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Orientation dependent elastic interaction between a truncated stacking fault tetrahedron and a glissile dislocation

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Abstract

The orientation dependence of elastic interaction between a stacking fault tetrahedron (SFT) and mobile dislocations is investigated for the possibility of unfaulting and subsequent absorption of the SFT. The obtained result indicates that 60° dislocations have stronger interaction with the spontaneously truncated SFT than pure screws or edges. Due to the high activation energy, the collapse and absorption of the SFTs seems to be limited to the cases where the approaching dislocations along $\langle 1\,1\,0\rangle$ directly cut the SFTs symmetrically. The anisotropic energetics can contribute to the spatially limited growth of defect-cleared channels observed in the irradiated materials.

1. Introduction

The defect-dislocation interaction has been the major issue for determination and prediction of the mechanical response of materials in the high-energy environment. While network dislocations play major roles in macroscopic plastic deformation as carriers of plastic strain, cascade induced nanoscale defect clusters greatly influence the macroscopic behavior through their collective pinning effects on glissile dislocations. Due to the high density of defect clusters, significant hardening is commonly observed in irradiated materials, often accompanied by yield drops and instability, i.e. stress serration in stress–strain profiles [1–3]. Knowledge of the local defect clusters and their unfaulting mechanisms are essential to explaining microstructure evolution such as defect-cleared channels, and the strain localization [4]. In materials with high stacking fault energy (SFE) the elastic field of the approaching dislocations can unfault the Frank sessile loops [5]. On the other hand, in low SEF materials, the interaction between a dislocation and a perfect SFT of size of few nm is not strong enough to cause unfaulting of the SFT [6]. Similar results are obtained in molecular dynamics simulations [7].

Hirsch [12] suggested a SFT absorption mechanism by a screw dislocation followed by formation of a helical dislocation configuration: Shockley partials (SPs) cutting the SFT constrict at contact with the stair-rods (SRs) of the SFT, and cross-slip to another plane of the SFT. Then each SP moves in the opposite direction by removing the stacking fault [8]. Another possible SFT absorption mechanism is discussed for cases of a mixed dislocation interacting with a truncated SFT [9]: once SPs are introduced on the SFT by the reverse glide (truncation), they can strongly interact with the leading SP of the glissile network dislocation, and annihilate each other in certain cases. In this paper, the elastic interaction between a truncated SFT and glissile dislocations is investigated in various cases for a copper sample, and the possibility of associated SFT unfaulting mechanism is reported.

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2. Elastic interaction energy between a truncated SFT and straight Shockley partial dislocations

Here we consider a pair of infinitely long Shockley partials (SPs) directed in the positive x direction approaching a single SFT from either positive y direction in cases 1–4, and from positive z direction in cases 5 and 6 (see Figs. 1 and 2). The origin of the coordinates is set on the center of the base (ABC in Fig. 1) of the SFT. Various combinations of different SFT orientations (symmetric, and rotated by 30°), glide planes (($\bar{1}\,1\,\bar{1}$) and (1 1 1)), and Burgers vectors (edge, screw, 60° mix, and 30° mix) for a total of six cases (case 1 through 6 below) are investigated in this study (Fig. 2). The allowable changes in each case are the relative position of the SPs (y, z), and the truncation of the SFT. Degree of the truncation is measured by a ratio (t) of the segment length of the shorter stair-rods (L') to size of SFT (L) defined as $t = L'/L$. a typical value for copper, L is fixed to be 10b, [1] and the intervals (d) between a pair of SPs is the equilibrium distance without any applied stress, for instance, $d = 6.26b, 12.2b, 14.2b$ for screw, mixed (60°), and edge dislocations, respectively. All other degrees of freedom such as the curvature of the incident dislocations are suppressed in the current elastic energy calculations.

The self-energy of the SFT (E_{self}) and the interaction energy between SFT and the partials (E_{int}) are computed by decomposing the SFT configurations into Volterra dislocation loops, and applying Blin's formulas [8,9]. In this work, lengthy but closed analytical form of the interaction energy between a truncated SFT and an edge dislocation is obtained for the first time. For mixed and screw dislocations, the analytical expressions obtained in previous work are used [9].

The stability of the truncated SFT with respect to the perfect SFT is checked by computing the energy gap ΔE of the net energy ($E_{\mathrm{self}} + E_{\mathrm{int}}$) between the truncated and the perfect SFTs. For instance, the negative ΔE (positive ΔE) indicates that the truncated SFT is more stable (unstable) than the perfect, and the elastic interaction of the incident SPs assists (obscures) the possible collapse of SFT and unfaulting. The force field is also computed from gradient of the energetic landscape.

