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Effects of Schmid factor and slip nucleation on deformation mechanism in columnar-grained nanotwinned Ag and Cu

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We report the results of a molecular dynamics study of the effect of texture on the yield and peak stresses in columnar-grained nanotwinned Ag and Cu. The simulations suggest that in pure nanotwinned face-centered cubic metals, the strength is determined primarily by the cooperation or competition between two major factors: the magnitude of the Schmid factors for the available slip systems and the effectiveness of grain boundaries (and their triple-junctions) in generating dislocations. These factors and their relative impact depend on the geometry of the specimen relative to the applied stress, which is typically reflected in the texture of the material in experimental studies. The detailed mechanisms of plastic deformation are discussed for seven specific geometries that represent a range of different textures.

I. INTRODUCTION

Nanotwinned materials have been actively studied for the last decade due to their superior and unique mechanical properties compared to conventional polycrystalline and nanocrystalline materials. Nanotwinned metals have shown enhanced strength and ductility, as well as improved electrical performance, fracture toughness, and stability against cyclic loading, compared to ultrafine-grained and nanocrystalline materials.1–8 These materials contain a high density of coherent twin boundaries (CTBs) that appear to serve as effective barriers to dislocation motion: these boundaries are the loci of changes of crystal orientation between matrix and twin, and discontinuities in most of the slip systems across the CTBs. Tensile tests of nanotwinned materials with various twin densities show that the yield strength, hardness, and ductility increase with decreasing twin spacing down to some critical spacing.9–17

With very pronounced preferred orientations of CTB planes, the orientation of CTBs with respect to a loading direction is a factor that can play a significant role in the deformation behavior of nanotwinned materials in a tensile test. With changes of CTB orientation, the deformation mechanisms can also change, leading to new kinds of orientation-dependent plastic response, and observably anisotropic plasticity.9,15 Although some researchers argue that the influence of crystallographic texture (orientation of CTBs) on the deformation behavior is minimal,10 others have found that texture is one of the key factors that affect the mechanical behavior of nanotwinned materials.14,15,18 A clearer understanding of the orientation-dependent plastic response of these materials is essential if they are to be used in engineering applications.

II. MOLECULAR DYNAMICS SIMULATIONS OF NANOTWINNED Cu AND Ag UNDER TENSILE LOADING

Molecular dynamics simulations were performed using the LAMMPS package, which was designed to allow parallel simulations of systems containing millions of atoms.20 Interatomic interactions were described by an embedded-atom method (EAM) potential for the Cu-Ag system.21 Using this potential, we modeled pure Cu and pure Ag systems, as discussed below. To study a behavior of the nanotwinned materials under tensile loading, we used a simulation cell containing two parallel sets of twins, separated by grain boundaries, as shown in Fig. 1. In the images of the simulation cells (or their fragments) provided throughout this paper, the atoms are colored according to the Common Neighbor Analysis (CNA).22,23 The CNA allows assigning a structure type (face-centered cubic (fcc), hexagonal close-packed (hcp), body-centered cubic (bcc), etc.) to every atom. Analysis and visualization of MD simulation snapshots were performed using the software package OVITO (Open Visualization Tool).24,25

The simulation cells were constructed by joining two parts of the system (containing CTBs), which had been tilted around the y-axis ((110)) (see Fig. 1). After joining the two parts, the whole system was relaxed at T = 0 K with periodic boundary conditions applied in all three principal directions.

