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Effects of structural relaxation on the generalized stacking fault energies of hexagonal-close-packed system from first-principles calculations

Yuchen Dou [a], Jing Zhang [a,b,*]

[a] College of Materials Science and Engineering, Chongqing University, Chongqing 400044, China
[b] National Engineering Research Center for Magnesium Alloys, Chongqing 400044, China

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ABSTRACT

In this paper, the effects of relaxation parameters on the first-principle-calculated generalized stacking fault energy (GSFE) were investigated. Two relaxing directions were considered, out-of-plane (N-direction) and in-plane (P-direction). N-direction is normal to the slip plane. P-direction is parallel to the slip plane and perpendicular to the slip direction. The results show that relaxation along the N-direction is essential, especially for the high-index slip plane; relaxation along the P-direction is needed when the atoms on the two sides of the slip direction are unsymmetrical. Discussions were made based on the first-principle calculated forces and the geometry of the atomic configurations of different slip systems.

1. Introduction

The GSFE, introduced by Vítek in 1986 [1], is a fundamental parameter intimately related to the mechanical behavior of a material. It stems from the relative slip between two adjacent atomic planes during the shear deformation of a given slip system. Particularly, the local minimum/maximum of the GSFE is called stable/unstable stacking fault energy (abbreviated as γ_{SF} and γ_{USF} in the following). The GSFE can be used to model a large number of atomic-scale phenomena, such as intrinsic ductility based on the Peierls concept [2], solid-solution strengthening and the thermal cross-slip stress of dislocations [3,4]. Successful modeling is highly dependant on the precision of the obtained GSFE values. Since experimental measurement of GSFE is almost impossible, the first-principle method has been widely used in various cases, such as metallic systems (Al [5], Fe [6], Mg [7], Mo [8], Ni [9]) and compounds (GaN [10], Al_2O_3 [11]). In calculating the GSFE, a procedure called lattice relaxation must be carried out before the calculation of a supercell's total energy. A survey of literatures reveals that the calculated GSFE is sensitive to the degree of freedom adopted in the relaxation procedure.

Taking magnesium alloys as a prototype, which have attracted significant interest in recent years due to the need for weight reduction in automobile and aerospace industries. Commonly, magnesium alloys have poor room temperature ductility which stems from their hexagonal close packed (HCP) crystal structure. The easiest basal slip system provides only two independent slip systems, far from enough to meet the von Mises requirement for five independent slip systems [12]. Early experiments on pure Mg single crystals have demonstrated that the critical resolved shear stress (CRSS) of the prismatic $\langle a \rangle$ and pyramidal $\langle c+a \rangle$ slip systems are 50–100 times larger than that of the basal slip system at room temperature; as a consequence, the activation of non-basal slip systems is harder. Fortunately, the CRSS can be modified by alloying elements. It is reported that addition of Zn and Al promotes the activation of the prismatic $\langle a \rangle$ slip [13], and addition of Li eases the activation of the pyramidal $\langle c+a \rangle$ slip [14]. In this context, it is supposed that the lowered CRSS results from the decreased γ_{USF} caused by alloying element addition. To design new magnesium alloys with satisfactory ductility, the effects of alloying elements on the GSFE has largely been studied by means of first-principle calculation in recent years.

Published GSFE data [15–25] (by no means complete) for pure magnesium by first-principle calculation are listed in Table 1, where slip systems $\{0001\}\langle 1-100\rangle$ (for staking fault $\boldsymbol{I}_2$), $\{1-100\}\langle 11-20\rangle$ and $\{11-22\}\langle 11-23\rangle$ are involved. For the $\{0001\}\langle 1-100\rangle$ slip system, the published data coincide well with

* Corresponding author at: College of Materials Science and Engineering, Chongqing University, Chongqing 400044, China. Tel.: +86 23 65111167; fax: +86 23 65102821.
E-mail address: jingzhang@cqu.edu.cn (J. Zhang).