The stability analysis indicates that a slightly truncated SFT down to $t = \sim 0.8$ is as stable as a perfect SFT ($t = 1$) in symmetric orientations (see cases 3–6). Hence, short segments of glissile SPs (such as A′B′ or B′C′ in Fig. 1) can be introduced in the truncated part of the SFT, and they contribute to new core reactions with incident SPs as those shown in the next section. In general, perfect and the nearly perfect SFTs are confirmed to be much more stable than the highly truncated SFT when a pair of incident partial dislocations are distant from the SFT by more than 0.5 nm. Due to its high positive value of ΔE, thermal activation process of spontaneous truncation or unfaulting of the SFT into Frank sessile loop in copper seems practically impossible unless dislocations are piled up in front of the SFT [9] or direct dislocation core reactions are involved. This implication is consistent with previous stability analysis indicating that a perfect SFT is stable even under the influence of the incident dislocation [6]. Having considered the robustness of the perfect SFT, core reactions via SFT truncation can provide possible destruction mechanisms: the incident SPs may react with glissile SPs in the truncated part of the SFT as well as the sessile stair-

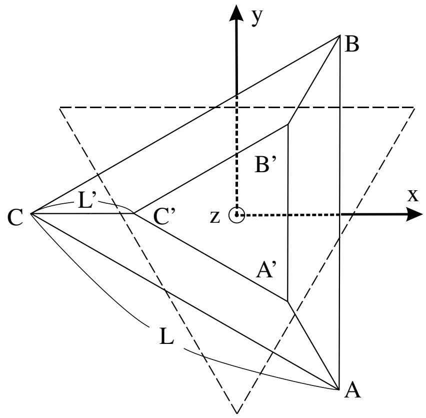

Fig. 1. Coordinate for a truncated SFT. Incident Shockley partials are aligned parallel to the x direction, and their position is measured at the nearest point on the leading partial to the center of the base of the SFT.

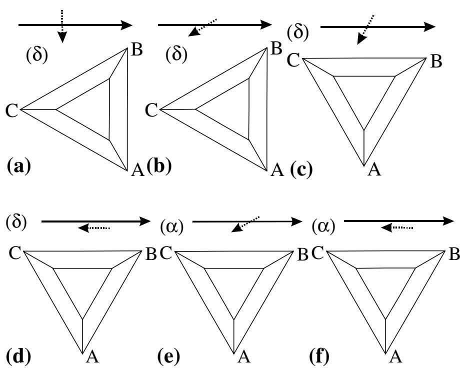

Fig. 2. Tested configurations. Cases 1–6 correspond to (a)–(f). (α) and (δ) denote ($\bar{1}\,1\,\bar{1}$) and (1 1 1) glide planes, respectively. One polarity of perfect Burgers vectors is shown as a dashed arrow.

[1] b is the magnitude of the Burgers vector, and $b = 0.256$ nm fo copper. Other used material parameters in this calculations are the shear modulus $= 54.6$ Gpa, and Poisson ratio $= 0.324$.

rods (SRs). In the following, the main result of the energetics in each case is shown when the leading dislocation collides with truncated SFT segments, together with possible core reactions.

3. Results of interaction energy profile and core reactions

Noticeable energy reduction due to the incident dislocation is found in case 1 (edge dislocation: $b_{SPlead} = \delta A$, $b_{SPtrail} = B\delta$), case 3 (60° dislocation: δA, $B\delta$), and 5 (60° dislocation: αD, $B\alpha$). Fig. 3(a) denote the profile of $\Delta E(t, y = 0, z)$ around the center of the SFT in case of the edge dislocation (case 1). Local minima on the curves correspond to the position where the leading incident partial comes into contact with SPs of the SFT. In the proximity of such contact position, the interaction force between the leading SP and the SP of the SFT is attractive as can be seen in Fig. 4(b).

Larger energy reductions are found in certain positions such as cases 3 and 5 due to core reactions. The possible reactions between the leading SP and SR/SP of the truncated SFT in case 3 are: $b_{SPlead} + b_{SFT} = \delta A + D\alpha \rightarrow D\delta/\alpha A$ (SR), and $\delta A + \alpha\delta \rightarrow \alpha A$ (Frank sessile). Since these junctions are sessile, the SFT is likely to stay intact. On the other hand, in case 5, the SFT can be destroyed by an annihilation, i.e. $\alpha D + D\alpha$. Scanning over various relative positions (y, z) with constraint of each glide plane, we obtain the activation path with an energy of ~0.16 eV/atom to truncate the SFT down to $t \sim 0.1$ in case 1, ~0.1 eV/atom in case 3, and no energy required in case 5. This junction formation as seen in the case 3 may cause strong pinning effects, which is qualitatively different from simple pinning and the formation of cusp of the incident dislocation at the intersection with SFT segments as previously reported [9].