In this paper, we report the results of a systematic series of molecular dynamics (MD) simulations of the plastic deformation of textured nanotwinned Ag and Cu films. Our results demonstrate that the activation of slip is determined primarily by the Schmid factors of the available slip systems19 and the effectiveness of the grain boundaries (GBs) as dislocation sources. The molecular dynamics simulations indicate that changes in the texture of columnar-grained nanotwinned Ag or Cu may lead to significant variations of the yield and peak stresses of the material.
We investigated deformation for seven distinct tilt angles ($\alpha$ and $-\alpha$) covering a range from $|\alpha| \sim 2^\circ$ to $|\alpha| \sim 45^\circ$ using simulation cells corresponding to the angles of 2.38°, 8.28°, 14.01°, 22.58°, 27.47°, 31.96°, and 44.95°. The tilt angles we selected were tuned to these values so the simulation system would be periodic in the z-direction. The separation distance between the CTBs is set initially at $\sim 10.5$ nm. The simulation cell dimensions varied slightly, depending on the value of the tilt angle $\alpha$, with the average size of the system being $44$ nm $\times 12.8$ nm $\times 44$ nm in the x, y, and z directions, respectively, so that the total number of atoms in the system was approximately $2 \times 10^6$. We note that these microstructures are similar to those of sputtered thin films produced and tested experimentally. However, the simulation system we use is simplified compared to fully three-dimensional columnar-grained experimental samples because all of the GBs were initially parallel to each other and there are no GB triple junctions in the simulated systems (although there are triple junctions between GBs and TBs). At this stage, our goal is to determine the unit mechanisms that govern the basic behavior of the material, rather than to simulate the precise behavior of real experiments in every detail.

At least two mechanisms can contribute to the plastic deformation of nanocrystalline materials: one is based on dislocation nucleation and propagation, while the other one is associated with GB sliding (see, e.g., Ref. 26 for a review). A transition between these two mechanisms usually occurs at a grain size of around 20 nm, with dislocation glide dominating at larger sizes and grain boundary sliding at smaller ones. In our study, we have focused on nanotwinned materials where the TB separation is small ($\sim 10$ nm) but the GB separation is much larger (e.g., the columnar-grain size ranged from 43 to 80 nm in Ref. 5). The GB sliding mechanism is not expected to operate in this case. However, the GB separation in our simulation cell is only about 20 nm because larger GB separations would require larger simulation cell and, therefore, would be more computationally expensive. Therefore, to explore qualitatively similar deformation mechanisms to those which operate in experimentally produced nanotwinned materials, we applied uniaxial stress only in the x-direction, which is normal to the GBs in the computational cells, effectively suppressing grain boundary sliding.

Our simulation cells include a variety of distinct grain boundaries. If we arbitrarily designate the alternating crystal orientations in each grain as "matrix" and "twin," then the grain boundary parameters depend on whether the abutting crystals are "matrix-matrix," "twin-twin," "twin-matrix," or "matrix-twin." As illustrated schematically in Figure 2, these grain boundary variants include two asymmetric tilt grain boundaries (ATGBs) with misorientations of $|2\alpha|$ that are identical to each other except for a rotation of $180^\circ$ about the $z$-axis, corresponding to the "matrix-matrix" and "twin-twin" cases. The "matrix-twin" and "twin-matrix" cases produce distinct symmetric tilt grain boundaries (STGBs) with misorientations of $|2\alpha + 70.53^\circ|$ and $|2\alpha - 70.53^\circ|$, modulo $90^\circ$. Each simulation thus contains three distinct grain boundary variants, in addition to the coherent twin boundaries, and the negatives of each of the grain boundary variants. A complete list of all of the grain boundary misorientations is given in Table I.

It was demonstrated recently that annealing the atomic configurations at high temperatures is necessary for equilibrating grain boundaries in computer-generated polycrystals. Therefore, after the initial relaxation, all systems were annealed at $T = 1200$ K and zero stresses for 4 ns using the isothermal-isobaric (NPT) ensemble method. The models were then cooled to $T = 300$ K before tensile loading was applied in the x-direction. The tensile loading simulations were carried out using an ensemble with a fixed number of atoms, $N$, and a fixed simulation temperature of $T = 300$ K. A constant engineering strain rate of $10^4$ s$^{-1}$ was applied in the x-direction and the stresses in the y and z directions were fixed (at zero). Periodic boundary conditions were applied in all directions.

