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First-principles calculations of stacking fault energy in titanium alloys

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Abstract

The research of plastic deformation of metals attaches great importance to stacking fault energy (SFE). In this paper, we derive the expressions of four types (I_1, I_2, E and T_2) of basal plane SFEs of hcp-Ti within the framework of the Ising model. Based on this model, alloying effects on the stacking fault energy (SFE) of titanium alloys are investigated via first-principles calculations. It is found that SFE always decreases with addition of alloying elements. The distribution of lattice parameters of all the studied $Ti_{95}X_5$ has a direct relationship with alloying element's atomic radii. Additionally, SFEs decrease linearly with the solutes concentration increasing in the Ti-based alloys. This work provides some useful data for new Ti alloys design.

Key words: Stacking fault energy; Ising model; Alloying and concentration effects; First-principles calculations

1. Introduction

Titanium-based alloys are attractive for structural applications owing to their high strength, light weight, corrosion resistance and so on[1], particularly in the automotive and aerospace industries. Poor creep resistance is a “bottleneck” of the high-temperature applications of titanium alloys. Thus, one of the key issues of the design of high-temperature titanium alloys is to improve the creep resistance.

One of the main influencial factors of steady state creep rate is the mobility of the dislocations, which result in the change of dislocation structure, as well as the stacking fault energies. The stacking fault energy can hardly be accurately measured experimentally and the fundamental knowledge of the alloying effects on the creep properties of titanium alloys is still limited although vast experimental research has been performed and reported in literature.

With the extraordinary improvements in modern computing facilities, computational alloy design has recently become more feasible, many stacking fault energies (SFEs) have been calculated by first-principle theory. Legrand had introduced an explicit treatment of the electronic degrees of freedom in a tight-binding (TB) approach[2,3,4,5], which obtained a prismatic spreading in an hcp metal (Ti) for the first time. Guo et al. [6] calculated the steady-state creep rate of commercially-pure titanium and TiAl alloys. Their creep behavior was found to follow power-law creep when the dependence of SFE on the aluminium content was taken into account in the calculation.

Employing density functional theory (DFT)， a first-principles calculation on the generalized-stacking-fault(GSF) energies and surface properties for several HCP metals on Mg, Be, Ti, Zn, and Zr has also been presented in recent years. [7] P. Kwasniak[8] gave a comprehensive review of the present theoretical knowledge of the bulk properties, stacking faults and γ-surfaces, which are essential properties to gain a deeper understanding of the relationship between the electronic structure of hcp-Ti and its plastic behavior. Additionally, they had also computed the effect of four elements on the GSFE of hcp-Ti by ab-initio calculations.[9] In a recent work, [10] bulk properties of hcp-Ti, relevant for the description of dislocations, such as elastic constants, stacking faults and γ-surface, are computed using density functional theory (DFT) and two central force embedded atom interaction models.

The remainder of this paper is organized as follows: Section 2 describes the theory and computational techniques used in our calculations. In section 3, we present the results of stacking fault properties of pure Ti, as well as the effects of alloying elements and solute

concentration on SFE.

2. Theoretical methods

2.1 Stacking fault energy of basal-plane

There are four kinds of basal plane stacking faults in hcp Ti, namely I_1, I_2, E and T_2 [11], with the stacking sequences as follows:

I_1: $(AB)^mABCBC(BC)^n$,

I_2: $(AB)^mABCAC(AC)^n$

E: $(AB)^mABCAB(AB)^n$

T_2: $(AB)^mABCBA(BA)^n$

2.2 The method of calculation of stacking fault energy based on Ising model

According to the Ising model [12], the SFEs of hcp-Ti can be derived. For example, the SFE of E is:

$$E_E - E_0 = 2E_{fcc} + 2E_{dhcp} - 4E_{hcp}$$

In which E_{hcp} stands for the energy of the perfect hcp structure with repeating AB units. The energy E_{fcc} for the perfect fcc structure with repeating ABC units, E_{dhcp} standing for the energy of the dhcp structure with repeating ABAC units. Note that the energies of the systems with fcc, hcp and dhcp structures can be readily calculated by using first-principles methods.

