Anomalous deformation twinning in fcc metals at high temperatures

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Nanotwinned structures have shown strong promise as optimal motifs for strength, ductility, and grain stability in fcc metals—in sharp contrast to their nano-grained counterparts where gains in strength are disappointingly offset by loss of ductility. However, their high temperature stability has remained relatively unaddressed. Here we investigate the high temperature response of twin boundaries that constitute these nanostructured metals, by way of molecular dynamics simulations. At low and intermediate temperatures, the twin boundaries exhibit normal motion coupled to shear deformation as expected. However, our simulations at higher temperatures (above 0.5–0.7 T_m), reveal considerable deformation twinning, an occurrence that has not been observed before in fcc metals. Although the origins of this intriguing behavior are not yet clear to us, we discuss a possible conjecture by addressing the following questions: (i) Why is the high temperature response of some fcc metals different? (ii) Why do we observe a transition from twin migration to stacking fault nucleation and subsequent twin formation at high temperatures? © *2011 American Institute of Physics*. [doi:10.1063/1.3596517]

I. INTRODUCTION

Research over the past few years has provided compelling evidence for the extraordinary properties of nanotwinned metals as compared to their nanocrystalline and fine-grained counterparts (see Ref. 1 for review). Some of their remarkable properties revealed through extensive experimental studies and mechanistic modeling include ultrahigh yield strength, high strain rate sensitivity, and enhanced ductility.[2–8] By nanotwinned metals, we refer herein to fcc metals with an average grain size of 200–500 nm containing twins with lamella thickness below 100 nm. It is well established that the coherent twin boundaries (CTBs) serve as effective barriers for impeding dislocation motion, thus constituting a strengthening motif, and also serve to accommodate large plastic strains by absorbing dislocations which leads to enhanced ductility. This is in contrast to nanocrystalline metals which undergo a severe loss of ductility with decreasing grain size and increasing strength (see Ref. 9 for review). Furthermore, nanocrystalline metals are known to exhibit stress-driven grain coarsening at low temperatures.[10–13] They also lose their stability at higher temperatures by grain growth, driven primarily by grain boundary (GB) mediated processes such as sliding, migration, and diffusion.[14–16] An extensive atomistic study of GB migration and sliding over a range of temperatures has been performed by Cahn *et al.*[17]

Although such structural instability is a critical issue that limits the benefits of nanostructuring, it has remained relatively unaddressed so far in the context of nanotwinned metals, especially at high temperatures. Recent studies by Shute *et al.*[18] and Saldana *et al.*[19] show the enhanced stability of nanotwinned Cu at cryogenic and ambient temperatures. The experimental studies of Lu *et al.*[20] performed at room temperature, also reveal that there exists a critical twin lamella thickness below which there is a decline in the strength (and possibly other properties) of the nanotwinned structure due to twin-twin interactions. These observations have been confirmed by the simulations of Kulkarni and Asaro[21] and Li *et al.*[22] Investigating the mechanical response of CTBs at low temperatures, Sansoz and Molinari[23] and Kulkarni *et al.*[24] observe that CTBs, being highly symmetric low energy interfaces, exhibit a very high shear strength compared to most GBs and undergo normal motion coupled to shear. On the other hand, the atomistic study by Li and Ghoniem[25] reveals a competition between deformation twinning and twin migration when the CTB is subjected to different kinds of loading at room temperature.

As a prelude to addressing the question of the high temperature strength and stability of nanotwinned metals, we investigated the high temperature response of CTBs by way of atomistic modeling. To this end, we performed molecular dynamics simulations of shearing of a bicrystal specimen containing a CTB. The runs were performed for various fcc metals over a range of temperatures. Our idealized bicrystal simulations enable us to understand the interplay between the three modes of deformation associated with the twin or the slip plane, namely, TB motion, slip, and deformation twinning. We define the three modes as follows. TB motion refers to the apparent motion of the TB normal to its plane, that is, along the [111] direction, when subjected to shear along the [112] direction (Fig. 5(a)). Slip refers to the formation of an intrinsic stacking fault (Fig. 5(b), Step I). Deformation twinning refers to the formation of a pair of CTBs under deformation. This is a two-step process, as illustrated in Fig. 5(b).