![FIG. 1. Simulation system. The case of $|\alpha| = 27.47^\circ$ (pure Ag) is shown as an example. The atoms are colored according to CNA. The color-coding is as follows: green—fcc, red—hcp, grey—other.](image)

![FIG. 2. Illustrating the various grain boundary types present at the outset of our simulation experiments. The orientations of the individual grains are indicated, relative to an uninclined “matrix” orientation. CTB refers to coherent twin boundaries, STGB to symmetric tilt grain boundaries, and ATGB to asymmetric tilt grain boundaries. The expressions above the grain boundary types give the rotation angle in degrees, about the [110] axis normal to the page.](image)
III. RESULTS

Figure 3 shows the stress-strain curves for models with angles $\alpha \sim 8.28^\circ$ and $\sim 44.95^\circ$: for the smaller angle, there is a distinct “peak stress” at the onset of deformation, which then proceeds at a moderately uniform flow stress. In our simulations, we observed a significant decrease in the peak and yield stresses, as the angles $\alpha$ were increased up to $45^\circ$.

Figures 4 and 5 show the dependence of the yield and peak stresses on the angle $\alpha$ for the pure Ag and pure Cu systems, respectively. The yield stress drops dramatically as the angle $\alpha$ increases from $\sim 14.28^\circ$ to $\sim 22.58^\circ$ and the peak stress decreases substantially, though somewhat less dramatically. To understand the reasons for the sharp decreases in the yield and peak stresses, we examined snapshots of the atomic configurations generated at various stages during the tensile loading. We will use the Ag model as an example, noting that the results obtained for Cu are qualitatively very similar.

Figure 6 shows a snapshot from the MD simulation of tensile loading of pure Ag system for $|\alpha| = 14.01^\circ$, corresponding to 4.8% strain in the x-direction. At this point, plastic deformation has just started. Only some of the slip systems are active, and, in particular, these are the ones which are not parallel to the y axis ($(110)$).

A summary of all systems studied is given in Fig. 8. The snapshots from the MD simulations shown in Fig. 8 correspond to initial stages of plastic deformation and the active slip systems are easily identifiable. The slip systems in a twin and its corresponding matrix grain can be illustrated using a double Thompson tetrahedron as illustrated in Figure 9. For lower values of the angle $\alpha$, we observe that the most active slip systems lie on the ADC ($A^4D^4C_7^4$) and BDC ($B^4D^4C_7^4$) slip planes. We observe Shockley partial dislocation loops enclosing semi-circular intrinsic stacking fault on these slip systems and we will refer to this type of

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$2\alpha$</th>
<th>$\Sigma$</th>
<th>$2\alpha + 70.53^\circ$</th>
<th>$\Sigma$</th>
<th>$2\alpha - 70.53^\circ$</th>
<th>$\Sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.38°</td>
<td>4.76°</td>
<td>1</td>
<td>75.29°</td>
<td>3</td>
<td>65.77°</td>
<td>3</td>
</tr>
<tr>
<td>8.28°</td>
<td>16.56°</td>
<td>$R$</td>
<td>87.09°</td>
<td>17</td>
<td>53.97°</td>
<td>11</td>
</tr>
<tr>
<td>14.01°</td>
<td>28.02°</td>
<td>19</td>
<td>8.55°</td>
<td>1</td>
<td>42.51°</td>
<td>9</td>
</tr>
<tr>
<td>22.58°</td>
<td>45.16°</td>
<td>$R$</td>
<td>25.69°</td>
<td>19</td>
<td>25.37°</td>
<td>19</td>
</tr>
<tr>
<td>27.47°</td>
<td>54.94°</td>
<td>11</td>
<td>35.47°</td>
<td>9</td>
<td>15.59°</td>
<td>$R$</td>
</tr>
<tr>
<td>31.96°</td>
<td>63.92°</td>
<td>3</td>
<td>44.45°</td>
<td>$R$</td>
<td>6.61°</td>
<td>1</td>
</tr>
<tr>
<td>44.95°</td>
<td>89.90°</td>
<td>17</td>
<td>70.43°</td>
<td>3</td>
<td>19.37°</td>
<td>$R$</td>
</tr>
</tbody>
</table>