2.3 The first-principles calculation

The exact muffin-tin orbitals (EMTO) method [13, 14] was applied to calculate the SFE of Ti-based random alloys. Combined with the coherent potential approximation (CPA)[15, 16], this method is more successful in studying stacking faults, e.g. in austenitic stainless [17, 18] ,Fe-Mn alloys [19] and so on.

3. Results and discussion

3.1 The stacking fault properties of pure Ti

Table 1 lists virious lattice parameters for HCP-Ti. Compared with previous data [20], c is 4.7014 in this work, which is more adjacent to the experimental value 4.6862.

It is well known that stacking fault energy (SFE) plays a vital part in predicting the plastic deformation mechanisms of metals. The calculated stacking fault energies of four kinds of basal plane stacking faults in pure Ti, namely, I_1, I_2, E, T_2 are listed in Table 2. It can be found that the EMTO method has generated fault formation energies, which are in good agreement with experimental and other theoretical results. Since the lattices involved in this type of calculation are all close-packed and thus the errors associated with the shape approximation can be kept at a minimal level, there is no surprise that a muffin-tin approach performs well for the metastable faulted alloys.

3.2 Effects of alloying elements on the SFEs properties of hcp-Ti

Table 3 lists the calculated equilibrium lattice parameter a, c/a of Titanium alloys $Ti_{95}X_5$. As a matter of fact, the variation of equilibrium lattice parameter with atomic radii has a close relationship, namely, the larger the atomic radii, the larger the equilibrium lattice parameter. This is understandable because a larger atom tends to occupy a larger space.

DFT computation also gives the values of the stacking fault energies (I_1, I_2, E, T_2) in $Ti_{95}X_5$, which is exhibited in Figure 1. The horizontal line in this figure corresponds to the SFE of the pure Ti, whereas the addition of an alloying element has decreased the energy. By the same token, a larger atomic radii corresponds to a larger stacking fault energy. Microscopically speaking, the alloying element's movement may cost more energy if it has a larger atomic radii. Therefore, the stacking fault energy rises with the increase of atomic radii.

For the hexagonal close-packed (hcp) $Ti_{95}X_5$, a perfect dislocation is more likely to dissociate into two partials, compared with the pure Ti. The lower SFE makes the dislocation cross-slip easier and climb more difficult.

3.3 Effects of solute concentration on SFE

In order to further understand the mechanical properties of HCP metals, the relationship between lattice parameter and solutes concentration has been investigated and the results are shown in Figure 2. Additionally, the composition dependence of the SFEs of metals containing alloying elements has been investigated. Figure 3 presents the variation of stacking fault energies with solutes concentration. Obviously, the stacking fault energies decrease as the solutes' concentration increases. These lower SFEs means that the hcp Ti is more likely to slip along the basal plane, with the addition of the alloying elements. With the solutes concentration increasing, the Ti-based alloys SFEs decrease linearly. At the solute concentration 20%, the SFE with Sc is the largest. On the contrary, the SFE with element W is

the smallest at this concentration.

4. Conclusion

In this work, we have investigated systematically the four kinds (I_1, I_2, E and T_2) of basal plane SFEs of 16 alloying hcp Ti alloys by using first-principles calculations based on the Ising model. We can summarize our theoretical study as follows：

1. All studied solutes reduce the basal-plane SFEs (I_1, I_2, E and T_2), which makes the hcp Ti alloys cross-slip easier and more difficult to climb.

2. The distribution of the lattice parameters of all the studied $Ti_{95}X_5$ is consistent with the distribution of the SFEs, which has a direct relationship with alloying element's atomic radii.

3. With the solutes concentration increasing, the Ti-based alloys SFEs decrease linearly.

Overall, this work provides a database for new Ti alloys design.