Section II presents the details of our simulations and results. In Sec. III, we analyze our results based on the energetics of these competing mechanisms and discuss a possible

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conjecture for the anomalous response of twin boundaries at high temperatures by addressing the following questions: (i) Why are the high temperature responses of some fcc metals different? (ii) Why do we observe a transition from twin migration to stacking fault nucleation and subsequent twin formation at high temperatures? Finally, Sec. IV summarizes our findings and discusses possible avenues for future work.

II. SIMULATION METHOD AND RESULTS

A. Methodology

The response of CTBs to shear deformation at a range of temperatures was studied by way of molecular dynamics simulations using LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator).[26] The simulations were performed in the canonical (NVT) ensemble using the Nose-Hoover thermostat. The effect of the thermal expansion was incorporated by expanding the simulation cell uniformly, prior to the MD simulation, according to the thermal expansion factor at the desired temperature. The thermal expansion was determined *a priori* through separate MD simulations on a periodic cell in the NPT ensemble. The fcc metals studied herein include Cu, Pd, Ag, and Al. Our choice of materials is based on the fact that these four metals differ widely in some of the relevant material parameters, thus covering a range of elastic moduli and stacking fault energies as well as twinnability. The embedded atom (EAM) interatomic potentials used in this work are those developed by Liu *et al.*[27] for Al, Mishin and co-workers for Cu[28] and Ag,[29] and Voter and Chen[30] for Pd. Our digital specimens were bicrystals of size $80 \times 80 \times 120$ Å with a coherent twin boundary (CTB) located at the center and normal to the z-axis as shown in Fig. 1. The simulation cells, containing 50 176 atoms, were aligned along the $[1\bar{1}0]$, $[11\bar{2}]$, and [111] crystallographic directions with periodic boundary conditions applied in the x- and y- directions. A few layers of atoms at the top and bottom of the bicrystal were treated as rigid slabs and did not participate in the MD runs. The shear was then applied by displacing the top slab along the $[11\bar{2}]$ direction with a constant velocity of 0.01 Å ps^{-1} while the bottom slab was held fixed. Thus, the strain rate in our simulations was on the order of 10^8 s^{-1}, which is typical for MD calculations. The defect structures were extracted using the centro-symmetry parameter[31] and were visualized using AtomEye.[32] The

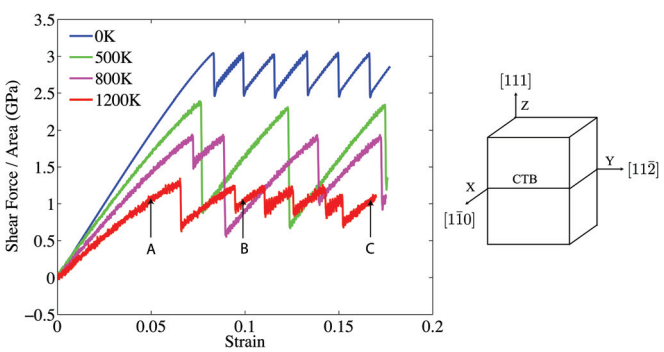

FIG. 1. (Color) Shear stress vs strain plots for Cu bicrystals at various temperatures, and the crystallographic orientation of the bicrystals. The atomic structures at A, B, and C are shown in Fig. 4.

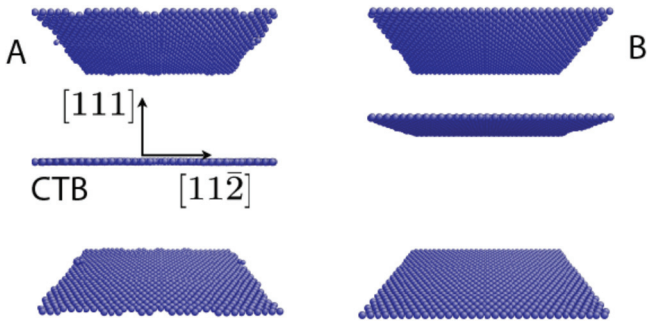

FIG. 2. (Color online) The position of the CTB at (a) 5% (initial position), and (b) 18% shear strain during shear deformation at $T = 0$ K.

observations of the shear tests are summarized and discussed in the following sections.

