

Multiplane-induced widening of stacking faults in fcc metals

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Using an *ab initio*-based parametric dislocation dynamics approach we show that Shockley partials on successive glide planes greatly assist the widening of stacking faults (SFs) in Al and Ag. This effect is amplified when all trailing partials are pinned. Subsequent placement of Shockley partials on adjacent planes enhances further the widening of the SF width. In sharp contrast, dislocations with zero net Burgers vector across three successive planes form very compact cores in both Al and Ag, in agreement with recent experiments. © 2007 American Institute of Physics.

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Nanocrystalline (nc) metals exhibit mechanical properties, which are markedly superior to those of conventional materials, such as dramatically enhanced strength and hardness,^{1,2} which can coexist, in a few cases, with very good ductility.¹⁻³ These exceptional properties have been attributed to their unique deformation mechanisms, which may be different from those in their coarse-grained (CG) counterparts.⁴⁻⁷ These include partial dislocation emission from grain boundaries (GBs), deformation twinning (DT), full dislocation gliding, and GB sliding. The ratio $\gamma_{ut} - \gamma_{isf} / \gamma_{us} - \gamma_{isf}$ provides a measure of the competition between deformation twinning and full slip in fcc metals, where γ_{us} is the unstable stacking fault energy required to nucleate the leading partial on the first glide plane, and γ_{isf} and γ_{ut} are the intrinsic stacking fault (ISF) and unstable twin fault energies,^{8,9} respectively. The numerator (denominator) represents the energy barrier to nucleate the twinning (trailing) partial on the adjacent (same) glide plane in the presence of the leading partial.

Molecular dynamics (MD) simulations, using extremely high strain rates in the order of $10^6 - 10^8 \text{ s}^{-1}$ predict that nc Al deforms via Shockley partial dislocation emission from GBs.¹⁰⁻¹² Consequently, these partials form DT and partial-dislocation-enclosed SF ribbons *within* the grains, the so-called *homogeneous* twinning mechanism.¹⁰ Interestingly, the observed SFs were found to be much wider (1.5–11 times) than both the experimental value in CG Al and the theoretical value predicted by atomistic simulations. Such wide SFs are unexpected because Al has very high ISF energy. On the other hand, in nc metals (Cu or Ag) with low γ_{isf} , no SF ribbons within the nanograins have been observed, while SFs across whole grain are ubiquitous.¹³ These wide SFs are attributed to both the small grain size and the presence of high stress concentration in nc metals.^{14,15} Another twinning mechanism predicted by MD simulations¹⁰ and recently confirmed by experiment¹³ is the *heterogeneous* one in which the twins are nucleated on GBs.

An intriguing question is the orientation of the Burgers vector of the trailing partial with respect to that of the leading partial that generated the SF.¹⁵ The trailing partials are generally believed to have *identical* Burgers vector, the so-called *monotonic activation of partials*. However, recent experiments¹⁶ find evidence of a twinning mechanism in nc metals, the so-called *random activation of partials* (RAPs) on successive (111) planes, which produce a zero net macrostrain, i.e., $\sum_{i=1}^3 \mathbf{b}^{(i)}$. In this letter, we use an *ab initio*-based parametric dislocation dynamics (DD) approach¹⁷ to investigate the effect of multiplanes on the SF width in Al and Ag, with different ISF energies. We demonstrate that identical partials greatly assist the widening of SFs, especially in low-ISF materials. This effect becomes further amplified when all trailing partials are pinned. We find that subsequent placement of leading partials on successive planes acts as a cascade process in enhancing further the widening of SFs of the previously placed partials. In sharp contrast, the dislocation configuration of zero macrostrain has very compact core in both Al and Ag, consistent with recent experiments.

The approach is an extension¹⁷⁻¹⁹ of the Peierls-Nabarro model to multiplanes, where n full dislocations nucleate on successive (111) slip planes, the dislocation spreading over all planes is explicitly accounted for, and both edge and screw components of the atomic displacements are treated on an equal footing. This allows for the dislocation dissociation into Shockley partials and utilizes the entire generalized stacking fault surface (GSFS) to capture the essential features of the core structure.^{17,19} Each full dislocation is represented by a set of N dislocations with fractional Burgers vector having both edge and screw components. The net force on each fractional dislocation comprises of the elastic forces from all other fractional dislocations on all slip planes, the lattice restoring force across the glide plane derived from the GSFS, and the externally applied Escaig stress. The equilibrium structure of the dislocation core is obtained by seeking the equilibrium configuration of these fractional dislocations in all slip planes, using a simple viscous damping equation. The *ab initio* calculation of the GSFS was carried out using the projector augmented-wave method,²⁰ as implemented in the VASP code.²¹ The ISF energy for Al is 0.166 J m^{-2} compared to 0.030 J m^{-2} in Ag.