Figures and tables

Figure 1. Effects of alloying elements on the SFEs properties of hcp Ti

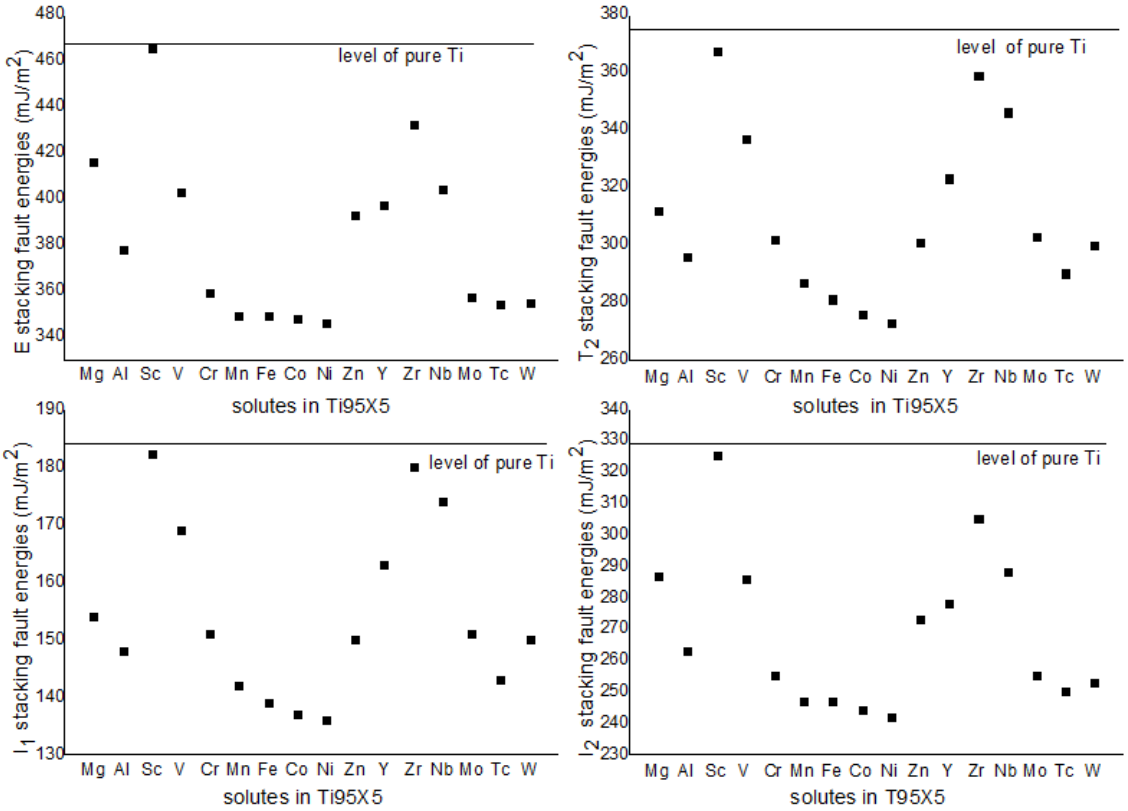


Figure 2. Relationship between lattice parameter and solutes concentration