B. Response at low and intermediate temperatures

The shear stress versus strain curves for Cu bicrystals at different temperatures are plotted in Fig. 1. The stress increases linearly as the bicrystal deforms elastically until it reaches a critical value when the CTB moves normal to the twin plane. With increasing temperature, we note an expected trend of softening due to the effect of thermal expansion, and reduced shear strength owing to the increase in the thermal energy content in the system. At 0 K, the CTB exhibits normal motion with a high shear strength of about 3 GPa, as reported by Kulkarni *et al.* previously.[24] Each drop in the curve corresponds to the motion of the CTB by one lattice plane in the [111] direction. Figure 2 shows a sequence of positions of the CTB at strain values of 5% (a) and 18% (b) separated by a distance of about 14 Å or 7 atomic layers. At higher temperatures ranging from 300 K to 800 K, the shear stress displays a similar stick-slip behavior, but with drops much larger than in the 0 K case, which correspond to the normal motion of the CTB through multiple lattice planes simultaneously. This difference is attributed to the thermal fluctuations that provide the excess energy to

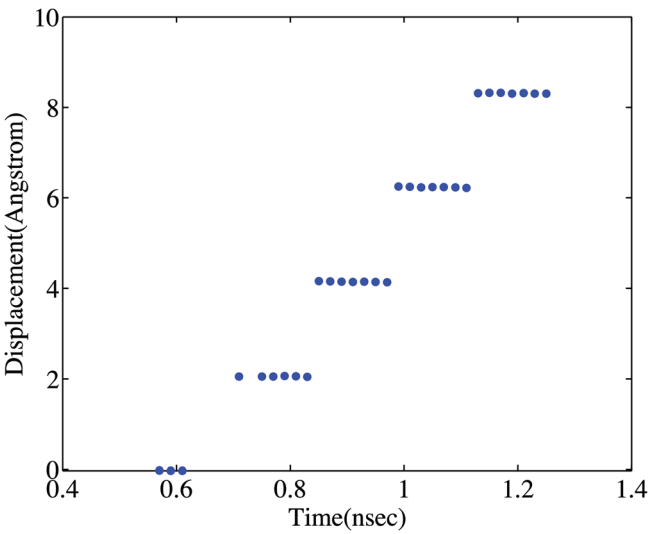

FIG. 3. (Color online) The normal displacement of the CTB with time in the shear simulation of a Cu bicrystal at 0 K.

overcome the activation barrier for twin migration at lower stresses.

These general observations are consistent with earlier MD simulations[17,23] on a series of symmetrical tilt boundaries over a range of temperatures. We note that at the temperatures considered here, we do not observe any sliding or spontaneous CTB motion, unlike some GBs considered by Cahn *et al.*,[17] which begin to exhibit spontaneous normal motion at about 800 K. In the absence of sliding, the ideal coupling relation between the applied shear and the shear induced by the normal motion can be defined as[17]

$$\kappa = \frac{v_{\|}}{v_n} \tag{1}$$

where v_b is the normal velocity and $v_{\|}$ is the applied shear velocity. Our calculation of κ for a CTB at different temperatures from 0 K to 800 K confirms the observation of Cahn *et al*. that κ remains almost constant with temperature and thus behaves like a geometric factor. Figure 3 illustrates the CTB displacement during the shear simulation. Using this plot, the κ for CTB motion is found to be about 0.72.

C. Response at high temperatures

In this section, we present the results for the shear deformation of Cu bicrystals at temperatures ranging from 800 K to 1200 K ($\sim$0.9 T_m with $T_m \sim 1357$ K). As seen in Fig. 1, the stress versus strain curve at 1200 K also shows a stick-slip behavior although the height of the drops is less uniform. Figure 4 illustrates the associated evolution of the bicrystal structure with increasing shear strain. Image (b), taken at about 9% strain, shows two additional CTBs separated by a lattice plane in the upper crystal, which indicates the formation of the first new twin. Continued deformation twinning is observed with increasing strain, as shown in image (c) which consists of two new pairs of CTBs in the upper crystal. On further shearing, oppositely oriented CTBs (indicated by arrows) move closer and eventually annihilate after approaching a critical separation. This is evident from image (d) taken at 24% strain. After the annihilation of CTBs, the process of twinning is repeated as the simulation continues.