**TABLE I.** Summary of the misorientations of the (initially) asymmetric and symmetric grain boundary segments for each of our simulations. The characteristic $\Sigma$-value is given wherever a boundary corresponds to a coincidence-site lattice within the error allowed by the Brandon criterion. Although none of these boundaries falls at an exact coincidence misorientation.
dislocation as type II, following the notation introduced in Ref. 28. As the angle $\alpha$ increases, the slip systems on the ADB (A$^1$D$^3$B$^1$), and ABC (A$^1$B$^1$C$^1$) slip planes become the most active during the initial stages of the deformation process. The dislocations we observed in motion on these slip systems are extended 60° full dislocations,28 each of which splits into a 30° leading partial, an intrinsic stacking fault and a 90° trailing partial.29 We will refer to this type of dislocations as type I.

We now describe the observed deformation processes for different angles $\alpha$. In the system with $|\alpha| \approx 2.38^\circ$, we mostly observed type II dislocations. The peak on the stress-strain curve corresponds to the strain level at which the type II dislocations are first activated. In this system, we observed nucleation of type II dislocations on the slip planes associated with the dislocations that make up the $\approx 4.76^\circ$ ATGBs (see Fig. 10) and also near the triple junctions of CTBs, ATGBs and STGBs.

In the system with $|\alpha| \approx 8.28^\circ$, we observed both type I and type II dislocations. However, the type II dislocations are more abundant and the peak of the stress-strain curve corresponds to the strain level at which the first type II dislocation appears. In this system, we observed nucleation of the type II dislocations on the slip planes associated with the dislocations that make up the $\approx 16.56^\circ$ ATGBs and near the places where type I dislocations intersect the CTBs. The type I dislocations nucleated near the triple junctions of CTBs, ATGBs, and STGBs, as well as on the STGBs. In the system with $|\alpha| \approx 14.01^\circ$, we mostly observed type II dislocations.
that nucleated near the triple junctions of CTBs, ATGBs, and STGBs (see Fig. 11).

In the system with $|x| \sim 22.58^\circ$, we observed both type I and type II dislocations. However, the type I dislocations, particularly those corresponding to ABC(A$^3$B$^3$C$^3$) slip planes of the double Thompson tetrahedron (see Fig. 9), were activated first. The embryos of these dislocations are structural units of the 25.69$^\circ$ STGBs in the initial configuration (before the imposition of strain). Under strain, the leading partials of these dislocations run across the whole grains on slip planes parallel to the twin boundaries, leaving stacking faults behind (see Fig. 12). When the strain is increased to $\sim 4\%$, type II dislocations are activated. These nucleate at the triple junctions of CTBs, ATGBs and 25.69$^\circ$ STGBs (see Fig. 13). At about the same level of strain, type I dislocations corresponding to the ADB (A$^3$D$^3$B$^3$) slip planes are activated. These nucleate at the triple junctions of CTBs, ATGBs, and 25.37$^\circ$ STGBs.

In the system with $|x| \sim 27.47^\circ$, type I dislocations predominated. The dislocations corresponding to ABC (A$^3$B$^3$C$^3$)
slip planes nucleated on the 35.47° STGBs. On the other hand, dislocations corresponding to ADB (A^TD>T^B) slip planes were present even without any imposed strain, because these dislocations are structural components of the 15.59° STGBs in the initial configuration. Under strain, the leading partials of the type I dislocations corresponding to both slip systems ran completely across the columnar grains, leaving stacking faults behind (see Fig. 14).

In the system with |z| ~ 31.96°, we observed only type I dislocations during yielding, and the deformation scenario is similar to the case of |z| ~ 27.47° presented above. The embryos of the dislocations corresponding to ADB (A^TD>T^B) slip planes were present in the initial (unstrained) configuration because they make up the 6.61° STGBs. Dislocations on the ABC (A^TB>C^T) slip planes first nucleated on the 63.92° ATGBs and later, at higher strain, they also nucleated on the 44.45° STGBs. Under strain, the leading partials of all these dislocations ran across whole columnar grains, leaving stacking faults behind. The peak stress was reached immediately before type II dislocations nucleated.