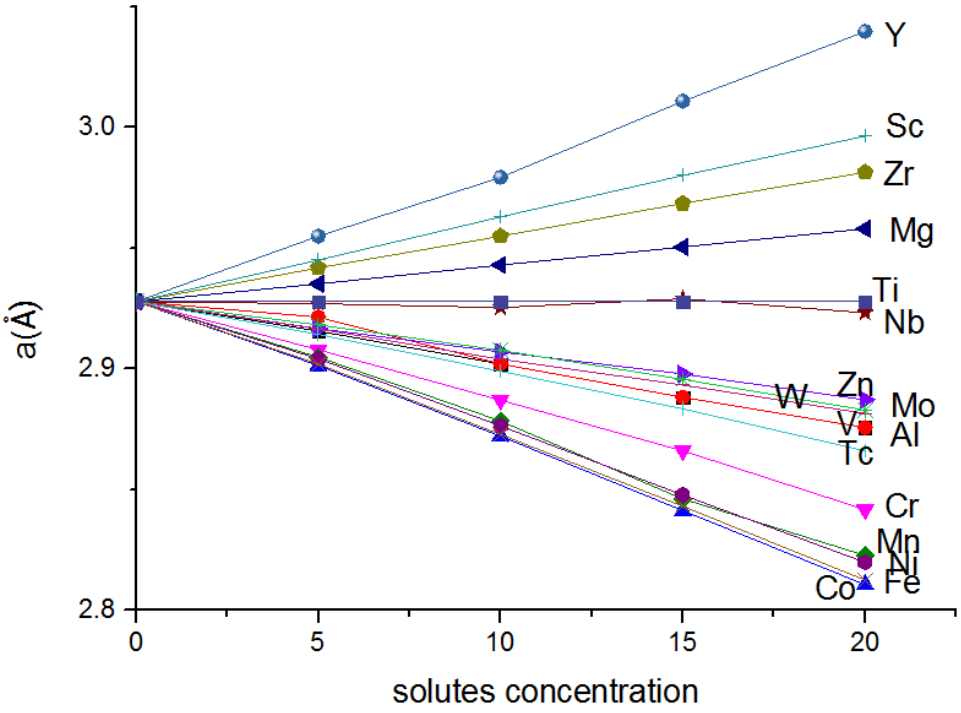
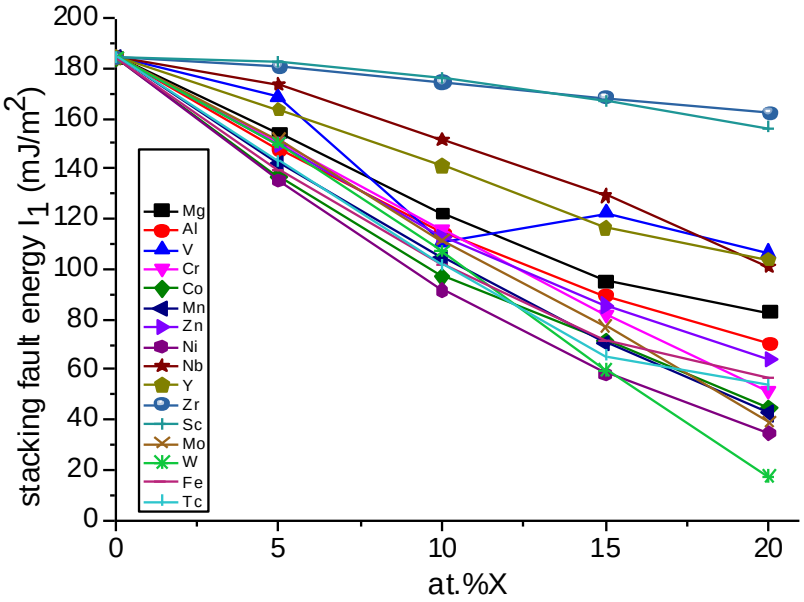
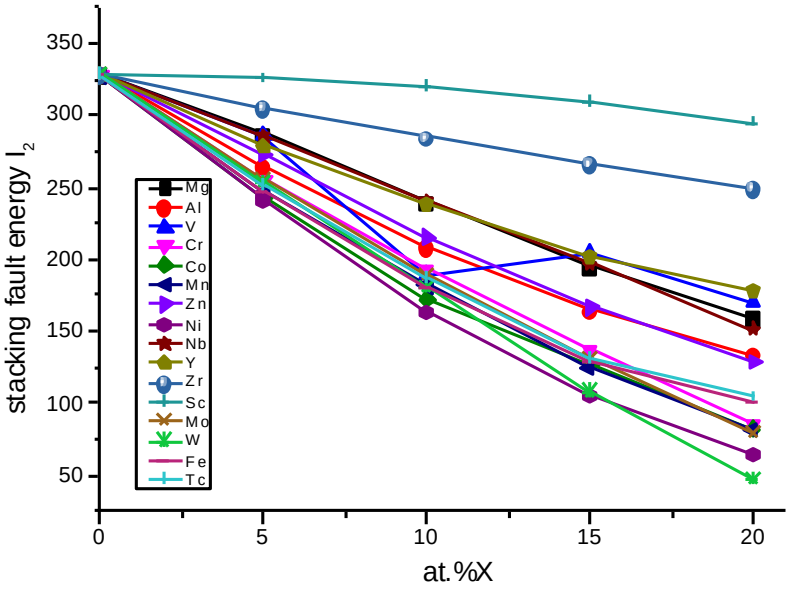
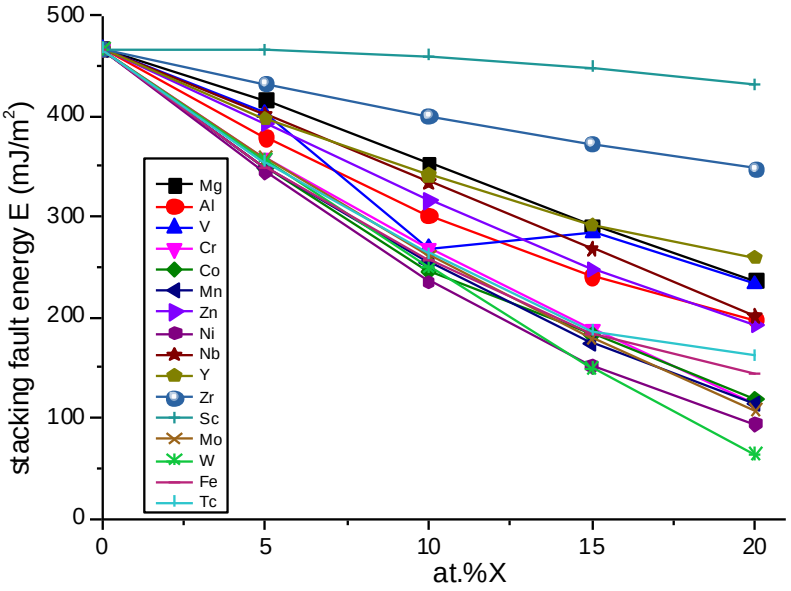