These results show that there is a transition in the response to shear from coupled CTB motion to formation of twins at higher temperatures. Our simulations at intermediate temperatures predict the transition temperature for Cu to be about 0.65 T_m ($\sim$850 K). No twinning is observed till 800 K. At 900 K, twinning is first observed at 15% strain. With further increase in temperature, twinning becomes predominant with almost negligible normal motion of the original CTB. As mentioned above, closely spaced oppositely-oriented CTBs are found to be more susceptible to normal motion under shear followed by subsequent annihilation.

Using the ABCABC… stacking sequence in the [111] direction for fcc metals, Fig. 5 depicts the process of normal motion and that of twin formation under shear along the $[11\bar{2}]$ direction. Twin migration occurs through the emission of a partial dislocation on a plane adjacent to the existing CTB. Twinning proceeds with the creation of a micro-twin, as observed in earlier works.[25,33–35] It is a two-step process, which involves the nucleation of two partial dislocations on successive [111] planes. The emission of a partial can be depicted by a sliding process. To illustrate this, consider Fig. 5(a), in which the atomic layer B (immediately above the CTB layer C) slides along $\langle 112 \rangle$ direction to the only other possible position, i.e., A (marked by the dashed arrow). All the layers above shift accordingly. The net result of this sliding is the (apparent) motion of the CTB by one lattice plane as depicted in Fig. 5(a). In Fig. 5(b), this sliding process, when initiated at a random layer in the upper (perfect) crystal, leads to the formation of an intrinsic stacking fault marked by step I. Repeating the sliding process starting one

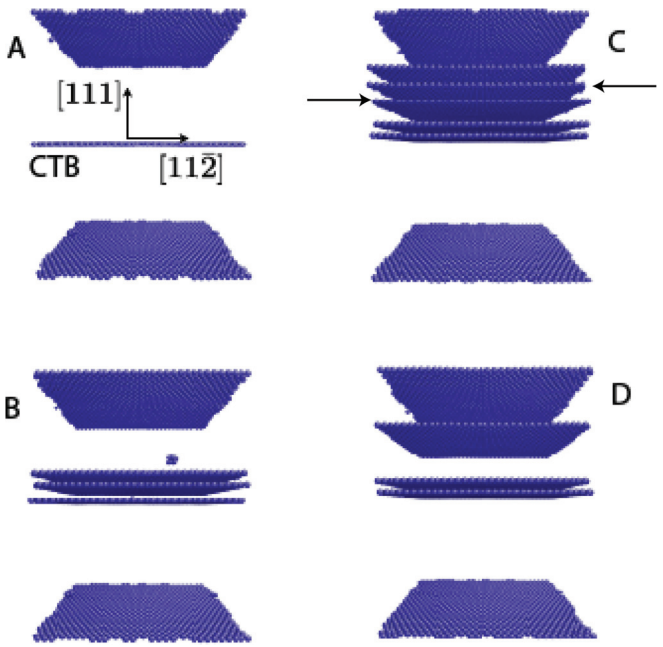

FIG. 4. (Color online) The atomic structures at different strains (a) 1%, (b) 9%, (c) 18% (d) 24% at T = 1200 K during shear deformation. The crystallographic orientation and the initial location of the CTB with respect to the top and bottom surfaces is shown in (a). The sequence of images shows the process of twinning (b,c) and the eventual annihilation of closely spaced, oppositely oriented CTBs (d).

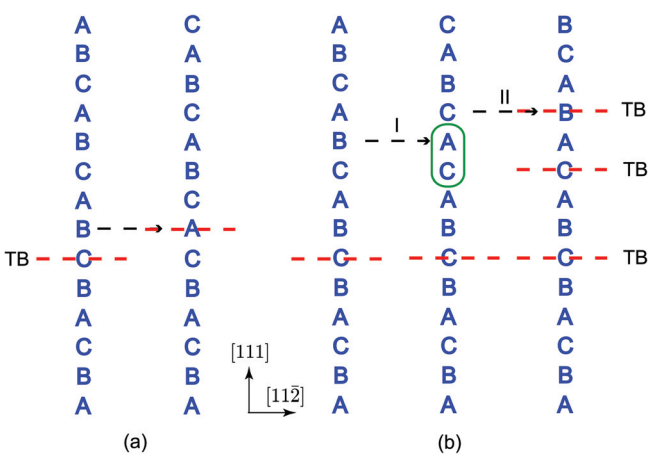

FIG. 5. (Color) Schematic representation of (a) twin motion, and (b) twin formation in a bicrystal with a CTB. The red line marks a CTB as the stacking sequences along [111] on either side of a red line are in reverse order (or mirror images). The green box shows a two-layer intrinsic stacking fault.

