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Energy pathways and directionality in deformation twinning

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We present *ab initio* density functional theory calculations of twinning energy pathways for two opposite twinning modes, $(111)[11\bar{2}]$ and $(111)[\bar{1}\bar{1}2]$, in fcc materials to examine the directional nature of twinning which cannot be explained by classical twin nucleation models or the "twinnability" criterion. By accounting for these energy pathways in a multiscale model, we quantitatively predict the critical twinning stress for the $(111)[\bar{1}\bar{1}2]$ mode to be substantially higher compared to the favorable $(111)[11\bar{2}]$ mode (whose predicted stresses are in agreement with experiment), thus, ruling out twinning in the $(111)[\bar{1}\bar{1}2]$ mode. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2800806]

The role of twinning energy pathways called the generalized planar fault energy (GPFE) on deformation twinning in face centered cubic (fcc) materials is well recognized.[1–6] It is now well established that nucleation of twins in fcc materials occurs due to passage of Shockley partial dislocations on successive {111} planes, permitting twinning shear in one direction but not in the opposite.[7] Unlike slip, reversal of shear in case of twinning does not result in activation of the same twin system in opposite direction. While the directional nature of twinning is known on geometric grounds,[8] a rigorous mechanistic argument for twinning directionality is needed. In this letter, we link the directionality in twinning to its energy landscape, i.e., GPFE, and unravel the role of twinning barriers to be overcome by Shockley partials for activation of fcc twinning modes.

Classically, the directional nature of twinning has been explained through the minimum shear hypothesis proposed by Jaswon and Dove.[9] They suggested that twinning modes accommodating twins through smallest possible shear will be favored. Figure 1 shows two possible opposite twinning modes, the $(111)[11\bar{2}]$ mode and the $(111)[\bar{1}\bar{1}2]$ mode, that result in identical final twin configurations in the fcc lattice. Since the $(111)[\bar{1}\bar{1}2]$ mode requires twice the shear for the $(111)[11\bar{2}]$ mode, it is precluded by the Jaswon and Dove hypothesis.[9] Note that $(111)[\bar{1}\bar{1}2]$ mode involves intermediate $\cdots AA\cdots$ configuration and requires surmounting an unfavorably high energy barrier; however, the magnitude of this barrier and the associated increase in the twinning stress has not yet been calculated. A physical basis for twinning directionality can be provided through these twinning pathways and associated barriers. Therefore, here, we calculate the energy pathways GPFE to explain the observed twinning modes quantitatively based on the critical shear stress criterion.

For fcc materials, the GPFE $\gamma(u_x)$ is the energy per unit area required to form m-layer faults by shearing m successive {111} layers along the $\langle 112\rangle$ direction through displacement u_x. Most GPFE were reported for two-layer thick faults considered as twins,[1–4] with γ_{us} as the stacking fault nucleation barrier or unstable stacking fault energy (SFE), γ_{isf} as the intrinsic SFE, γ_{ut} as the two-layer fault nucleation barrier (or unstable twin SFE), and $2\gamma_{tsf}$ as twice the twin SFE (or twin boundary energy) of the metastable two-layer fault considered as a twin. Typically, the GPFE curves are determined for the experimentally observed twinning modes. Presently, we contrast the GPFE pathways for minimum shear $(111)\times[11\bar{2}]$ mode with the pathways for the larger shear, exactly opposite $(111)[\bar{1}\bar{1}2]$ mode that results in the same final twin configuration (see Fig. 1). For $(111)[\bar{1}\bar{1}2]$ mode, we denote the unstable SFE as γ_{us}^{*} and the unstable twin SFE as γ_{ut}^{*}. Here we determine the GPFE curves associated with these two twinning modes for following fcc metals which are known to twin: Cu, Ag, Au, and Pb.

