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First-principles calculations of twin-boundary and stacking-fault energies in magnesium

Y. Wang,[a,*] L.-Q. Chen,[a] Z.-K. Liu[a] and S.N. Mathaudhu[b]

[a] *Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802, USA*
[b] *Materials and Manufacturing Sciences Division, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD 21005-5069, USA*

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The interfacial energies of twin boundaries and stacking faults in metal magnesium have been calculated using first-principles supercell approach. Four types of twin boundaries and two types of stacking faults are investigated, namely, those due to the $(10\bar{1}1)$ mirror reflection, the $(10\bar{1}1)$ mirror glide, the $(10\bar{1}2)$ mirror reflection, the $(10\bar{1}2)$ mirror glide, the I1 stacking fault and the I2 stacking fault. The effects of supercell size on the calculated interfacial energies are examined.

Keywords: Magnesium; Interfaces; Twinning; First-principles calculation

Magnesium alloys are increasingly being used in a wide range of applications due to their light weight and high strength. One of the current research frontiers on Mg alloys is to understand, estimate and improve their low plastic formability to operate under increasingly demanding conditions. At the atomic scale, the plastic formability is closely related to the ease of the formation of planar defects along the close-packed planes, namely, twin and stacking faults [1–5]. Experimentally, direct measurements of interfacial energies require very delicate techniques and the results often show large uncertainties. For instance, the measured stacking-fault energies [6–8] (and references therein) for magnesium are scattered in the range of 50–280 mJ m^{-2}. Alternatively, the steady improvement in both computer power and the efficiency of computational methods in the past few years has enabled the calculation of defect energetics at reasonable computational cost [9]. For the case of metal magnesium, existing first-principles results are scattered among specific types of twin boundaries, stacking faults, approximations to exchange–correlation energy and supercell size [10–14]. The main purpose of this paper is to report the calculation of interfacial energies of twinning and stacking faults in magnesium from a unified theoretical framework. In particular, we report our calculated results for the $(10\bar{1}1)$ mirror reflection, the $(10\bar{1}1)$ mirror glide, the $(10\bar{1}2)$ mirror reflection and the $(10\bar{1}2)$ mirror glide twin boundaries, together with the I1 and I2 stacking faults. The effect of supercell size on the calculated interfacial energies will be discussed.

Since we employ a first-principles approach with periodic boundary conditions, the interfaces due to twinning and stacking faults are modeled using a supercell. In fact, the crystallographic theory of twinning [2] is rather complicated for a hexagonal close-packed (hcp) metal. For the special cases of $(10\bar{1}1)$ and $(10\bar{1}2)$ twins, following Morris et al. [11], the supercells are built by first transforming the hcp structure into the orthogonal structure (see Fig. 1) by which both the $(10\bar{1}1)$ and $(10\bar{1}2)$ planes can be seen more clearly. Secondly, the $\boldsymbol{a}$ lattice vector of the supercell is taken as that parallel to paper surface and within the $(10\bar{1}1)$ or $(10\bar{1}2)$ plane, and the $\boldsymbol{b}$ lattice vector of the supercell is taken as that vertical to paper surface and within the $(10\bar{1}1)$ or $(10\bar{1}2)$ plane. Furthermore, the $\boldsymbol{c}$ lattice vector of the supercell is derived in the direction perpendicular to both $\boldsymbol{a}$ and $\boldsymbol{b}$. The atoms that above the interfacial plane that pass through $\boldsymbol{a}$ and $\boldsymbol{b}$ are then cut away, and a mirror reflection with respect to the interfacial plane that passes through $\boldsymbol{a}$ and $\boldsymbol{b}$ is made. The last step is to shift the atoms that are nearest to the interfacial plane to the interfacial plane for the mirror reflection twin or to shift the reflected atoms by $\boldsymbol{b}/2$ for the mirror glide twin. Examples of the built supercells for the $(10\bar{1}1)$ and $(10\bar{1}2)$ twins are illustrated in Figures 2 and 3, respectively. The supercells for the I1 and I2 stacking

* Corresponding author. E-mail: yuw3@psu.edu

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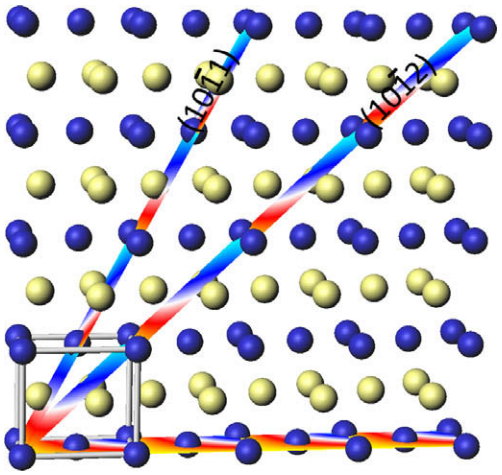