layer above (step II) results in two new CTBs marked by red lines. Both these processes can also be simulated using MD to obtain the generalized planar fault curves and the twin migration curves in order to estimate the associated activation energies for stacking fault nucleation, twin formation, and twin migration in different fcc metals.[36]

D. Response of various fcc metals

The transition temperature is investigated further by performing similar shear simulations on a few other fcc metals, namely, Pd, Ag, and Al. The melting temperatures are taken to be 1828 K for Pd, 1235 K for Ag, and 933 K for Al. Figure 6 compares the stress-strain response for these metals at 0.7 T_m which corresponds to about 1000 K for Cu, 1300 K for Pd, 900 K for Ag, and 700 K for Al. The deformation mechanism at low and medium temperatures is found to be coupled normal motion in all the cases. However, the transition to twinning at high temperatures and the associated transition temperature is observed to vary in different metals, as described below.

Pd displays a response very similar to that of Cu with a transition temperature of about 0.65 T_m (~1250 K for Pd). At 1300 K, twinning is first observed at 15% strain, which is in agreement with our Cu simulations described earlier. In the case of Ag, twin formation becomes the dominant mode of deformation at a much lower transition temperature of about 0.5 T_m (~600 K for Ag). In sharp contrast, Al shows no transition at all even up to temperatures as high as 0.86 T_m (~800 K for Al) and continues to exhibit twin migration. Thus, in Fig. 6, the load drops correspond to twin migration for Al and deformation twinning for Cu, Pd, and Ag.

III. DISCUSSION

Our simulations reveal an intriguing temperature dependence of the behavior of twin boundaries, which is not expected based on earlier studies. We now seek to analyze these results by addressing the following questions: (i) Why are the high temperature responses of some fcc metals different? (ii) Why do we observe a transition from twin motion (Fig. 5(a)) to stacking fault nucleation (Step I, Fig. 5(b)) at high temperatures? (iii) Why does twin formation (Step II, Fig. 5(b)) occur before or instead of subsequent stacking fault nucleation?

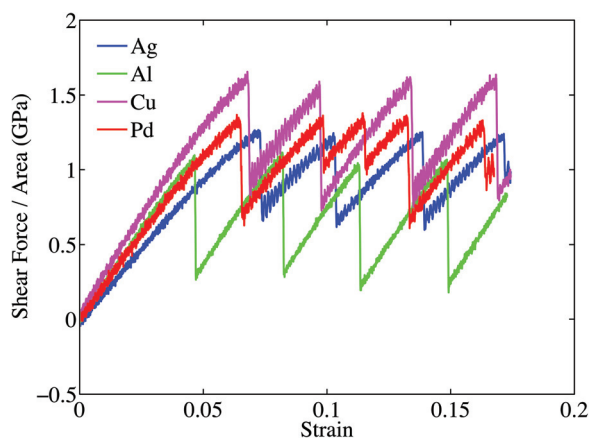

FIG. 6. (Color) Shear stress vs strain plots for bicrystals of Ag, Al, Cu, and Pd at ~0.7 T_m.