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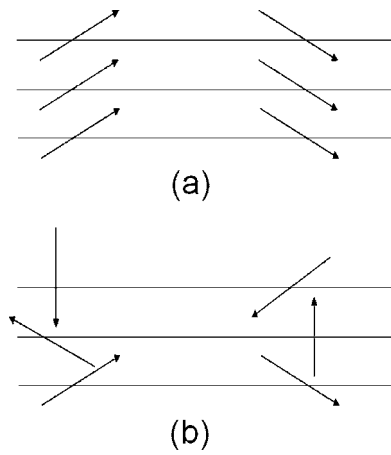


FIG. 1. Schematic configurations of edge dislocations on three successive (111) slip planes. (a) All dislocations have identical Burgers vectors. (b) Dislocations have different Burgers vectors such that $\sum_{i=1}^3 \mathbf{b}^{(i)} = 0$.

In Fig. 1(a), we show the configuration of three full edge dislocations on the successive slip planes having identical Burgers vectors, i.e., all leading partials have $\mathbf{b}_p^L = a/6[2\bar{1}\bar{1}]$ and all trailing partials have $\mathbf{b}_p^T = a/6[1\bar{2}\bar{1}]$. In Fig. 1(b), we show the configuration corresponding to the RAP DT mechanism, where the three full dislocations have different Burgers vectors with the constraint that $\sum_{i=1}^3 \mathbf{b}_{i,p}^L = \sum_{i=1}^3 \mathbf{b}_{i,p}^T = 0$.

Figure 2(a) shows the results for the partial separation on the first slip plane $d_1^{(n)}$ in Al as a function of the applied Escaig stress normalized to its critical value τ_c for a single (squares), two (circles), and three (triangles) identical ($b_1 = b_2 = b_3$) edge dislocations placed on a single, two, and three successive slip planes respectively, ($n = 1-3$). The same Escaig stress is applied on each slip plane. The corresponding results for Ag are displayed in Fig. 2(b). Here, $\tau_c = 2\gamma_{\text{isf}}/b_p$ is the critical stress at which the partial separation becomes infinite for a single glide plane.²² This expression is derived using a simple model where the width of the ISF is determined by the balance between the elastic repulsion among the partials, the constant lattice restoring force (CLRF), and the external stress. τ_c is 2.0 GPa (0.25 GPa) for Al (Ag). For comparison, we also display in Figs. 2(a) and

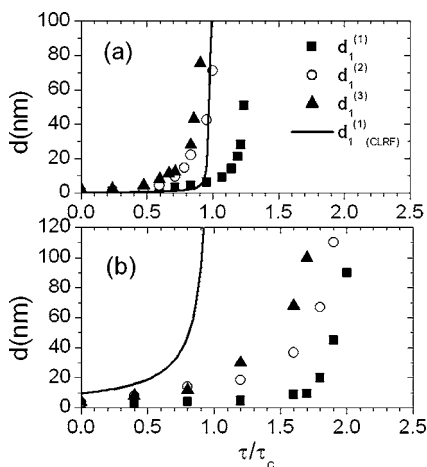


FIG. 2. Partial separation $d_1^{(n)}$ on the first slip plane for (a) Al and (b) Ag vs applied Escaig stress normalized to τ_c for a single (squares), two (circles), and three (triangles) identical edge dislocations placed on a single, two, and three successive slip planes. The symbols denote the results of the hybrid DD-*ab initio* (CLRF) approach.

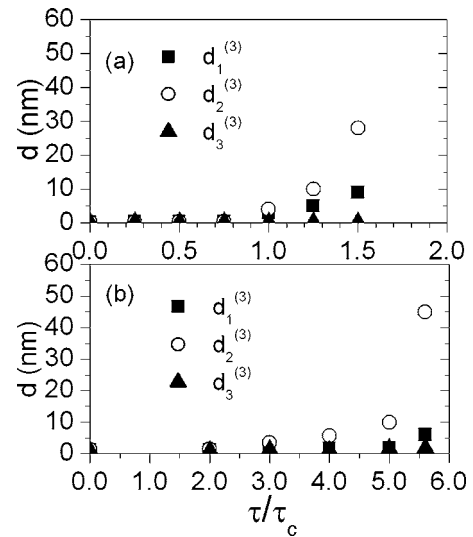


FIG. 3. Partial separation $d_i^{(3)}$, $i = 1, 2, 3$ on the first, second, and third slip planes for (a) Al and (b) Ag vs applied Escaig stress normalized to τ_c for three dislocations placed on successive slip planes, where $b_1 + b_2 + b_3 = 0$.

2(b) the results for $d_1^{(1)}$ obtained from the simple CLRF model.