Figure 1. The (10$\bar{1}$1) and (10$\bar{1}$2) planes in hcp metals. The heavy (blue) and light (yellow) balls are used to represent the A and B atomic layers in the *c* direction conventionally used for the hcp structure. The gray box shows the orthogonal cell mapped from the hcp cell. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

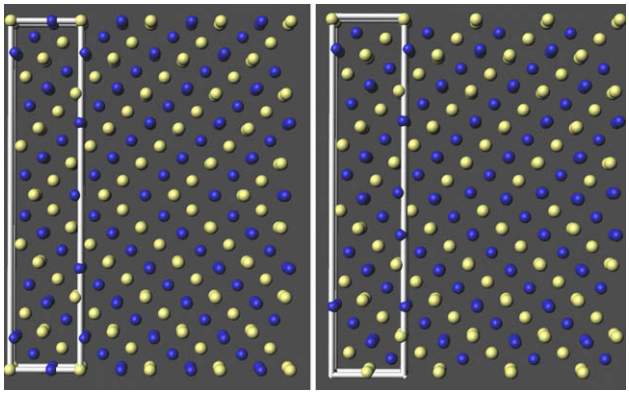

Figure 2. Structures of the (10$\bar{1}$2) mirror reflection twin boundary (left panel) and the (10$\bar{1}$2) mirror glide twin boundary (right panel). For the meanings of the balls, see Figure 1.

faults are relatively easier to build. Taking the case of 32-atom supercell (16-layer) as an example, they are just the ABABABABCBCBCBCB and ABABABABCACA CACB arrangements, respectively, for the I1 and I2 stacking faults [12]. Note that in the supercell approach each supercell contains two interfaces. The effect of the supercell sizes on the calculated interfacial energies was studied. The built supercells with different sizes are listed in Table 1.

To calculate the 0 K energies, we employed the Vanderbilt ultrasoft pseudopotential [15] within the generalized gradient approximation (GGA) [16] to the exchange–correlation energy as implemented in the Vienna ab initio Simulation Package (VASP) package [17,18]. The plane wave energy cutoff was 132.7 eV, which is an automatic value when setting the key "Prec = High" in VASP. The calculation of interfacial energy involves finding the difference between two total energies. We therefore adopted very dense *k* points (see Table 1), and the gamma-centered scheme was used. We extracted the interfacial energy, ζ, by

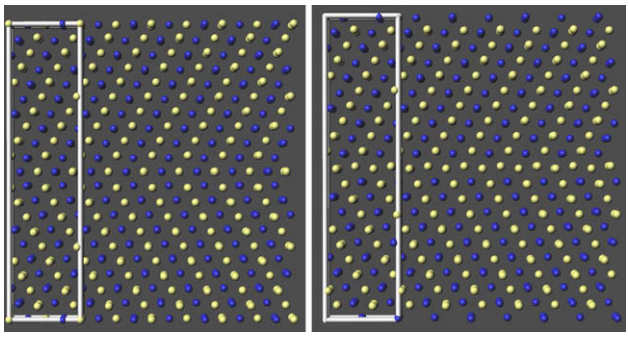

Figure 3. Structures of the (10$\bar{1}$1) mirror reflection twin boundary (left panel) and the (10$\bar{1}$1) mirror glide twin boundary (right panel). See also Figure 1 for meanings of the balls.

$$\zeta = (E_{Supercell} - E_{hcp})/2A,$$

noting that $E_{Supercell}$ is the total energy of the supercell, E_{hcp} is the total energy of hcp Mg scaled to the supercell size, and A is interfacial area which is scalar value of the cross product of lattice vectors $\boldsymbol{a}$ and $\boldsymbol{b}$. We note that, in the above procedure of extracting the interfacial energy, the elastic energy resulting from the formation of an interface has not been considered separately. This is a reasonable approximation for the twin boundary in hcp Mg, as it will be seen that the calculated interfacial energies are just weakly dependent on the supercell size (see Table 1).

The calculated interfacial energies are summarized in Table 1, together with the measured stacking-fault energies [6–8] and those previously calculated following different approaches [4,10–14]. For the twin boundaries, it is observed from our calculations that the effects of the gliding of the interfacial crystal planes on the interfacial energy are minor, and the interfacial energies of the twin boundary are one magnitude larger than those of stacking faults. Effects of the supercell size on the calculated interfacial energies are also seen. For the twin boundary, increasing the supercell size by up to 80 atoms can only decrease the interfacial energy by less than 5%. However, the calculated interfacial energies for stacking faults show strong dependence on the adopted supercell size, as it is seen from Table 1 (I1 and I2) that the calculated interfacial energies are reduced by 50% when the supercell size is increased from 8 to 32. This is because the interfacial energies for the I1 and I2 stacking faults are so small in number that their calculations have reached the accuracy limit of the current first-principles method.

