Generalized planar fault energies and twinning in Cu–Al alloys

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We report *ab initio* density functional theory calculations of generalized planar fault energies of fcc Cu–xAl (x=0, 5.0, and 8.3 at. %) alloys. We investigate the effects of substitutional solute Al on the unstable intrinsic γ_{us} and twin γ_{ut} stacking fault energies (SFEs). Our results reveal an increased tendency of Cu–Al to deform preferentially by twinning with increasing Al content, consistent with experiment. We attribute this mechanical behavior to appreciable lowering of the twinning barrier γ_{ut}, along with the stable intrinsic and twin SFEs. © *2006 American Institute of Physics*.
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In recent years, considerable attention has been given to the dependence of deformation mechanisms of coarse-grained and nanograined fcc materials on generalized planar fault energies (GPFEs).[1–6] It has been demonstrated, both experimentally and numerically, that partial dislocations nucleate from grain boundaries and lead to the formation of deformation twins in nanocrystalline (nc) fcc metals.[7–10] Recent molecular dynamics simulations[1,2] and mechanistic models[4] suggest that GPFE curves affect the nucleation of partials and twins in nc metals. Similar qualitative dependence of deformation twinning tendency on GPFE has been predicted for coarse-grained fcc metals as well.[5,6] However, limited studies have focused on the effect of GPFE curves on twinning in fcc alloys. Additionally, these studies[3] have considered low solute concentrations (up to 2.5 at. %).

Here we explore the effect of GPFEs and increasing solute content on twinning in Cu–Al alloys. We report the GPFE curves of Cu–(5.0 at. %)Al and Cu–(8.3 at. %)Al up to four-layer and five-layer thick twins, respectively, and compare them to that of pure Cu. Experimental studies have shown that, in contrast to Cu which does not undergo twinning except at high strain rates and/or low (4 K) temperatures,[11] Cu–5.0%Al and Cu–8.0%Al accommodate plastic deformation at 77.4 K and room temperature, respectively, by undergoing deformation twinning.[12–14] This increased twinning activity has been attributed to lowering of intrinsic stacking fault energy (SFE) γ_{isf} from 45 mJ/m^2 for Cu to about 20 mJ/m^2 for Cu–5.0%Al and about 9 mJ/m^2 for Cu–8.0%Al.[15,16] In particular, we examine the effect of increasing Al content on the nucleation barrier heights γ_{us} and γ_{ut} and its influence on competing slip and twinning mechanisms.

The generalized stacking fault energy (GSFE) and GPFE provide a comprehensive description of stacking faults[17] and twins,[1–6] respectively. In fcc alloys, GSFE is the energy per unit area required to generate single-layer stacking faults on {111} slip planes by shearing one elastic half space of the crystal relative to the other along ⟨112⟩ slip direction.[17] Recently, the intrinsic stacking fault width in fcc alloys was quantitatively shown to depend on GSFE curves.[18] For fcc alloys, the GPFE is the energy per unit area required to form n-layer faults (twins) by shearing n successive {111} layers along ⟨112⟩. Most GPFEs were reported for two-layer thick twins,[1–5] with γ_{us} as the stacking fault nucleation barrier, γ_{isf} as the one-layer SFE, γ_{ut} as the two-layer twin nucleation barrier, and $2\gamma_{tsf}$ as twice the twin SFE (or twin boundary energy) of the metastable two-layer twin. Some reported fcc GPFE curves are for up to five-layer thick twins,[6] and, in such studies, while γ_{us} and γ_{isf} are defined as before, γ_{tsf} and γ_{ut} are defined as their converged values on the GPFE curve.

We have computed the GPFE curves using Vienna *ab initio* simulation package[19,20] (VASP) using the generalized gradient approximation[21] and the projector augmented wave[22] (PAW) basis. We used periodic supercells consisting of N (111) fcc layers with four atoms per layer (no free surfaces). Fault energies for Cu were converged when $N \geqslant 9$. For these cells, Brillouin zone sampling was performed using $8\times8\times4$ special k-point mesh[23] with 273.2 eV energy cutoff, ensuring convergence of energy within 1 meV/atom. While internal relaxations were permitted, no external cell relaxations along [111] were included as fault energies are unaffected if the cell is large enough, as found for twins in Al–Ag alloys[24] and SFs in Hadfield steels.[18]

For Cu–5.0%Al (Cu–8.3%Al), we used a supercell with ten layers (nine layers) having a total of 40 (36) atoms. For 5.0%Al, one Cu atom was substituted by an Al within the

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TABLE I. Stacking fault energies (in mJ/m^2) for Cu and Cu–xAl using VASP-PAW. Computed energies are compared with the reported experimental values (enclosed in parentheses) and first principles calculations in literature.

