion is found to be a precursor for the nucleation of two Shockley partial dislocations from opposing surfaces, and then glide in opposite directions along the (111)-twin interface. The two dislocation loops have opposite Burger's vectors so that the sum of their Burger's vector is zero. The dislocation loops glide under the applied shear strain and finally get absorbed at surfaces. As a

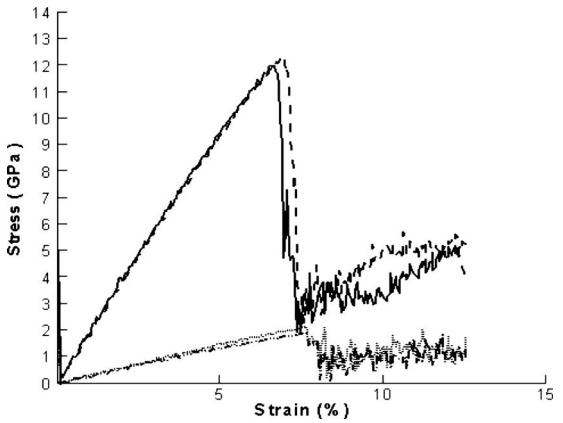

FIG. 5. Stress-strain curves for deformed copper crystals. (a) Solid line: tension of a single crystal, (b) dashed line: tension of a twinned crystal, (c) dotted line: shear of a single crystal, and (d) dashed dotted line: shear of a twinned crystal.

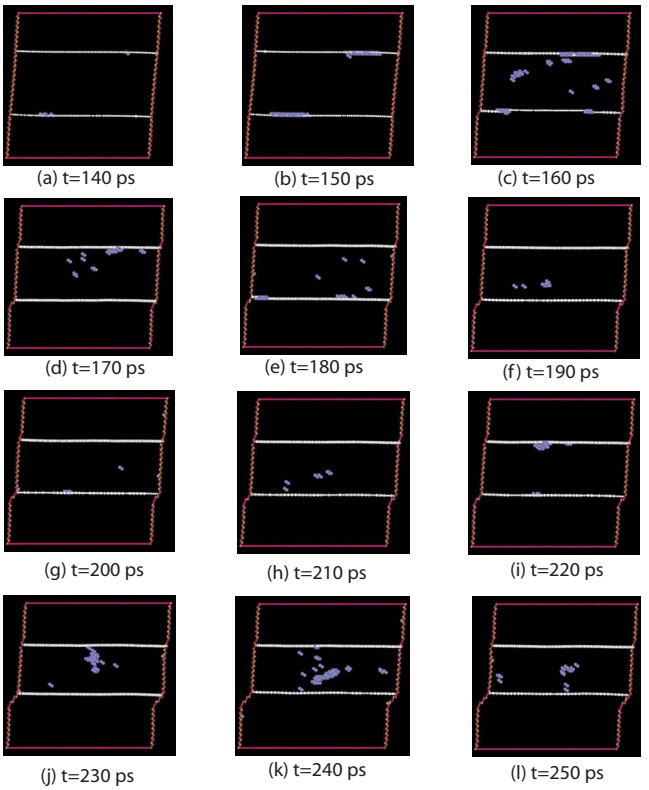

FIG. 6. (Color online) Time sequence of atoms in defect positions in a three-layer twinned copper crystal subjected to a high shear strain rate of 5×10^{8} s^{-1}.

result of dislocation glide over the entire twin plane, the twin interface moves one layer up or down depending on the twin orientations. To understand the critical step involved in twin boundary interface migration, we modified the Burgers' circuit analysis so as to enclose the twin interface. Figure 7 shows a Burgers circuit around the twinning dislocation core, where we show two circuits for two segments of the same curved Shockley partial dislocation, which was originally emitted from the surface. The Burgers vector is $\frac{1}{6}[112]$, as indicated on the figure. The two segments of the dislocation line illustrated in Fig. 7 are of the edge type. However, the Shockley dislocation loop is curved, and is thus of the mixed type depending on the curve orientation relative to the Burgers vector. Twin boundary migration is a consequence of Shockley partial nucleation and motion in an fcc crystal, consistent with earlier descriptions (e.g., Ref. 20). However, our current MD simulations clearly show the conditions, configuration, and motion of Shockley partials leading to twin boundary migration. For a twinned crystal with layer

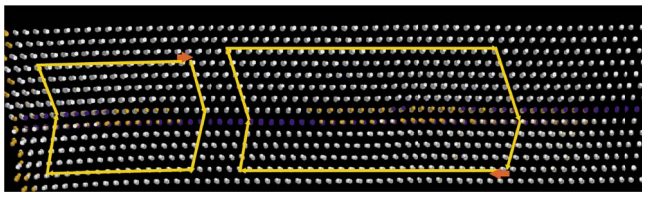

FIG. 7. (Color online) Burgers circuit for the curved partial dislocations.

stacking as ABCAB|C|BACB, if a partial dislocation glides over a (111)-type plane adjacent to the twin boundary, it will move all lattice atoms in an area above its slip plane a distance equal to the magnitude of one Burgers vector. So the layer of atoms in B positions will be moved to an A position. Simultaneously, atoms in C positions will move to B positions, and those in an A position will move to a C position, etc. As the Shockley partial glides over the twin boundary interface, all atoms in the upper part of the crystal will be moved according to the described sequence outlined here. Finally (111)-type atomic planes in the crystal lattice will have the following sequence: CABC|A|CBACB, and thus the upper half of the lattice will still have the layout of ABC, while the lower half remains in the layout of CBA, but the twin interface has moved one layer upward and A is the new twin interface.