In case 2 (30° dislocation: $b_{SPlead} = \delta C, b_{SPtrail} = B\delta$), 4 (screw dislocation: δC, $B\delta$), and 6 (δC, $B\alpha$), either very weak energy change or mainly energy increase is found. For instance, the shift of the $\Delta E(t = 0.6, y = 0, z)$ due to the incident dislocation just about +0.005 eV/atom in case 2, −0.015/ + 0.04 eV/atom in case 6, as compared with −0.0375 eV/atom in case 1. Fig. 4(a) and (b) illustrate the energy profile $\Delta E(t, y = 0, z)$ and force field for the screw dislocation for the case 4. In a symmetric position like this, the net interaction between the truncated SFT and the screw components becomes zero, so small changes in the curve in Fig. 4(b) are caused by the edge component of the SPs. While further self-truncation cannot be expected in these cases, in case 4 the following core reaction between the leading SP and the SR of the base of the SFT can destroy the SFT: $b_{SPlead} + b_{SFT} = \delta C + \alpha\delta \rightarrow \alpha C$ (SP). Since the resulting Shockley partial αC is mobile on the $(\bar{1}\,1\,\bar{1})$ plane, further reaction can propagate to the neighboring segments, i.e. $\alpha C + \beta\alpha \rightarrow \beta C$, which is also able to move on the neighboring $(1\,\bar{1}\,\bar{1})$ plane, and so on. Another SR formed through the core reaction with SP in the truncated part ($\delta C + \alpha D \rightarrow D\delta/\alpha C$) is unstable, and it is unlikely to affect the stability of the SFT.

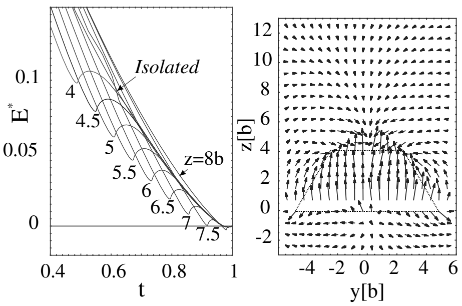

Fig. 3. Energy gap vs. truncation factor for case 1 (left, Fig. 3(a)), and the corresponding profile of forces exerting on the leading partial interacting with the SFT (illustrated with dotted lines) at $t = 0.5$ (right, Fig. 3(b)). E^* is the energy gap per vacancy in the unit of eV.

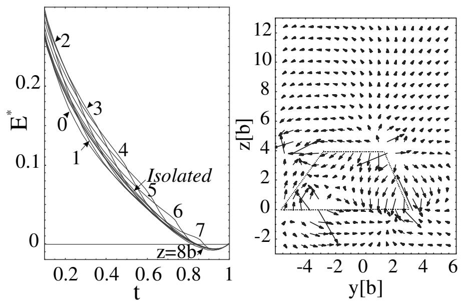

Fig. 4. Energy gap vs. truncation factor for case 4 (left, Fig. 4(a)) and the corresponding profile of forces exerting on the leading partial at $t = 0.5$ (right, Fig. 4(b)). E^* is the energy gap per vacancy in the unit of eV.

4. Discussion

In addition to the core reactions in the cases 4 and 5 described above, changes in the glide planes of a screw dislocation between (1 1 1) plane and $(\bar{1}\,1\,\bar{1})$ plane by cross-slip can also contribute to the destruction of the SFT. Namely, changes in SP as $\delta C + B\delta \rightarrow \alpha C + B\alpha$ in case 4, and $\alpha C + B\alpha \rightarrow \delta C + B\delta$ in case 6, introduce a mobile SP on different planes of the SFT, and cause chain core reactions as described above. While the leading SP has to hit certain segments of the SFT to collapse the SFT by the formation of a mobile junction or segments annihilation, the SFT destruction by cross-slip is more efficient at expanding the defect free area since it can take place when a screw dislocation hits and gets pinned on one of the SFT planes [5,11]. The SFT absorption by screws and the subsequent formation of defect free channels has been indeed observed in irradiated copper samples using in situ transmission electron microscopy [13]. The experimental data [10] of weak temperature dependence of the growth of defect-cleared channel and the channel formation even at a cryogenic temperature of 4 K suggest that the growth process is mostly mechanical rather than thermal. On the other hand, the corresponding thermal energy of a typical deformation temperature is not sufficient to cause the frequent cross-slips (with the activation energy of ~eV) in copper. Atomistic study on the energetics [14] indicates that the reduction of the activation enthalpy of the constrictions and the cross-slips requires significantly high (Escaig) stress due to its low activation volume. In irradiated metals, a high stress concentration in front of local defect clusters such as the SFTs can provide the sufficient mechanical work to drive the cross-slip. The relative roles of the cross-slip with respect to the annihilation/formation of a mobile SP junction require further investigations. Annihilation and combination of the leading partial with other non-parallel dislocation segments such as those in 30° rotated positions take place less frequently since the reaction requires local bending of the segments and need to form higher energy configurations. In such cases, partial dislocations cut through the SFT by leaving unit jogs on the segments [9]. Hence, all of the SFT destruction processes by annihilations, mobile junction formations, and cross-slips are preferentially caused by incident partials directed close to ⟨1 1 0⟩ directions.

5. Conclusion

The effect of the elastic field of glissile network dislocations on the stability of a truncated SFT is examined for various configurations using isotropic elasticity. Symmetric orientations have stronger elastic interactions and more effective core reactions to collapse the SFT than 30°-rotated orientations. The crystallographic constraint of the SFT destruction and absorption by incident Shockley partials can lead to the anisotropic growth of defect free areas into channels.

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