	a_0 (Å)	γ_{us}	γ_{isf}	γ_{ut}	$2\gamma_{tsf}$	δ_{us}^{ut}	T
Cu	3.64	181	41	200	40	19	1.05
	(3.61)[a]	180[b]	(45)[c]	210[b]	(48)[a]		
Cu–(5.0 at. %)Al	3.65	170	20	179	32	9	1.09
	(3.6364)[d]	⋯	(20)[a]	⋯	(34)[a]		
Cu–(8.3 at. %)Al	3.65	169	7	176	11	7	1.11
	(3.6466)[d]	⋯	(9)[a]	⋯	⋯		

[a]Reference 16.
[b]Reference 6; see Ref. 24 for sensitivity of SFE on cell size.
[c]Reference 15.
[d]Reference 30.

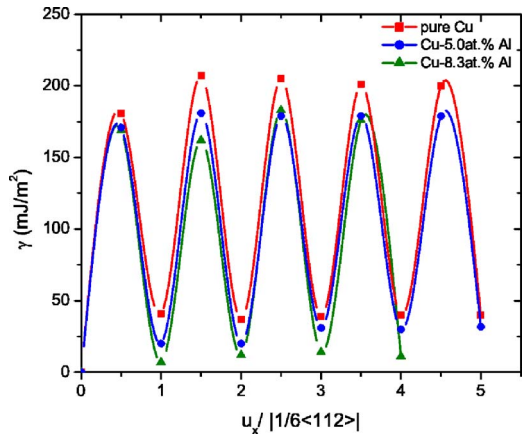

FIG. 1. (Color online) VASP-PAW GPFE curves for Cu and Cu–Al.

second and sixth layer. The intrinsic stacking fault was created by sliding the layers 5–10 relative to layers 1–4 in $[11\bar{2}]$ through one twinning partial Burgers vector $|\mathbf{b}_p|=a_0/\sqrt{6}$, based on the translation in cubic coordinates of $T_1=[10\bar{1}]$ and $T_2=[01\bar{1}]$ in the [111] plane and $T_3=m\mathbf{b}_p+N\times[111]$, where layers above the twin (including those in the next periodic supercell) shift rigidly through $m\mathbf{b}_p$ for an m-layer twin always maintaining fcc symmetry across the periodic supercells. The two-layer twin was then generated by sliding layers 6–10 in similar fashion, three-layer twin by sliding layers 7–10, and so on to generate the GPFE curve up to five-layer twins. For 8.3%Al, one Cu atom was replaced by an Al within the second, fifth, and eigth layers, and then layers 6–9 were successively displaced through $|\mathbf{b}_p|$ relative to layers 1–5 to generate the GPFE curve. Due to this atomic arrangement, Cu–8.3%Al supercell can be sheared only up to four-layer twins. Since the solute-fault interaction is short ranged,[3,25,26] our supercells with multiple solute atoms are good representatives of Cu–Al alloys.

For all Cu–Al configurations, we placed Al atoms equidistant on either side of the twin boundaries (TBs) such that mirror (positional) symmetry was maintained in all n-layer twin configurations (while solute symmetry may be destroyed during the shear), as these positions always lead to the lowest energy configurations.[24] Moving the position of Al atoms further away from the TB violated mirror symmetry in one or more configurations during shearing, while bringing them closer increased the Al–Al interaction, leading to an extremely unfavorable increase in γ_{isf} (from 20 up to 154 mJ/m^2). The selected Al atom positions in the layers 2 and 6 within the ten-layer supercell permit a continuous shear to generate multiple twins with high symmetry. The fault energies of these high symmetry metastable configurations (intrinsic and twins) generated from initial configurations lead to a good agreement with the observed values, see Table I.

Our calculated GPFE curves for Cu–xAl are shown in Fig. 1, with values summarized in Table I. For Cu, our γ_{us} and γ_{ut} agree with previous calculations. For Cu–xAl our lattice constants a_0 and planar energies γ_{isf} and γ_{tsf} are in good agreement with available data. Thus, our trends for Cu–xAl energy barriers (γ_{us} and γ_{ut}), which must be overcome to attain the stable stacking fault and twin configurations, are expected to be reliable.

The figure and table clearly show that the addition of Al to Cu dramatically decreases γ_{isf}, while γ_{tsf} also reduces but not as dramatically. (As an aside, based on hard-ball model,[27] the intrinsic and twin stacking fault energies for elements are related by $\gamma_{isf}\approx 2\gamma_{tsf}$. However, our results for Cu–xAl indicate that this relation is not obeyed by inhomogeneous alloys for reasons explained recently.[24]) Compared to Cu, the 12% decrease in unstable twin SFE γ_{ut} with increasing Al content is twice as much as that for the unstable SFE barrier γ_{us}, see Table I. However, increasing Al from 5.0% to 8.0% in Cu–xAl, the barriers γ_{ut} and γ_{us} remain unchanged, within the relative error.