The present simulations indicate that nucleation of Shockley partials involved in the TBM mechanism is found to be heterogeneous, initiated at three sites: on the layer directly adjacent to the twin boundary, at the surface of the crystal, and at stress concentration regions associated with the motion of a nonlinear elastic wave through the crystal. When two Shockley partial dislocation loops with the same Burgers vector merge together in the middle of the slip plane, the local stress is so large that a new dislocation loop nucleates on top of the merging area, and on the plane adjacent to the newly formed twin boundary. Thus, the mechanism is repeatable with alternating nucleation sites of Shockley partial loops between the boundaries and the center, and lead to the continuous motion of the twin boundary.

B. Strain rate effects

To investigate the deformation behavior of nanotwinned copper under strain rate control, we set up simulations for Cu twin structure with wavelengths of 3, 4, 5, 6 nm, respectively. Single crystals are also simulated to provide a reference for understanding the influence of the twin size on mechanical deformation. Twin orientations were randomly selected, for both tension and shear at 300 K, with a time step of 5×10^{-15} s. Under tensile strain loading, an abundance of mechanical twins were observed to nucleate. Figure 8 shows a time sequence for a nanotwinned copper crystal (wavelength of 3 nm) under an applied tensile strain rate of 10^{10} s^{-1}. We observe from the figure that many new stacking fault planes [green (light gray) atoms here] grow from the original twin interface and gradually fill the space between the original twin interfaces, resulting in a high areal density of stacking faults. Figure 9 gives a clear view of nucleated stacking fault layers, where blue (dark) atoms represent original matrix atoms and green (light gray) atoms designate nucleated stacking fault layers. We observe here that the stacking fault layers always show up in pairs, indicating that mechanical twinning is initiated. Twin orientations are shown by the yellow line in Fig. 9. It is observed that double layers of Shockley partials are nucleated, resulting in new nanotwins at high strain rates, in qualitative agreement with experimental observations.[11,21] In order to understand the conditions for mechanical twinning as a dominant deforma-

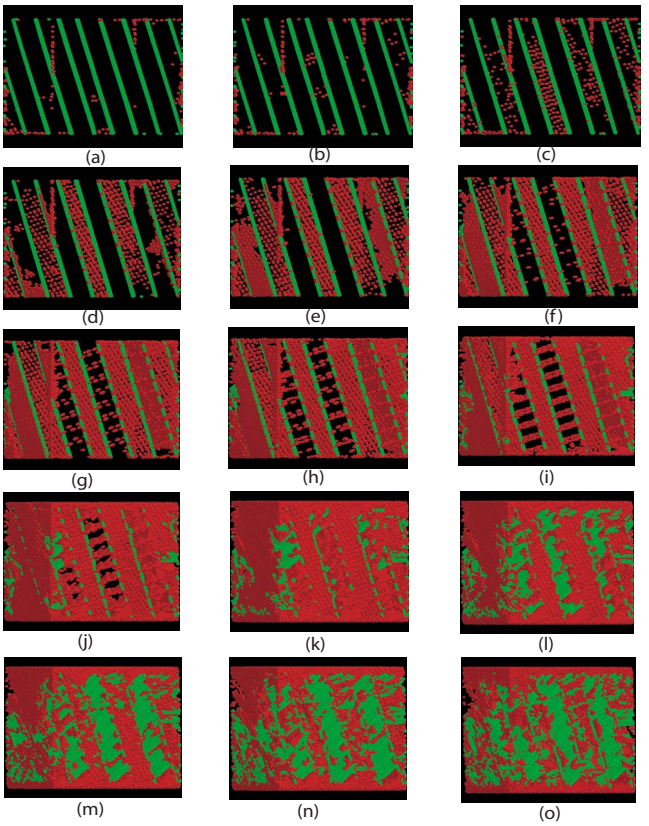

FIG. 8. (Color online) Time sequence showing the progression of deformation in a nanotwinned copper crystal under an applied tensile strain rate of 10^{10} s^{-1}. The time (picoseconds) sequence is as follows: (a) 3, (b) 3.5, (c) 4, (d) 4.5, (e) 5, (f) 5.5, (g) 6, (h) 6.5, (i) 7, (j) 7.5, (k) 8, (l) 8.5, (m) 9, (n) 9.5, and (o) 10. Green (light gray) atoms are for the stacking fault layers, while red (dark) represents other defects such as atoms, vacancies, and dislocations.

tion mechanism, we study the effect of the strain rate on the density of mechanical twins. As shown in Fig. 10, the system under a fast strain rate (10^{10} s^{-1}) achieves very high stacking fault density; close to 20% when the total applied strain reaches 10%, while the slower strain rate (10^{9} s^{-1}) shows the stacking fault density to be around 7%–8%. Therefore a higher deformation rate results in a higher nanotwin density.