Figure 3. Variation of stacking fault energies with solutes concentration




stacking fault energy I_2
at.%X
Mg
Al
V
Cr
Co
Mn
Zn
Ni
Nb
Y
Zr
Sc
Mo
W
Fe
Tc


stacking fault energy E (mJ/m^2)
at.%X
Mg
Al
V
Cr
Co
Mn
Zn
Ni
Nb
Y
Zr
Sc
Mo
W
Fe
Tc

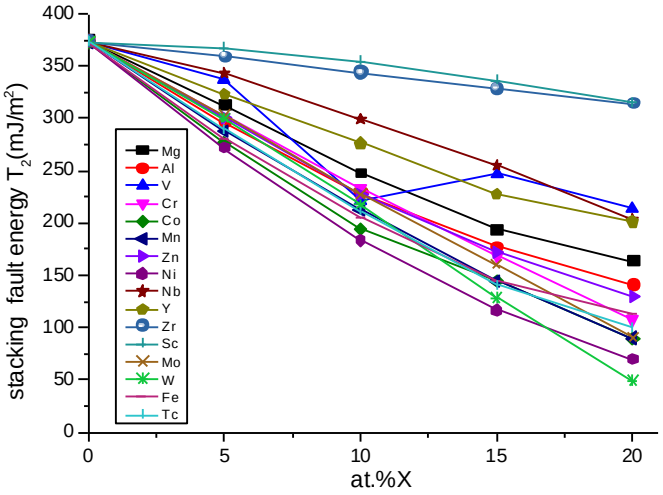


Table 1 The calculated and experimental lattice parameters (a, c/a) for pure Ti

	a(Å)	c/a
This work	2.9291	1.61
Ref[3]	2.9510	1.59
Ref[7]	2.9000	1.55
Ref[10]	2.9960	1.59
Ref[20]	2.9340	1.59

Table 2 the calculated and experimental stacking fault energy (In mJ/m2) for the four types (I1, I2, E and T2)

	I_1	I_2	E	T_2
This work	184	327	466	373
Ref[7]		287		
Ref[8]		307		367
Ref[10]	148	259	353	
Ref[11]	180	310	440	360
Ref[21]		291		
Ref[22]		292		
Ref[23]		>300		

Table 3 Calculated equilibrium lattice parameters of titanium alloys Ti95X5.

$Ti_{95}X_5$	a(Å)	c/a
Mg	2.9351	1.61
Al	2.9213	1.61
Sc	2.9449	1.60
V	2.9155	1.61
Ti	2.9291	1.61
Cr	2.9078	1.61
Mn	2.9047	1.60
Fe	2.9018	1.60
Co	2.9013	1.60
Ni	2.9014	1.60
Zn	2.9183	1.61
Y	2.9548	1.61
Zr	2.9417	1.61
Nb	2.9269	1.61
Mo	2.9181	1.61
Tc	2.9141	1.61
W	2.9164	1.61

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