In the system with |z| ~ 44.95°, we observed only type I dislocations. The dislocations corresponding to ADB (A^TD>T^B) slip planes nucleated at |z| ~ 2.8% strain at the triple junctions of the CTBs, 89.90° ATGBs, and 70.43° STGBs (see Fig. 15(a)). At a strain of |z| ~ 3.2%, type I dislocations belonging to the ABC (A^TB>C^T) slip planes nucleated at 89.90° ATGBs, and their leading partials traversed the columnar grains, leaving stacking faults behind (see Fig. 15(b) and also the corresponding image of Fig. 8).

IV. DISCUSSION

To explain the MD simulation results, we need to consider two factors: the values of the Schmid factors for all available slip systems and the effectiveness of the grain
boundaries as dislocation sources. Both factors depend on the angle $\alpha$.

Table II summarizes the locations at which dislocations nucleated at the beginning of the plastic deformation process for all angles $\alpha$ that we studied. In our simulations, all STGBs and ATGBs were initially normal to the tensile loading direction: any change in the orientation of a grain boundary with respect to the loading direction, or change in a type of load applied (e.g., tensile, shear, etc.), should be expected to lead to changes in preferred dislocation nucleation sites.

We calculated the Schmid factor values for all slip systems and all angles $\alpha$ considered in the present study. Figure 16 shows the maximum values of the Schmid factors for the three groups of slip systems (see the double Thompson tetrahedron in Fig. 9):

(1) BCD, $B^T C^T D^T$, ACD, and $A^T C^T D^T$ planes;
(2) ABD and $A^T B^T D^T$ planes;
(3) ABC and $A^T B^T C^T$ planes.

Note that in our MD simulations, the tensile axis always lies symmetrically between BCD and ACD and is always perpendicular to the intersection of ABD and ABC (AB), imposing a fairly high level of symmetry. Figure 16 also shows the Schmid factor values that correspond to the slip systems that were activated first in our MD simulations.

**TABLE II.** Observed places of the dislocation nucleation in the beginning of the plastic deformation.

<table>
<thead>
<tr>
<th>$\alpha$ (°)</th>
<th>Dislocation of type I</th>
<th>Dislocation of type II</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.38</td>
<td>Not observed ATGBs, triple-junctions</td>
<td></td>
</tr>
<tr>
<td>8.28</td>
<td>STGBs, triple-junctions</td>
<td>ATGBs</td>
</tr>
<tr>
<td>14.01</td>
<td>Not observed</td>
<td>Triple-junctions</td>
</tr>
<tr>
<td>22.58</td>
<td>STGBs, triple-junctions</td>
<td>Triple-junctions</td>
</tr>
<tr>
<td>27.47</td>
<td>STGBs</td>
<td>Not observed</td>
</tr>
<tr>
<td>31.96</td>
<td>STGBs, ATGBs</td>
<td>Not observed</td>
</tr>
<tr>
<td>44.95</td>
<td>ATGBs, triple-junctions</td>
<td>Not observed</td>
</tr>
</tbody>
</table>

For the smallest angles $\alpha$ (2.38°, 8.28°), the maximum values of the Schmid factor correspond to the slip systems that belong to BCD ($B^T C^T D^T$) or ACD ($A^T C^T D^T$) planes of the Thompson octahedron. In the MD simulations, we observed that the type II dislocations (Shockley partial dislocation loops) that belong to these slip planes are activated first and they are the most abundant dislocations in the strained crystals. Even though the embryos of the dislocations that correspond to ABC ($A^T B^T C^T$) slip planes of the Thompson octahedron are present from the very beginning in the simulation systems with $\alpha \approx 2.38°$ (where they make up the $\sim 4.76°$ ATGBs) and $\alpha \approx 8.28°$ (where they make up the $\sim 16.56°$ ATGBs), these slip systems remain inactive throughout the entire MD simulation, probably because of the extremely low Schmid factors associated with them (see Fig. 16).