IV. SIZE EFFECTS ON THE DEFORMATION OF NANOTWINNED COPPER

Since the existence of surfaces, whether external or internal (e.g., twin boundaries) is essential to the nucleation of nanotwins and dislocations, plastic deformation of nanocrystals is expected to depend on its size. On the other hand, the degree by which dislocations and nanotwins spread and engender plastic deformation should also depend on the interference of such interfaces with dislocation motion, which is also determined by size. In this section, we study the effects of nanotwinned crystal size on its subsequent deformation. We present MD simulations for the deformation of nanotwinned Cu crystals of various twin layer thickness (wavelength), and focus on understanding the influence of the twin

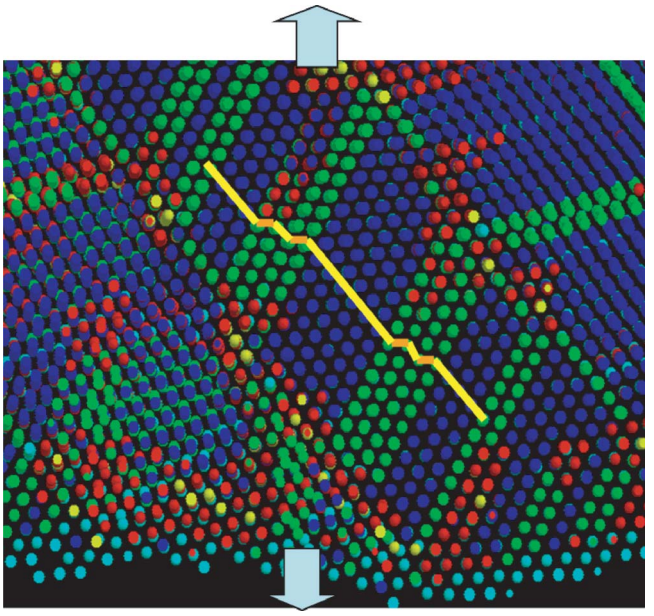

FIG. 9. (Color online) A detailed view of mechanical twinning under an applied tensile strain, at 10 ps and with 10% strain. Blue (dark) atoms represent original matrix atoms and green (light gray) ones show the stacking fault layers.

layer thickness on hardening and plastic deformation mechanisms. We present results for both strain rate control and stress control.

A. Deformation under strain rate control

Figure 11 shows a time sequence for the deformation behavior of a 3 nm wavelength nanotwinned structure under a constant shear strain rate of 10^{9} s^{-1}. We note that the stacking fault [green (light gray) atoms in the figure] is always nucleated on adjacent (111)-plane pairs, forming a nucleus for the spread of a mechanical twin. Red (dark) atoms delineate dislocations leading the spread of the stacking fault. We can see that dislocations are well confined by twin interfaces in the 3 nm nanotwin case. While dislocations in the single-

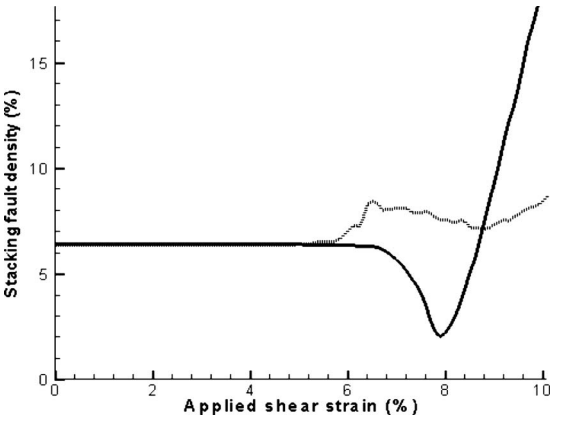

FIG. 10. Growth of the relative stacking fault areal density for rapid quench of 10^{10} s^{-1}, solid line, and for slower quench rate of 10^{9} s^{-1}, dotted line.