We used Vienna *ab initio* simulation package[10,11] (VASP) with the generalized gradient approximation[12] and the projector augmented wave[13] basis for our computations. Our periodic supercells (i.e., having no free surfaces) consisted of ten (111) fcc layers having 1 atom per layer. The details of our computations are already summarized elsewhere.[6,14] For the $(111)[11\bar{2}]$ mode, the intrinsic stacking fault was created

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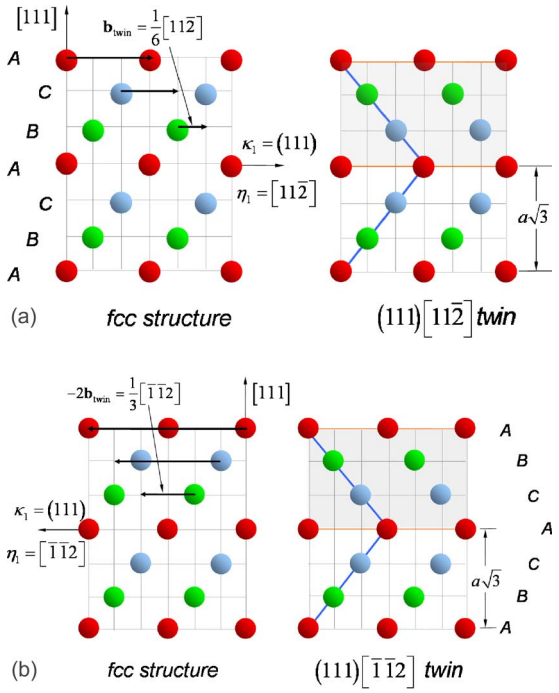

FIG. 1. (Color online) Schematic of two opposite fcc twinning modes giving identical final twin configurations: (a) $(111)[11\bar{2}]$ and (b) $(111)[\bar{1}\bar{1}2]$. As suggested by the minimum shear hypothesis (Ref. 9), the $(111)[\bar{1}\bar{1}2]$ mode is not observed experimentally indicating directional nature of deformation twinning.

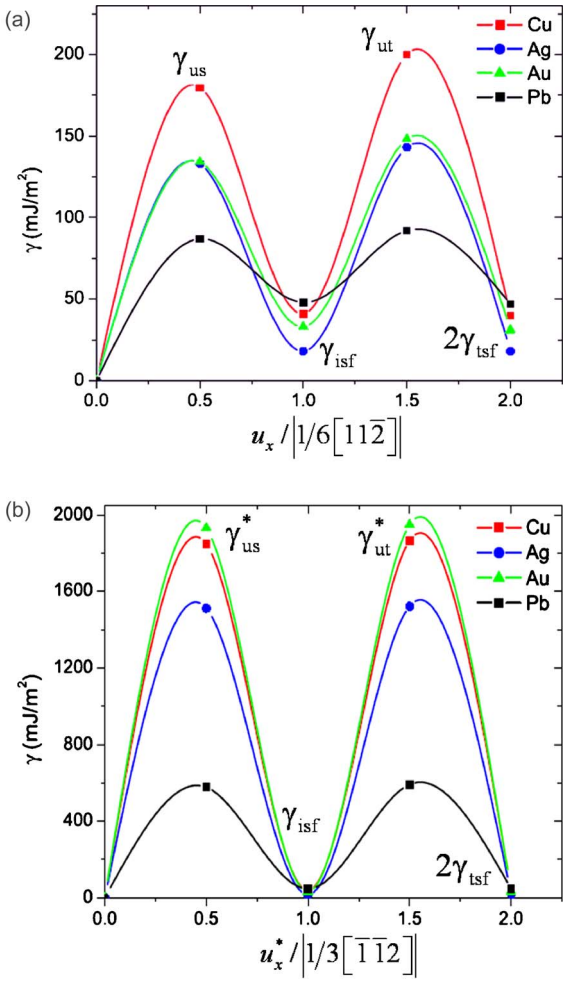

FIG. 2. (Color online) GPFE curves for two opposite twinning modes computed using VASP-PAW-GGA: (a) $(111)[11\bar{2}]$ and (b) $(111)[\bar{1}\bar{1}2]$. The energy barriers for the $(111)[\bar{1}\bar{1}2]$ mode are an order of magnitude higher than the corresponding values for $(111)[11\bar{2}]$ mode.

by sliding layers 7–10 relative to layers 1–6 in $[11\bar{2}]$ through one twinning partial Burgers vector $|\mathbf{b}_{twin}| = a_0/\sqrt{6}$. The two-layer twin was then generated by sliding layers 8–10. A similar procedure was adopted for the $(111)[\bar{1}\bar{1}2]$ twinning mode except the layers were sheared through $|\mathbf{b}^*_{twin}| = 2|\mathbf{b}_{twin}| = a_0/\sqrt{3}$ in $[\bar{1}\bar{1}2]$ direction.