We assume that the larger the supercell sizes are, the more accurate the calculated interfacial energies. For the six largest supercells of the six types of defects, our calculated interfacial energies are 85.5, 81.0, 118.1, 120.0, 8.1 and 21.8 mJ m^{-2}, respectively, for the (10$\bar{1}$1) mirror reflection, the (10$\bar{1}$1 mirror glide, the (10$\bar{1}$2 mirror reflection, the (10$\bar{1}$2) mirror glide, the I1 stacking fault and the I2 stacking fault. Overall, these numbers are in good agreement with the reported results from the previous publications. Yoo et al. [14] calculated the (10$\bar{1}$1) and (10$\bar{1}$2) mirror reflection twins employing the ab initio method (no information was given on the employed potential and the approximation to the

Table 1. Computational settings and interfacial energies.

	k-mesh	Supercell size	Interfacial energy (mJ m^{-2})		
			This work	Previous calculation	Measurements
hcp Mg	$25 \times 25 \times 15$	2	0		
$(10\bar{1}1)$	$7 \times 25 \times 4$	40	84.2	70[a]	
	$9 \times 31 \times 3$	80	85.5		
$(10\bar{1}1)$g	$7 \times 25 \times 4$	40	84.2		
	$9 \times 31 \times 3$	80	81.0		
$(10\bar{1}2)$	$17 \times 39 \times 7$	20	122.3		
	$11 \times 25 \times 3$	40	118.8	114[b];114[a]	
	$13 \times 31 \times 2$	80	118.1		
$(10\bar{1}2)$g	$17 \times 39 \times 7$	20	125.3		
	$11 \times 25 \times 3$	40	120.8	114[b]	
	$13 \times 31 \times 2$	80	120.0		
I1	$25 \times 25 \times 12$	8	17.8	9[c]; 10[d]; 4[f]	<25[g]; 39[h]; >45[i]; 51–140[j]
	$25 \times 25 \times 9$	16	13.1		
	$25 \times 25 \times 6$	32	8.1		
I2	$25 \times 25 \times 12$	8	38.3	18[c]; 22[d]; 16[e]; 8[f]	
	$25 \times 25 \times 9$	16	27.7		
	$25 \times 25 \times 6$	32	21.8		

For the I1 and I2 stacking faults, the reported stacking-fault energies in the literature [6–8,10,12,13] were divided by a factor of two since I1 and I2 contain two interfaces [12].

[a] Yoo et al. [14], ab initio calculation (see the text).
[b] Morris et al. [11], ab initio calculation (see the text).
[c] Smith [12], ABINIT 24-atom supercell within the GGA.
[d] Chetty and Weinert [10], LDA.
[e] Uesugi et al. [13], GGA.
[f] Hu et al. [4], EAM.
[g] Court and Caillard [7].
[h] Sastry et al. [6].
[i] Fleischer [8].
[j] Quoted by Fleischer [8] (and see references therein).

exchange–correlation energy by Yoo et al.), and reported the calculated interfacial energy values of 70 and 114 mJ m^{-2}, respectively; Morris et al. employed the same ab initio method to calculate the $(10\bar{1}2)$ mirror reflection and the $(10\bar{1}2)$ mirror glide twins using 20-atom supercells and reported the same interfacial energy of 114 mJ m^{-2} for both the $(10\bar{1}2)$ mirror reflection and the $(10\bar{1}2)$ mirror glide twins. The interfacial energies of the I1 and I2 stacking faults calculated by Smith [12] were, respectively, 9 and 18 mJ m^{-2} using the 24-atom supercells (12 layers of Mg) and the ABINIT package [19] within the GGA. The calculated interfacial energies of the I1 and I2 stacking faults by Chetty and Weinert [10] were, respectively, 10 and 22 mJ m^{-2} using the 24-atom supercells (12 layers of Mg) within the local density approximation (LDA) [20]. The calculated interfacial energies of I2 stacking fault by Uesugi et al. [13] was 16 mJ m^{-2} using the CASTEP package [21] within the GGA. Other results for stacking-fault energies are from the embedded atom method (EAM) by Hu et al. [4], who reported that the interfacial energies for the I1 and I2 stacking faults are 4 and 8 mJ m^{-2}, respectively.

In summary, the interfacial energies for four types of twin boundaries and two types of stacking faults observed in metal magnesium have been obtained through first-principles calculations. It therefore offers a unified picture of the interfacial energies for these lattice mismatches within the same theoretical framework. The calculated values can also serve as the input for the future simulation of the growth process of these planar defects or the estimation of the effects of these lattice mismatches on the mechanical properties of magnesium alloys.

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