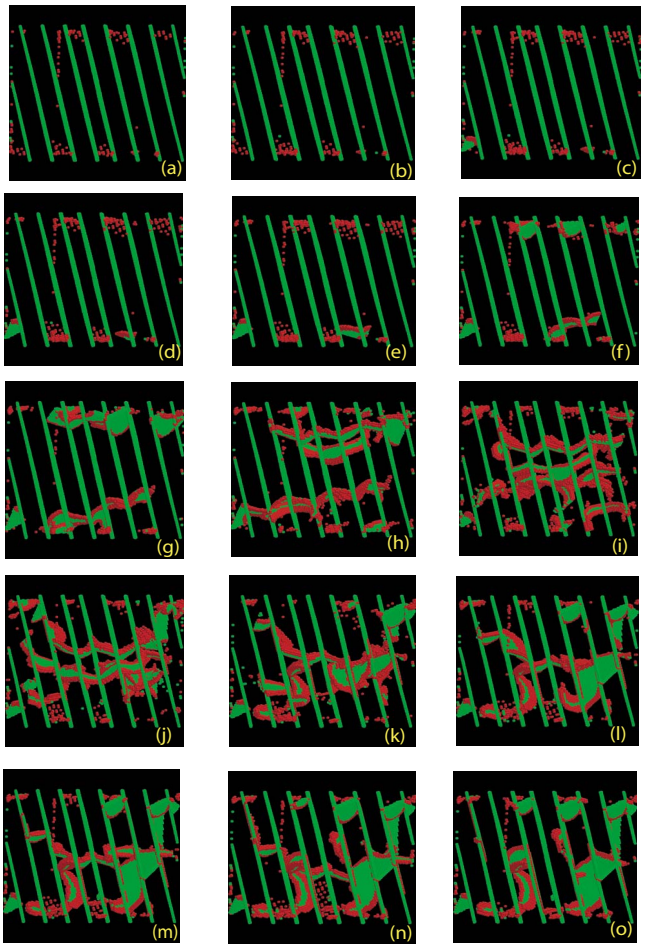

FIG. 11. (Color online) Time sequence of the deformation of a nanotwinned copper structure with a wavelength of 3 nm at an applied shear strain rate of 10^9 s^{-1}. The time (picoseconds) sequence is as follows: (a) 54, (b) 57, (c) 60, (d) 63, (e) 66, (f) 69, (g) 72, (h) 75, (i) 78, (j) 81, (k) 84, (l) 87, (m) 90, (n) 93, and (o) 96.

crystal case can easily glide on their slip planes, dislocations inside the 3 nm nanotwin structure cannot continue gliding once they encounter a twin boundary, and they are essentially trapped within narrow nanotwin channels. When two confined dislocations are close by within the channel, they cross slip and the screw segments annihilate one another, as can be seen in Figs. 11(h)–11(l). If we take a closer look at the deformed crystal shown in Fig. 12, we observe both twin boundary migration and mechanical twinning. For example, the twin boundary [green (light gray) atoms] resides on two adjacent (111) planes in two regions of the crystal. Between the two regions, red (dark) atoms delineate a Shockley partial dislocation, giving rise to twin boundary migration. Between layers of original twin planes, a new stacking fault nucleus [green (light gray) atoms] is observed to form as a pair of adjacent planes. Thus, in this case, deformation proceeds by a mixed mode though mechanical twin nucleation as well as twin boundary migration.

To understand the competition between the deformation modes discussed earlier is Sec. III, we focus our attention on the dislocation motion and stacking fault extension mechanisms. Figure 13 shows a side-by-side comparison of deformation structures found at a shear strain of 10% in nanotwinned copper (left, layer thickness=3 nm) versus single a single crystal (right). It is clear that the number of dislocation nucleation sites in the 3 nm nanotwin system is much higher than the corresponding number in the single-crystal case. Another observation is that in the nanotwinned structure, we see many full dislocations (stacking faults surrounded by a leading and a trailing Shockley partial dislocation), while very few full dislocations are observed in the single-crystal case. We also compare in Fig. 14 the relative stacking fault areal density (SFAD), defined as the ratio of number of atoms in stacking fault area (excluding grown-in twins) to the total number of atoms in the crystal, at an applied shear strain of up to 10%. The graph also shows the results for a single copper crystal for reference. As we can see from the figure, the SFAD of the single crystal reaches close to 3.5% in about 90 ps, while the SFAD in the nanotwinned structure remains relatively low (typically less than 1%).

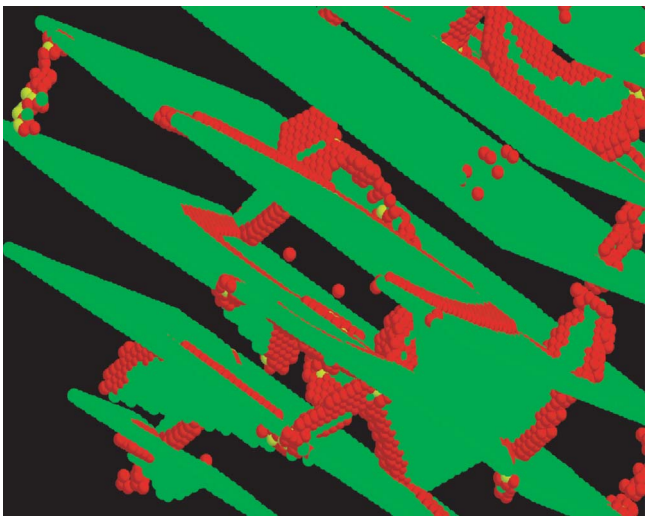

FIG. 12. (Color online) Dominant deformation modes of nanotwinned copper crystals. The figure shows the operation of the twin boundary migration mechanism (see fourth boundary from the bottom), and mechanical twinning, which is evident in the double layers bound by Shockley partial dislocations.