This differing degree of effect of solute content on energy barriers has important implications on deformation twinning in Cu–Al. Based on the analysis by Rice,[28] a simple criterion for twinning activation is given by relative barrier height difference $\delta_{us}^{ut}\equiv\gamma_{ut}-\gamma_{us}$.[1,3] The values of δ_{us}^{ut} for Cu and Cu–Al are given in Table I. The δ_{us}^{ut} decreases significantly with addition of Al, which is primarily due to the lowering of γ_{ut}, see Fig. 1. This indicates that twinning is likely to be activated more easily in Cu–Al than in Cu. However, since γ_{ut} is greater than the trailing partial nucleation barrier γ_{us} for Cu as well as these Cu–Al, the relative barrier difference criterion does not predict twinning to be the dominant deformation mechanism.

Tadmor and Bernstein[5] have proposed a measure called *twinnability* (denoted by τ in their papers and by T here), which quantifies the propensity of fcc metals to twin as opposed to slip, and have suggested the following approximate expression.[5]

$$T=\left[1.136-0.151\frac{\gamma_{isf}}{\gamma_{us}}\right]\sqrt{\frac{\gamma_{us}}{\gamma_{ut}}} \tag{1}$$

that gives correct qualitative trends for several fcc metals. We have computed the twinnability of Cu and Cu–Al using (1), see Table I. Our results show that both Cu–8.3%Al and Cu–5.6%Al will undergo twinning more readily than Cu and that we can expect more active twinning systems with more twin-based texture in the alloys, consistent with observations.[12,29] Thus, the twinnability measure predicts correct trends for twinning in Cu–Al. Our defect results, however, also indicate that ⟨100⟩ twinning texture is expected to increase monotonically with decrease in γ_{isf}, in agreement with experiments.[29] Further, Ratuszek and Karp[29] have noted a dramatic increase in ⟨100⟩ texture with increase

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in Al content from 5 to 7.65 at. % and higher. We attribute this jump in texture to the dramatic decrease in intrinsic SFE and twin SFE by a factor of 3 with increase in Al content from 5.0 to 8.3 at. %, see Table I. This dramatic decrease in γ_{isf} and γ_{tsf} is not reflected in either the twinnability or the relative barrier difference criterion. As such, these criteria fail to provide a qualitative measure of the solute effect on $\langle 100 \rangle$ texture that we find reflected in γ_{isf} and γ_{tsf}.

Our calculated GPFE curves indicate that increased twinning tendency in Cu–xAl is primarily due to (i) a decrease in intrinsic SFE and twin SFE and (ii) a relatively larger decrease in twinning barrier γ_{ut} which dominates a smaller decrease in the unstable SFE barrier γ_{us}. The twinnability criterion accounts for this more general dependence of deformation twinning on γ_{ut} and γ_{us} in addition to γ_{isf}. The twinning criterion δ_{us}^{ut} based on relative barrier heights also captures the correct twinning trend in Cu–Al alloys, but it does not account for changes in γ_{isf} and γ_{tsf}.

Finally, the size of twin embryos in fcc alloys can be predicted based on convergence behavior of GPFE curves.[6] Ogata *et al.* have observed convergence of fault energies from second layer sliding onwards for pure fcc metals.[6] They predicted a two-layer microtwin as the possible twin nucleus in fcc metals. Our GPFE curves in Fig. 1 show that the twin SFE γ_{tsf} converges at third layer sliding for Cu as well as Cu–(5.0 at. %)Al and Cu–(8.3 at. %)Al.[31] The unstable twin SFE γ_{ut} converges after third layer sliding. These results suggest that the basic twin nucleus in fcc alloys is expected to be three layer thick. Using a dislocation model for twin formation, Mahajan and Chin[32] have also suggested a three-layer twin as the basic nucleus in fcc alloys. Our result is in agreement with their predictions.

In summary, we have calculated the GPFE curves for fcc Cu–Al alloys and correlated them to deformation twinning. Our results indicate an increased tendency of Cu-Al alloys to deform preferentially by twinning with increasing Al content. This mechanical behavior is attributed to a dramatic lowering of the twinning barrier γ_{ut} which dominates a relatively smaller decrease in the unstable SFE γ_{us}. Twinning tendency is further assisted due to a decrease in intrinsic and twin stacking fault energies with Al addition. Finally, we show that γ_{tsf} converges at third layer sliding for Cu–xAl alloys, suggesting that the twin nuclei in fcc alloys may be expected to be three layer thick to become mature twin embryos, a result consistent with predictions of dislocation-based twin models in fcc alloys.[32]

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