It is well-established through studies on single and polycrystalline metals that dislocation-mediated slip and deformation twinning are the primary mechanisms of deformation at temperatures below which individual atoms become mobile and that the latter is observed at subambient temperatures and/or high strain rates while slip is the dominant deformation mode at higher temperatures.[33,37] In contrast, our simulations, although performed at high strain rates, show deformation twinning to be the dominant mechanism at high temperatures (above 0.5–0.7 T_m). No twinning is observed at low temperatures where the deformation is governed by TB motion. To the best of the authors' knowledge, this has not been observed before in pure fcc metals although a similar behavior has been observed by Yapici *et al.*[38] in their experimental study on Ti-6Al-4V. They attribute this unexpected high temperature twinning to the high levels of stress and strains generated during their experiments. Consistent with these studies, our molecular dynamics simulations are also performed under high stresses and high strain rates. Furthermore, comparing our results with the work of Cahn *et al.*,[17] we note that they only observe normal GB motion and GB sliding at all temperatures. This is due to the fact that they apply the shear on the GB plane in their bicrystal simulations. Thus, the critical stress for GB motion or sliding is reached before the critical resolved shear stress on one of the slip planes can lead to slip or twinning. Since we apply the shear on the [111] plane, our bicrystal simulations involve two competing mechanisms, namely, slip or deformation twinning and twin migration. Thus, our simulations solely compare the shear stress on the slip plane required to nucleate a twin or move an existing twin boundary and its dependence on temperature. This is also a major difference from most prior studies on twinning which were performed on single and polycrystalline specimen and consequently, the major deformation modes were slip, deformation twinning, and ultimately grain-boundary mediated processes at high temperatures. In fact, we believe that a part of the reason for the anomalous deformation twinning we observe is the high shear stresses generated in our idealized simulations in addition to the absence of other high temperature deformation modes which are available in realistic nano- or poly-crystalline specimens.

We first address the different responses of various fcc metals at high temperature based on our earlier work (Kulkarni and Asaro)[21] on dislocation-twin interaction in different fcc metals and that of Bernstein and Tadmor[39] on the twinnability of fcc metals. Both studies use the Peierls framework for dislocation emission from a crack tip introduced by Rice.[40] Based on the predictions of Bernstein and Tadmor,[39] the fcc metals can be sorted according to their tendency to twin as

$$\mathrm{Pt} < \mathrm{Al} < \mathrm{Ir} < \mathrm{Au} < \mathrm{Cu} < \mathrm{Pd} < \mathrm{Pb} < \mathrm{Ag}$$

This trend is in agreement with the increasing values of the dimensionless parameters, β and β_t defined as

$$\beta = 1 - \gamma_{sf}/\gamma_{us}; \quad \beta_t = 1 - \gamma_{sf}/\gamma_{ut}$$

and computed by Kulkarni and Asaro[21] for Al, Cu, Pd, and Ag, where γ_{sf} is the stacking fault energy, γ_{us} is the unstable

stacking fault energy, and γ_{ut} is the unstable twinning energy. Taken together with our results for high temperature simulations, we conclude that metals which have greater twinnability (or higher β_t) also exhibit a greater tendency toward deformation twinning at higher temperatures. Consequently, Cu and Pd, which have intermediate but similar β_t, show similar transition temperatures ($\sim$0.7 T_m), whereas Ag, which has the highest twinnability, starts to show profuse deformation twinning at a lower transition temperature ($\sim$0.5 T_m). In contrast, Al has the lowest twinnability and does not exhibit twinning at any temperature. This response of Al is well known[33,39] and usually attributed to its high stacking fault energy, except for recent simulations and experimental observations of deformation twinning in nanocrystalline Al at ambient temperatures.[41,42]

In order to address questions (i) and (ii), we compare our bicrystal simulations with identical shear tests performed on single crystals of the same dimensions.[43] We observe that single crystal Cu exhibits twin formation according to the mechanism illustrated in Fig. 5(b), with more twinning observed at 1200 K as compared to 0 K. The stress-strain curve shows a saw-tooth behavior. The first peak in the shear stress drops from 3.5 GPa at 0 K to 1.3 GPa at 1200 K ($\sim$ 0.9 T_m). For Al, the first peak drops from 2.6 GPa at 0 K to 1.4 GPa at 800 K ($\sim$0.9 T_m). We note that these peaks correspond to the critical stress for the homogeneous nucleation of an intrinsic stacking fault. The subsequent peaks are smaller than the first and correspond to the stress required to form a twin according to step II in Fig. 5(b).