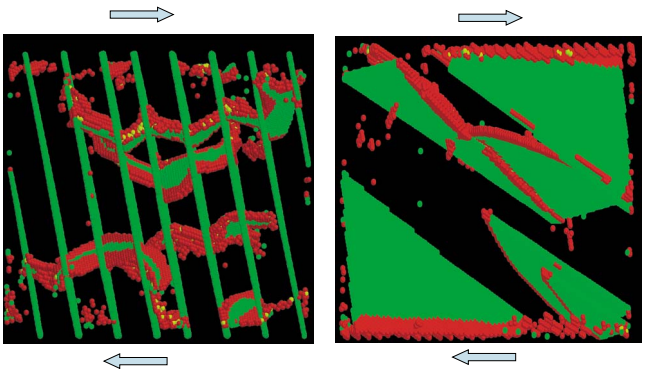

FIG. 13. (Color online) Comparison between the deformed structures of nanotwinned copper (left) and single copper crystal (right) at a strain of 10%. Note the abundance of dissociated dislocations in the nanotwinned case and of stacking faults in the single crystal.

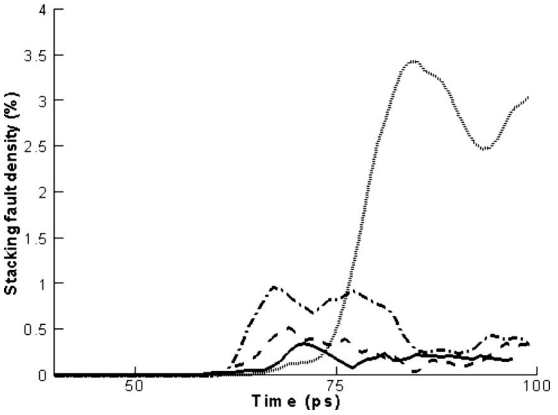

FIG. 14. Time evolution of the relative stacking fault areal density for various twin layer size. Simulations are performed at a constant strain rate of 10^9 s^{-1} up to a final strain of 10%. (a) Solid line—3 nm, (b) dash line—4 nm, (c) dash dot line—5 nm, (d) dotted line: single crystal.

Based on MD simulations of the deformation of nanotwinned copper crystals under an applied shear strain rate, the following is concluded: (1) the dislocation density in the nanotwinned structure is much larger than that in a single crystal, (2) the stacking fault density in nanotwinned crystals is lower than that in single crystal, (3) the trailing partial dislocation density in a nanotwinned structure is much higher than in a single crystal as a result of dislocation confinement in narrow channels. We also conclude that the rate of dislocation nucleation is higher in a nanotwinned crystal as compared to a single crystal under the same conditions. On the other hand, the rate of expansion of Shockley partials is much faster in a single crystal as compared to a nanotwinned crystal, resulting in a higher rate of deformation twinning in the single-crystal case. The nucleation rate difference is confirmed by the large number of dislocations in nanotwin and the observation that full dislocations are dominant in nanotwins. The reason for the high nucleation rate in a nanotwinned structure is explained to be a result of the large density of nucleation sites in nanotwinned structures, provided by twin boundaries themselves. Additionally, the confinement of dislocations and their motion in narrow channels concentrates the stored elastic energy near twin boundaries, which can be released by further nucleation of dislocations. Although the single crystal has fewer dislocations, a much higher stacking fault areal density is formed. Once dislocations nucleate, they start to spread at very high speeds (approximately at 1.3 km/s, compared to the sound speed at 273 K in copper of 3.57 km/s). As a result of the competition between dislocation nucleation rates and dislocation glide rates, we would expect an optimum nanolaminate thickness that maximizes the strength. In Sec. IV B, we discuss such optimization of nanotwinned structures for maximum strength.

B. Deformation under stress control

In the following, we present results of MD computer simulations for the deformation of single and nanotwinned crystalline copper under the conditions of constant stress. Constant tensile stress values (2, 2.5, and 3 GPa) are applied at 300 K for nanotwinned crystals with lamella thicknesses of 3, 4, and 5 nm, respectively. Figure 15 shows the time sequence for the evolution of defect structures and plastic deformation under a constant tensile stress of 2.5 GPa for nanotwinned crystals with a lamella thicknesses of 3 nm. Similar simulations were performed for lamella thicknesses of 4 and 5 nm, and for single crystals without twins. When the nanotwin lamella thickness is 3 nm at 2.5 GPa, we observe that fully dissociated dislocations (with leading and trailing partials) can easily cross the twin boundary and overcome the boundary resistance. A more detailed illustration of this boundary crossing process at 3 nm is shown in Fig. 16. A second mode of dislocation interaction with twin interfaces is that of cross slip of the leading partial from its original slip plane to the twin interface itself [which is a (111)-type plane], followed by glide of the leading Shockley partial along the interface. Interestingly, the trailing Shockley partial follows by cross slipping onto the twin boundary interface, but it glides in the opposite direction, expanding the new