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each other. The γ_{SF} (located at 1.0***b***; ***b*** is the Burgers vector) falls into the range from 33.8 to 48.2 mJ m^{-2}; the γ_{USF} (located at 0.5***b***) falls into the range from 84 to 99 mJ m^{-2}. However, for the $\{1-100\}\langle 11-20\rangle$ and $\{11-22\}\langle 11-23\rangle$ slip systems, the published GSFEs show significant discrepancies. In the case of $\{1-100\}\langle 11-20\rangle$, the γ_{USF} (located at 0.5***b***) falls into the range from 189 to 354 mJ m^{-2} (Note that there does not exist a γ_{SF} in this slip system). For the $\{11-22\}\langle 11-23\rangle$ slip system, there are two γ_{USF}. In this paper, only the larger one of the two γ_{USF} was discussed, whose value shows a much larger discrepancy than the smaller one, as listed in Table 1. The published γ_{SF} and γ_{USF} fall into the range from 221 to 399 mJ m^{-2} and from 463 to 1080 mJ m^{-2}, respectively. Meanwhile, even the location of the γ_{SF} exhibits disagreement. In detail, Wen [17] and Pei [21] proposed that the γ_{SF} is located at ~0.4***b***; Ghazisaeidi [18] and Nogaret [22] suggested that the γ_{SF} is located at ~0.33***b***; Wang [24] reported that the γ_{SF} is located at 0.5***b***. Experimentally, transmission electron microscopy (TEM) observation illustrate that the second-order pyramidal $\langle c+a\rangle$ dislocation exists in a dissociated form, i.e. two 1/2 $\langle 11-23\rangle$ partial dislocations with a $\{11-22\}$ stacking fault in between [14], providing strong support that the γ_{SF} must be located at ~0.5***b***. Toward this end, Wang [24] got the right result. The striking disparity in both the calculated GSFE value and its location is attributed to the different degree of freedom adopted in the relaxation procedure of first-principle calculation. However, the effects of relaxation parameters on the accuracy of the calculated GSFE have not been recognized and addressed.

The $\{1-100\}\langle 11-20\rangle$ and $\{11-22\}\langle 11-23\rangle$ slip systems play very important roles in the plastic deformation process of magnesium alloys. However, published GSEFs exhibit significant discrepancies. To set a benchmark for the GSFE calculations of Mg-based alloy systems in the future, it is necessary and timely to clarify the effects of relaxation parameters on the accuracy of the GSFE calculation.

2. Computational details

First principle calculations were carried out using the Vienna Ab initio simulation package (VASP) [26,27], with the generalized gradient approximation (GGA) in the Perdew–Burke–Ernzerhof (PBE) form [28]. The cut-off energy was set as 300 eV. The first order Methfessle–Paxton with smearing of 0.2 eV was used for structural relaxation until the total energy changes within 10^{-6} eV. Then the total energy calculation was performed using linear tetrahedron method with Blöchl correction; the Hellmann–Feynman force was calculated by first order Methfessle–Paxton with smearing of 0.2 eV. For $\{0001\}\langle 1-100\rangle$, $\{1-100\}\langle 11-20\rangle$ and $\{11-22\}\langle 11-23\rangle$ slip systems, supercells with 48 atoms were constructed, as illustrated in Fig. 1a, d and g. (In this work, effects of relaxation parameters were discussed under the same supercell size, although different supercell size does affect the calculated GSFE [29].) The Brillouin zone was sampled using a Monkhorst–Pack *k*-point mesh as following: $7\times8\times3$, $7\times4\times3$ and $4\times7\times3$ for $\{0001\}\langle 1-100\rangle$, $\{1-100\}\langle 11-20\rangle$ and $\{11-22\}\langle 11-23\rangle$, respectively. The slip process was simulated by gradually displacing the upper 6 atom layers with respect to the remaining 6 layers along ***b*** (Burgers vector). GSFE was derived with the following equation:

$$\gamma_{GSFE} = (E_n - E_0)/A \quad (1)$$

where E_n is the energy of the supercell with a displacement and E_0 is the energy of the original supercell, and A is the supercell's cross-sectional area.