Figure 2 contrasts the $(111)[11\bar{2}]$ and $(111)[\bar{1}\bar{1}2]$ mode GPFE curves for Ag, Au, Cu, and Pb. Note first that the γ_{isf} and γ_{tsf} are equal for the two modes, since each twinning mode leads to the same stable planar defect (stacking fault or a twin) configuration. However, the barriers γ^*_{us} and γ^*_{ut} for the $(111)[\bar{1}\bar{1}2]$ mode are an order of magnitude larger than the γ_{us} and γ_{ut} barriers for the $(111)[11\bar{2}]$ mode. This is due to the unfavorable $\cdots AA\cdots$ type stacking encountered during the relative sliding of the fcc layers along the $[\bar{1}\bar{1}2]$ direction, but not during shear along the $[11\bar{2}]$ direction. Further, in contrast to the $(111)[11\bar{2}]$ mode where barriers γ_{us} and γ_{ut} for Cu are higher than those for pure Au [see Fig. 2(a)], the barriers γ^*_{us} and γ^*_{ut} for pure Au are higher than those for pure Cu in the $(111)[\bar{1}\bar{1}2]$ mode, [see Fig. 2(b)]. The GPFE values for the two modes are summarized in Table I.

We have recently developed a sequential, multiscale approach to predict the true (experimentally observed critical) twinning stress in fcc metals without requiring empiricism at any length scale.[14] It is noted that dislocations are not explic-

TABLE I. Fault energies (in mJ/m^2) and twinning stress (MPa) computed for two opposite twinning modes in fcc metals. Present twinning stress criterion rules out the $(111)[\bar{1}\bar{1}2]$ mode in agreement with experiments.

	Mode			$(111)[11\bar{2}]$				$(111)[\bar{1}\bar{1}2]$		
	a_0(Å)	γ_{isf}	$2\gamma_{tsf}$	γ_{us}	γ_{ut}	τ_{crit}	τ_{expt}	γ^*_{us}	γ^*_{ut}	τ^*_{crit}
Pb	4.95	48	47	87	92	43	19–71[a]	578	592	190
Ag	4.09	13	12	133	143	64	38–71[b]	1512	1522	310
Au	4.08	33	31	134	148	77	85–100[c]	1930	1947	400
Cu	3.61	41	40	180	200	120	125–160[d]	1847	1865	370

[a]Reference 19.
[b]Reference 20 and 21.
[c]Reference 21.
[d]Reference 22.

itly modeled in the *ab initio* calculations and we focus on twinning in ideal (defect-free) fcc materials. Consequently, we have incorporated the barriers to twinning via GPFE into a heterogeneous, dislocation based mechanistic model for twin nucleation to determine a closed-form expression for twinning stress.[14] Our theory predicts that twin nucleus width d is $100-500b_{\text{twin}}$ for $(111)[11\bar{2}]$ mode. In the limit when core width w is very small compared to d, the original twinning stress equation for $(111)[11\bar{2}]$ mode simplifies to the following approximate form:

$$\tau_{\text{crit}} = \frac{2}{3Nb_{\text{twin}}}\left(\frac{3N}{4}-1\right)\left[\gamma_{\text{ut}} + \frac{(2\gamma_{\text{tsf}}+\gamma_{\text{isf}})}{2}\right] - \frac{2}{3N}\frac{(\gamma_{\text{us}}+\gamma_{\text{isf}})}{b_{\text{twin}}}.$$