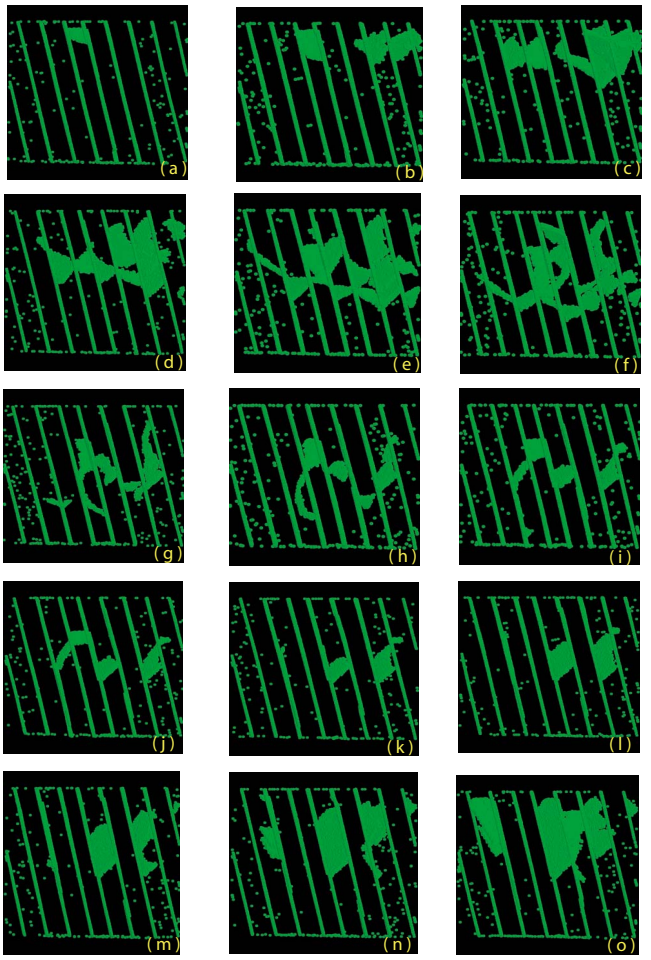

FIG. 15. (Color online) Time sequence (in picoseconds) for the deformation behavior of nanotwinned copper under a tensile stress of 2.5 GPa at 300 K, and with lamella thickness of 3 nm (ten layers are shown here). Simulations are conducted at 300 K, with a time step of 5 fs. (a) 32, (b) 34, (c) 36, (d) 38, (e) 40, (f) 42, (g) 44, (h) 46, (i) 48, (j) 50, (k) 52, (l) 54, (m) 56, (n) 58, and (o) 60.

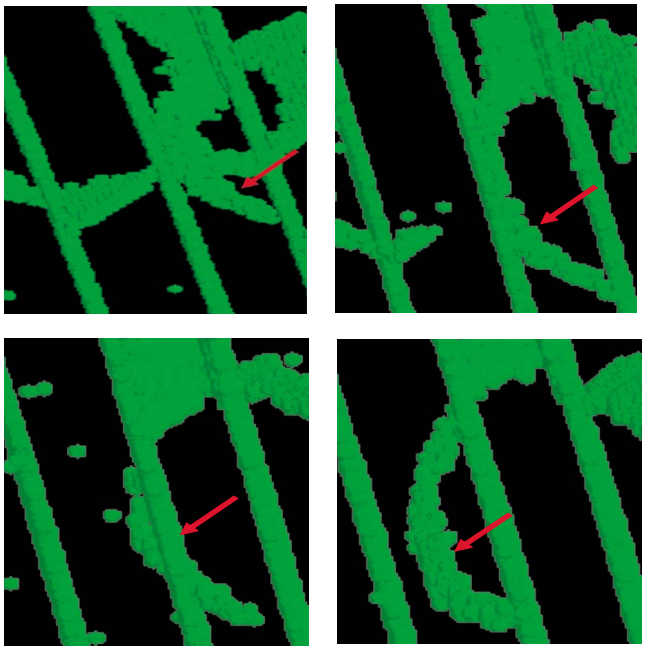

FIG. 16. (Color online) Illustration of the cross-slip mechanism for dislocations nucleated at one twin boundary crossing onto the opposing boundary.

stacking fault area bound by the two partials and resulting in TBM, as we discussed earlier. Under an applied shear stress of 2.5 GPa, the dislocation interaction mechanism with twin interfaces is observed to be quite different from the case the nanotwin lamella thickness is 4 nm. This interaction mechanism is shown is Fig. 17, where we present the time sequence for the deformation process, and focus attention on dislocation-twin boundary interaction. It is observed that under these conditions, once the leading partial is nucleated on one twin interface, it expands quickly to the other interface, while the trailing partial is almost stationary close to the nucleation site. Collision of the leading partial with the opposite interface results in its trapping, direction reversal, and shrinkage of the dissociated stacking fault zone. The leading partial, once it reverses direction, continues motion until the two partials recombine again at the nucleation site. This interesting behavior is shown in Fig. 17. For an applied shear stress of 2.5 GPa and lamella thickness of 5 nm, the previously described dislocation "trapping-recoil" mechanism is also observed. Nevertheless, fully dissociated dislocations are also observed to easily cross twin boundary interfaces, resulting in significant plastic strain. In the single crystal, which is a limiting case here, there is no barrier to dislocation motion. Many stacking faults are generated, which is a prelude to mechanical twinning as a deformation mode.