In this study, two relaxing directions were considered, out-of-plane (N-direction) and in-plane (P-direction). N-direction

Table 1
Calculated first-principle (within the GGA) values of stable stacking fault energy (γ_{SF}) and unstable stacking fault energy (γ_{USF}) for pure Mg, in mJ m^{-2}. For the $\{0001\}\langle 1-100\rangle$ slip system, the γ_{SF} and γ_{USF} are located at 1.0***b*** and 0.5***b***, respectively (***b*** is the Burgers vector). For the $\{1-100\}\langle 11-20\rangle$ slip system, there does not exist a stable value and the γ_{USF} is located at 0.5***b***. For the $\{11-22\}\langle 11-23\rangle$ slip system, there are two γ_{USF} and one γ_{SF}, located at different positions depending on the degree of freedom adopted in the relaxation procedures. Values without references are calculated in this work.

Relaxation procedure	$\{0001\}\langle 1-100\rangle$		$\{1-100\}\langle 11-20\rangle$		$\{11-22\}\langle 11-23\rangle$	
	γ_{SF}	γ_{USF}	γ_{USF}	γ_{USF}	γ_{SF}	γ_{USF}
0	33.8[a]	87.6[a]	354[c]	(0.27***b***) 452[c]	(0.42***b***) 399[c]	(0.67***b***) 1080[c]
	48.2[b]	99[c]		(0.25***b***) 240[d]	(0.33***b***) 235[d]	(0.68***b***) 475[d]
	34[c]					
1	36[e]	92[e]	189[f]	(0.3***b***) 318[g]	(0.4***b***) 298[g]	(0.7***b***) 559[g]
	36[g]	94[f]	212[g]	(0.27***b***) 243[h]	(0.33***b***) 236[h]	(0.68***b***) 485[h]
	34[i]	84[g]	218[i]			
		92[i]				
2			351[j]	(0.3***b***) 378[j]	(0.5***b***) 223[j]	(0.7***b***) 466[j]
			356[k]	(0.3***b***) 376[k]	(0.5***b***) 221[k]	(0.7***b***) 463[k]
3	36	93	288	(0.25***b***) 394	(0.35***b***) 376	(0.7***b***) 1029
4	35	86	169	(0.25***b***) 246	(0.35***b***) 236	(0.7***b***) 503
5	35	86	169	(0.3***b***) 244	(0.5***b***) 216	(0.7***b***) 413
6	35	86	169	(0.3***b***) 243	(0.5***b***) 184	(0.7***b***) 393
7	35	86	169	(0.3***b***) 242	(0.5***b***) 182	(0.7***b***) 390

Note: 0 – Ambiguous relaxation process. 1 – All atoms were fully relaxed along the N-direction. 2 – Atoms in the 6th and 7th planes were relaxed along the P-direction. Relaxation along the N-direction is ambiguous. 3 – All atoms are fixed. 4 – All atoms are fully relaxed along the N-direction. 5 – All atoms are fully relaxed along the N-direction. Atoms in the 6th and 7th planes are relaxed along the P-direction. 6 – All atoms are fully relaxed along the N-direction. Atoms in the 5th, 6th, 7th and 8th planes are relaxed along the P-direction. 7 – All atoms are fully relaxed along the N-direction and the P-direction. For 1 and 2, the relaxation of supercell's shape and volume is ambiguous; from 3 to 7, supercell's shape and size are fully relaxed.

[a] Ref. [15].
[b] Ref. [16].
[c] Ref. [17].
[d] Ref. [18].
[e] Ref. [19].
[f] Ref. [20].
[g] Ref. [21].
[h] Ref. [22].
[i] Ref. [23].
[j] Ref. [24].
[k] Ref. [25].