The first term represents the stress required to overcome the twin nucleation barrier γ_{ut} while the second term accounts for the barrier γ_{us} for competing cross-slip mechanism. An increase in γ_{ut} increases τ_{crit} and an increase in γ_{us} inhibits cross slip and reduces τ_{crit} making twinning more favorable. Above equation shows that the twinning stress depends on GPFE and the number of layer N in the twin nucleus. Classically, the smallest twin is commensurate with three layers,[15,16] as also suggested by the Mahajan-Chin twinning mechanism.[17] Hence, τ_{crit} is computed at $N=3$ in our theory using the above equation. The twinning stress τ^*_{crit} was determined from the original nonlinear τ_{crit} equation[14] by replacing γ_{us} and γ_{ut} with γ^*_{us} and γ^*_{ut}, respectively. We note that $w/d \ll 1$ does not hold for the unfavorable mode.

Table I compares the twinning stresses τ_{crit} and τ^*_{crit} to activate $(111)[11\bar{2}]$ and $(111)[\bar{1}\bar{1}2]$ modes, respectively. The predicted twinning stress τ_{crit} for the observed mode is in good agreement with experimental data.[14] Also, we have demonstrated a monotonic trend between τ_{crit} for $(111)\times[11\bar{2}]$-type modes and the corresponding twinning barrier γ_{ut}.[14] Our results in Table I show that a similar monotonic trend holds true between τ^*_{crit} and γ^*_{ut} for $(111)[\bar{1}\bar{1}2]$-type modes, as predicted. Moreover, it is seen that the twinning stress τ^*_{crit} required to activate $(111)[\bar{1}\bar{1}2]$ mode is about four to six times higher than the τ_{crit} stress for the $(111)[11\bar{2}]$ mode. This implies that twinning in fcc metals will occur through the favorable $(111)[11\bar{2}]$-type twinning modes but not through the energetically unfavorable $(111)[\bar{1}\bar{1}2]$-type twinning modes, although both modes result in identical final twinned lattices. Thus, our twinning stress criterion not only predicts the true (i.e., experimentally observed) twinning stress for observed $(111)[11\bar{2}]$-type modes but also it quantitatively *precludes* twin nucleation through unfavorable $(111)[\bar{1}\bar{1}2]$-type twinning modes in fcc lattices. Twinning directionality is, therefore, naturally incorporated in our theory for twinning stress.

The GPFE curves have been qualitatively correlated to the twinning propensity of fcc metals.[1,3,4] Tadmor and Bernstein[4] have defined a material property called *twinnability* that measures the propensity of fcc metals to undergo twinning. The predicted twinnability for $(111)[11\bar{2}]$ and $(111)[\bar{1}\bar{1}2]$ modes range from 1.02 to 1.05 and 1.11 to 1.13, respectively. While, twinnability criterion correctly predicts that fcc metals will twin when (observed) $(111)[11\bar{2}]$ is considered, it does not rule out twinning in the $(111)[\bar{1}\bar{1}2]$ mode. This is because the twinnability parameter depends on the ratios of fault barriers and not on their magnitudes. The twinnability criterion, therefore, does not account for directionality in twinning.

Finally, we note that several twinning stresses models available in the literature propose a relation of the form $\tau_{\text{crit}} \sim K\gamma_{\text{isf}}/b_{\text{twin}}$ with K as a fitting parameter.[18] Since, these models rely only on γ_{isf}, they do not account for the twinning barriers and, consequently, completely fail to predict twinning directionality.

In summary, we have calculated GPFEs for two opposite twinning modes, $(111)[11\bar{2}]$ and $(111)[\bar{1}\bar{1}2]$, in fcc materials using *ab initio* density functional theory. Our calculations have revealed that the fault energy barriers for the two twinning modes differ by an order of magnitude and contribute to the directional nature of twinning. It is also seen that twinning directionality cannot be explained using the qualitative twinnability criterion or the classical twin nucleation models. To quantitatively explain twinning directionality, we have incorporated the GPFE pathways in our multiscale model[14] and have predicted the critical twinning stress for $(111)\times[\bar{1}\bar{1}2]$ mode to be restrictively higher compared to the favorable $(111)[11\bar{2}]$ mode, in agreement with experiments.

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