Because of these differences in the deformation behavior of twinned structures of various size lamellae, an optimum lamella thickness for maximizing the strength of the nanostructure is found to be about 4 nm for copper. At this thickness, the Shockley partial dislocation emitted from one interface recoils from the opposite interface, and atomic displacements of the two partials represent a trapped wave in between the two twin interfaces. The stacking fault in between the two Shockley partials induces attraction between

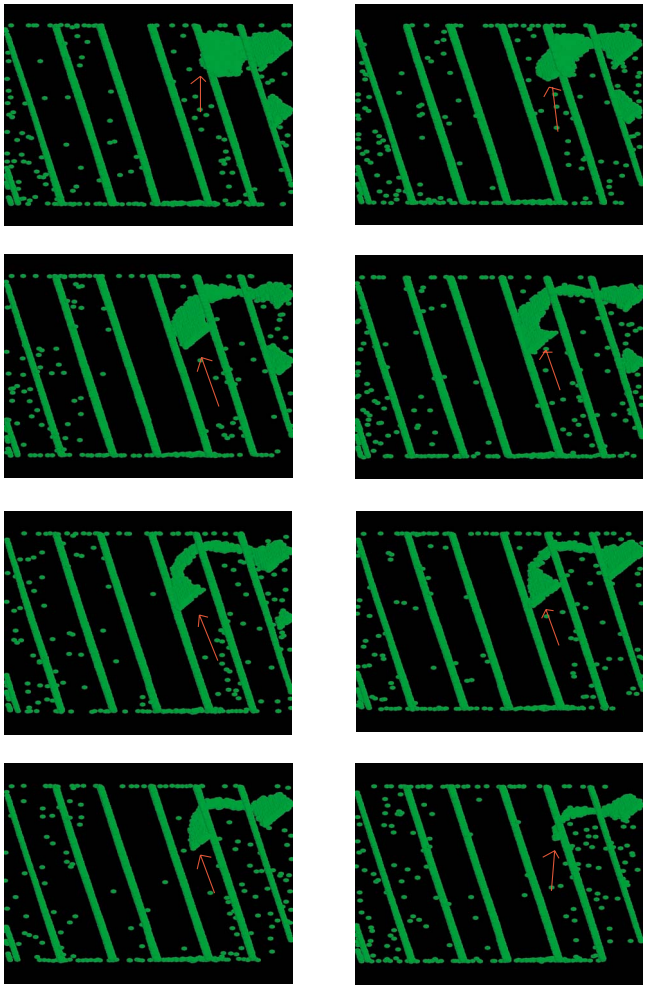

FIG. 17. (Color online) Dislocation collision with twin boundaries and rebounding back in twin lamella channels.

the two partials and shrinkage of the fault area. Thus, this trapping-recoil mechanism at 4 nm is the main reason for optimal strength in nanotwinned copper. To further quantify these observations, Figs. 18 and 19 show the time evolution of the accumulated strain of twinned copper structures of various lamella thicknesses at applied shear stress levels of 2 and 3 GPa, respectively. The resolved shear stress (RSS) on grown-in twin planes are 0.45, 0.675, and 0.9 GPa, respectively, while the RSSs on the dislocation glide planes intersecting with grown-in twins are 1.28 and 2.56 GPa, respectively. The strain oscillations in MD simulations are due to the dynamic extension and contraction of stacking faults and dislocation loops, as they interact with twin boundary interfaces or external surfaces. The results for 0 K deformation are the lower envelope bounding the strain values under dynamic conditions. The time evolution of strain, displayed in Figs. 18 and 19, clearly demonstrates that the lowest deformation is obtained when the lamella size is 4 nm. Plastic strain can also be measured in terms of the increase in the stacking fault surface area. The stacking fault areal density for nanotwin lamella size of 4 and 5 nm is relatively low, confirming the conclusion that an optimal lamella size of about 4 nm gives the most resistance to deformation.

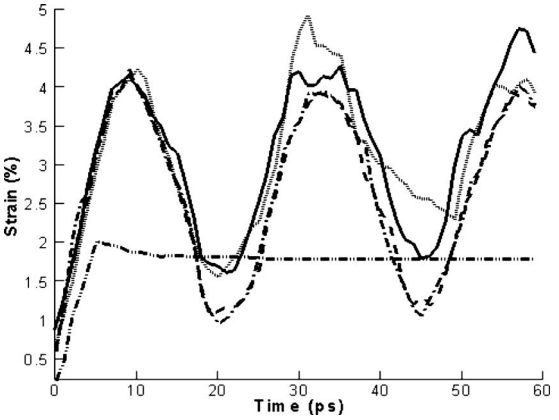

FIG. 18. Evolution of the shear strain for various size nanotwin lamella thicknesses at an applied shear stress of 2 GPa and 300 K. (a) Solid line—3 nm, (b) dash line—4 nm, (c) dash dot line—5 nm, (d) dotted line: single Cu crystal, (e) dash dot dot line—3 nm at 0 K.