These results demonstrate that the formation of leading and trailing partials on the second and third slip planes greatly assists in increasing the ISF width on the first plane. This effect is due to the elastic repulsion among the fractional dislocations on the $n = 2$ and $n = 3$ planes with those on the first plane. Consequently, for a given grain size, the presence of twinning partials on multiple slip planes reduces considerably the applied stress needed to move the leading partials across the grain. The partial separation assistance from the third plane is smaller (larger) in Al (Ag). It is interesting to note that when the applied stress lies in the range of 0.7–1.2 GPa, suggested by experiment, the partial separation is between 5 and 10 nm in Al and larger than 200 nm in Ag. These results are consistent with the experiment,² where partial-dislocation-enclosed SF ribbons have been observed within the grains in nc Al. The SF width in Al will increase by about an order of magnitude (≈ 100 nm) under stress concentration of ≈ 2 GPa found by MD simulations in the vicinity of SFs.²³

In Fig. 3, we show the partial separation $d_i^{(3)}$ ($i = 1-3$) on the first, second, and third planes for (a) Al and (b) Ag as a function of the Escaig stress normalized to τ_c , for the case of three nonidentical dislocations shown in Fig. 1(b), with $\sum_{i=1}^3 \mathbf{b}^{(i)} = 0$. Interestingly, this configuration of Burgers vector, which corresponds to zero net macroscopic strain, results in a very compact core structure in both low- and high-ISF materials. In this case, the full dislocations on the first, second, and third planes are pure edge, -30° , and 150° character, respectively. Thus, the negative edge components of the second and third dislocations are elastically attracted with the positive edge of the first one, resulting in a compact core. The partial separation remains smaller than 5 nm for $\tau \leq \tau_c = 2.0$ GPa. Even for high stress of $\tau \approx 3.0$ GPa = $1.5\tau_c$, the largest partial separation is ≈ 20 nm, much smaller than the corresponding value for the identical Burgers vector configurations in Fig. 2(a). We find similar trends in Ag, where, for example, an Escaig stress of $\tau = 1.0$ GPa = $4\tau_c$ leads to a small partial separation of 40 nm on the second plane. These results are in agreement with recent experiments¹⁵ which in-

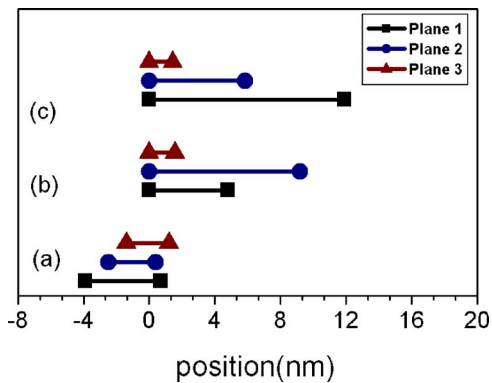


FIG. 4. (Color online) The equilibrium positions of the Shockley partials of three identical full dislocations nucleated on three successive slip planes in Al, for an external stress of $\tau=1.0$ GPa. (a) All partials nucleate simultaneously and are allowed to relax. (b) All partials are placed simultaneously and the trailing partials are pinned at the origin. (c) Leading partials are placed at different times.

dicating that DT in CG systems have partials of identical Burgers vectors, while the RAP configurations become the DT mechanism in nc materials.

In Fig. 4, we display the equilibrium configurations of the leading and trailing Shockley partials for three identical dislocations formed on the three adjacent slip planes in Al for an external stress of $\tau=1.0$ GPa. The results correspond to the following: (a) homogeneous twinning in coarse-grained Al (Fig. 2), where all fractional dislocations are placed simultaneously on adjacent planes and are allowed to relax until they reach their equilibrium configuration; (b) all fractional dislocations corresponding to the trailing partials are pinned at the origin, while all fractional dislocations corresponding to the leading partials are allowed to relax; and (c) the placement of the leading partials occurs at different times. We find a small overlap between SFs of about 3 nm in (a), and a partial separation $d_1^{(3)} > d_2^{(3)} \approx d_3^{(3)}$. On the other hand, in case (b), the SF width is enhanced by about a factor of 2–3, which is also in agreement with the experiment. The largest partial separation occurs in the second plane $d_2^{(3)} > d_1^{(3)}, d_3^{(3)}$ because it is assisted by the large elastic repulsive forces of all other leading and trailing partials on the first and third planes. Finally, in (c) we find that the average overlap of SFs increases further, consistent again with the experiment of heterogeneous nucleation, and that the largest partial separation occurs on the first plane. This is due to the fact that the leading partial on the first plane, nucleated at an earlier time, is repelled both by the leading partials on the second and third planes which are placed at subsequent times. This gives rise to a cascadelike effect where each leading partial nucleated at a later time on successive glide plane assists the widening of the SF of the previous plane, i.e., $d_1^{(3)} > d_2^{(3)} > d_3^{(3)}$. It is worth mentioning here that our work focuses on the widening of stacking faults in single crystals, where both leading and trailing partials are allowed to relax.

However, in contrast with our calculations, in the RAP of nanomaterials, the grain boundaries could emit the leading partial without having the trailing partial nucleated at the grain boundary.¹⁶ The pinned trailing partials are included in our calculations because the structure of the grain boundary is unknown to us. Therefore, the presence of the pinned trailing partials is assumed to compensate for the effect of grain boundaries.

In summary, we have found that the elastic interaction of partial dislocations in multiple planes leads to a widening of the SF when compared to its value for a single plane. Twin nucleation is expected to be more favorable in the case of identical partials when compared to the nonidentical case that yields zero strain. Pinning the trailing partials increases both the width of the SFs and their overlap distances on multiple planes making twinning easier compared to the bulk case.

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