A similar scenario is observed in case of $\alpha \approx 14.01°$. However, for this case, the values of the Schmid factors on the BCD ($B^T C^T D^T$) or ACD ($A^T C^T D^T$) planes are slightly lower than those on ABD ($A^T B^T D^T$). The higher values of the yield and peak stresses observed for the lower angles $\alpha$ (2.38°, 8.28°, 14.01°) (see Figs. 4 and 5) may be explained by the lower values of the maximum Schmid factors (over all available slip systems) and the fact that there were no pre-existing embryos of type II dislocations in the initial (unstrained) systems.

The behavior under tensile loading changes dramatically when we reach an angle $\alpha \approx 22.58°$. In this case, the structures of the 25.69° STGBs in the initial configuration incorporate embryos of the type I dislocations that belong to the ABC ($A^T B^T C^T$) slip planes. Even though the maximum Schmid factor values associated with these slip systems are much lower than the maxima of those associated with the BCD ($B^T C^T D^T$), ACD ($A^T C^T D^T$), or ABD ($A^T B^T D^T$) slip systems, these dislocations are activated first, at a relatively low strain level (~1.5%), which is the likely explanation for this case producing the lowest yield stress of all the angles $\alpha$ that we studied (see Figs. 4, 5). We note that the effect of
non-planar grain boundary structures on the behavior under deformation was recently reported, and these can occur in metals with low stacking fault energies. In particular, it was demonstrated that these non-planar structures (embryos of dislocations) make it easier for a grain boundary to emit a leading Shockley partial dislocation in order to accommodate the applied strain, which agrees with our observations for this particular case.

In the rest of the cases (angles $\sim 27.47^\circ$, $\sim 31.96^\circ$ and $\sim 44.95^\circ$), the behavior under the tensile loading is similar. The slip systems that belong to the ABD ($A^1B^1D^1$) and ABC ($A^1B^1C^1$) slip systems were activated for all low tensile strains (2%-3%). Thus, the lower values of the yield stresses that we observed for these angles may be explained by the combined effect of high Schmid factors for some of the slip systems and the ready generation of dislocations by some of the grain boundaries.

The peak stresses for the high angle cases (angles $\sim 22.58^\circ$, $\sim 27.47^\circ$, and $\sim 31.96^\circ$) were all reached immediately before type II dislocations nucleated. The peak stresses for these cases were lower than those for the lower-\(\alpha\) cases. However, the peak stresses do not vary monotonically with \(\alpha\) (see Figs. 4 and 5) which may be attributed to the fact that these systems already contain type I dislocations which can affect the nucleation of the type II dislocations. In the $\sim 44.95^\circ$ case, the type I dislocations so effectively reduce the stress that the type II dislocations never show up. Based on these assumptions, one can also suppose that the obtained values for the peak stresses may strongly depend on the strain rate. This question deserves further investigation.

Finally, we note that the geometry of all of our simulations is such that the applied stress is expected to produce lattice rotations that result in reducing the values of $\alpha$ or correspondingly, reducing misorientations across all of the various grain boundaries—though not the twin boundaries. Reducing the misorientation of a grain boundary calls for a reduction of its dislocation content so the formation of glide dislocations out of the grain boundary structures can be seen as meeting two needs of the deformation process: promoting plastic strain via glide, and maintaining the contiguity of the polycrystal as incompatible crystal rotations occur, by adjustment of the grain boundary structure. It is interesting that these work simultaneously in their “correct” directions through the dislocation emission process in the cases studied here. It deserves further study to see if this is true for all geometries, or if it is an artifact of the particular symmetry of our model.

V. CONCLUSIONS

The yield strengths of the nanotwinned materials simulated here are a result of the combined or competing effects of two major factors: the magnitudes of the Schmid factors for the available slip systems, and the effectiveness of grain boundaries (and their triple-junctions) in generating dislocations. Both of these factors depend on the texture of the material (which is reflected by the angle $\alpha$ in our simulations). When a slip system has both a large Schmid factor and an effective interfacial dislocation source, it is easily activated and becomes the dominant slip system. When the slip system with the highest Schmid factor does not have an effective dislocation source, it can be supplanted by a slip system with a moderate Schmid factor that has available a more effective source of dislocation nucleation.

ACKNOWLEDGMENTS

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