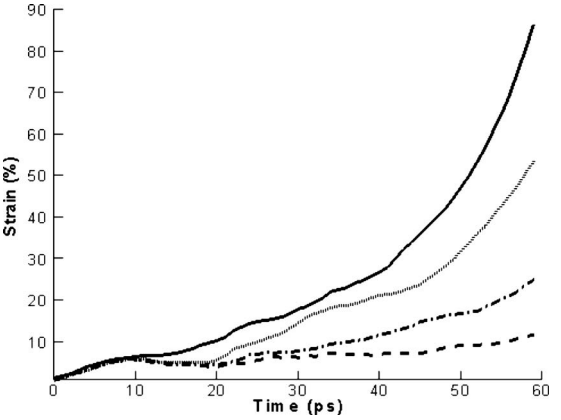

FIG. 19. Evolution of the shear strain for various size nanotwin lamella thicknesses at an applied shear stress of 3 GPa and 300 K. (a) Solid line—3 nm, (b) dash line—4 nm, (c) dash dot line—5 nm, (d) dotted line: single Cu crystal.

V. SUMMARY AND CONCLUSIONS

The present MD simulations of nanotwinned copper crystals reveal several atomistic mechanisms pertaining to the strength and ductility of nanotwinned copper crystals. In a three-layer twinned-structure simulation, shear stain was applied parallel to the twin interface. We observed that twin boundary migration is induced by Shockley partial dislocations in the following sequence:

(1) Nucleation of a partial is initiated by the coordinated thermal motion of atoms in a coherent "wave," where atomic positions are "shuffled," during this phase. The first partial nucleation site was observed to occur in three regions: on the layer directly adjacent to a twin boundary, at the surface of the crystal, and at stress concentrations.

(2) Partial dislocations glide under the applied shear strain leading to twin boundary migration by one atomic layer.

(3) When two partials with the same Burgers vectors merge together in the middle of the slip plane, the local stress is so large that a new dislocation loop nucleates on top of the merge point, and on the plane adjacent to the newly formed twin boundary. The continuous operation of this mechanism results in twin boundary migration under stress over long distances relative to interatomic spacings.

We also studied the effects of nanotwin lamella size on the deformation of nanotwinned copper. The deformation behavior of nanotwinned Cu with various twin thickness was simulated under several loading conditions. Simulations were performed for both constant applied shear strain rate and constant applied tensile stress. The relative stacking fault areal density and the number of nucleated dislocations were compare. Our simulations clearly demonstrate that the dislocation density in a nanotwin structured material is much more than the corresponding value in a single crystal, while the SFAD in a nanotwinned structure is much less than the corresponding value in a single crystal. In nanotwinned crystals, dissociated full dislocations were found to be dominant, while in a single crystal we observed very few full dislocations. Those observations lead to the conclusion that the degree of plastic deformation is determined by both the dislocation nucleation rate and rate of dislocation propagation, implying that an optimal thickness exists. MD simulation results confirmed the main mechanism of strengthening in nanotwinned copper as the restriction of dislocation motion in narrow channels (twinned layers). A critical twin thickness associated with maximum strength and minimum plastic deformation was found to be around 4 nm. For this thickness, the leading partial dislocation emitted from one twin interface propagates to the opposite interface, recoil there, reverses direction, shrinking the core of the emitted dislocation and confining it in the same twinning channel. For lamella thicknesses of 3 nm, MD simulations indicate that dislocations can easily cross twin interfaces. It is also found that the stress state greatly influences the dominant deformation mode. In the case of a large Schmid stress compared to normal components on the twin interface, the main mechanism of deformation is observed to be the TBM mechanism. When the Schmid stress on the twin interface is small compared to its value on intersecting (111)-slip planes, the main deformation mode is observed to be double layer nucleation and growth of Shockley partial dislocations.

Twin boundary migration was identified as a dominant deformation mode in nanotwinned Cu when the Schmid stress is high on the twin interface. On the other hand, dislocation nucleation and propagation in narrow twin channels is the main deformation mechanism when the Schmid stress is low on twin interfaces and high on conjugate (111)-glide planes. The large strength of nanotwinned copper structures is found to be derived from the resistance of twin boundaries to dislocation motion. Although twin boundaries act as nucleation sites for dissociated dislocation loops in twinned copper, they also act as barriers to their subsequent motion. At stress levels below a critical value, dislocations are generally confined in their motion to very narrow channels formed in between twin boundaries. This mode of restricted motion gives rise to strengthening of the structure. When the stress is raised above this critical value, dislocations are able to overcome the twin boundary barrier, and hence confinement is lost. It is found that at an optimal thickness of about

4 nm, Shockley partial dislocations emitted from the surface of one twin boundary recoil from the opposing boundary and are trapped in between. The dynamic effects of the recoils lead to further shrinkage of the stacking fault between the leading and trailing partials, and thus accumulated plastic deformation is recovered in this event. The results of both tension and shear show that TBM is the dominant deformation mode when twin boundaries have high Schmid factors, while mechanical twinning and dislocation glide are dominant when conjugate (111) planes have high Schmid factors.

ACKNOWLEDGMENTS

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