On the basis of our simulations, we are unable to provide a clear rationale for the transition from twin migration to deformation twinning at higher temperatures. However, based on the following reasoning, we conjecture that the transition possibly occurs due to the difference in the temperature sensitivity of the process of twin migration and that of nucleation of a stacking fault. Figure 1 shows the temperature dependence of TB motion in Cu from 0 K to 800 K (the mechanism in the plot for 1200 K is deformation twinning). The shear strength at 0 K is about 3 GPa. Since the peak stress versus temperature follows a linear relation as seen in our simulations, we estimate that the critical stress for TB motion at 1200 K would be about 1.5 GPa. Comparing this with the single crystal results above, we observe that the stress for homogeneous nucleation of a stacking fault is slightly more sensitive to temperature and becomes comparable or even lower than the stress for twin migration at high temperatures (possibly beyond 0.7 T_m, the estimated transition temperature for Cu). In contrast, for Al, the peak stress for TB motion drops from 1.5 GPa at 0 K to 1 GPa at 800 K, which is always lower than the stress required for stacking fault nucleation, and is consequently preferred at all temperatures. This provides a possible speculation for the transition from twin motion to twin formation for certain fcc metals at higher temperatures.

We now attempt to understand why we observe deformation twinning instead of dislocation or stacking fault nucleation only. To this end, we refer to the data compiled by Kulkarni and Asaro (see Table I in Ref. 21) and note that the values of β are very close to those of β_t for metals like Cu, Pd, and Ag. In other words, Kulkarni and Asaro's[21] γ_{us} and γ_{ut} are comparable to those obtained here. This is also indicated by the generalized stacking fault curves obtained by Swygenhoven *et al.*[33,36] which show γ_{us} and γ_{ut} to be almost the same for Cu. This implies that after an intrinsic stacking fault is created by homogeneous nucleation in a metal like Cu, it is energetically more favorable to move the two atomic layers of the stacking fault apart to create a deformation twin ($\gamma_{ut}-\gamma_{sf}$) than to create a new stacking fault by homogeneous nucleation (γ_{us}) or to migrate an existing twin (γ_{tm}). Once a new twin is created, the system now has multiple twin boundaries and the subsequent shear deformation depends, again, on the competition between twin motion and stacking fault nucleation.

IV. SUMMARY

Our simulations reveal an intriguing transition in the behavior of twin boundaries in fcc metals at higher temperatures as the mechanism changes from normal motion to deformation twinning. The response is studied for different fcc metals and we conclude that it correlates well with the twinnability of the material. We also speculate that in the metals which exhibit the transition, it occurs due to the different temperature sensitivity of the competing mechanisms, namely, twin migration and homogeneous nucleation of a stacking fault.

We would like to note that finite temperature molecular dynamics simulations are limited by high strain rates. To address this question within the limits of MD, we also performed identical shear simulations for Cu at 300 K and 1200 K at strain rates that vary by a factor of 10, namely 10^8 and 10^7 s^{-1}. At 1200 K, we do observe a slight strain-rate dependence as twin migration is also observed along with a slightly reduced tendency for twin formation at the slower strain rate, as compared with our observation of predominant twinning with no twin migration at the higher strain rate. No noticeable strain-rate dependence is observed at 300 K. A complete study of the strain-rate dependence is beyond the scope of MD. Using free-energy minimization methods and calculating the free-energy barrier for twin motion and twin formation in fcc metals at finite temperature could provide further insight into the strain-rate dependence of this response of twin boundaries. An interesting direction for future work is to investigate the dependence on load versus displacement controlled conditions. It would also be useful to study the entropic effects of these competing mechanisms based on the recent work of Ryu *et al.*[44] Our simulations do indicate that the behavior of nanotwinned metals should depend on the interplay between slip, twin migration, and mechanical twinning as the major modes of deformation. They also indicate that CTBs may maintain their stability with regards to twin migration even at high temperatures as twinning becomes preferable and the existing CTBs remain unaltered. Thus, it would be quite insightful to further investigate the response of realistic nanotwinned structures at high temperatures based on the competition between these mechanisms as well as GB mediated processes, which become dominant at higher temperatures. Although not discussed in detail as part of this paper, we also observe annihilation of oppositely oriented CTBs, which come closer than a critical separation. Taken together, these responses of twin boundaries observed in our

simulations may have an interesting effect on the structural stability of nanotwinned fcc metals and, hence, provide possible avenues for future investigations.

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