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The possibilities to lower the stacking fault energies of aluminum materials investigated by first-principles energy calculations

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ABSTRACT

The stacking fault energies (SFEs) of various aluminum solid solutions were investigated against temperature and solute concentration using first-principles energy calculations. Three types of impurities, including intrinsic defects, substitutional solute atoms and interstitial solutes were considered to study their effects on the SFEs in corresponding aluminum solid solutions. It is shown that the intrinsic defects hardly change the SFEs of aluminum, whereas substitutional solutes such as Ge, Y, Sc, Sr and interstitial solutes such as C, N, H, can drastically lower the SFEs of aluminum at low temperatures. Our study suggests that at circumstances the possibilities to introduce twins in aluminum materials can be increased significantly, since their SFEs can be lowered to the values smaller than 45 mJ/m^2. The physical mechanism of lowering the SFEs in those aluminum solid solutions were interpreted by their electronic structures around the SFs and the solutes or impurities.

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1. Introduction

Aluminum (Al) alloys are widely used in automotive, aerospace, defense, electronics and biomedical industries [1–3] due to their excellent performances, such as light weight, high strength and good fatigue resistance. The properties of Al materials depend strongly on their microstructures such as precipitates of alloying elements [4–7], grain size and texture, and as well their crystal defects such as dislocations, stacking faults (SFs), solutes of alloying elements, vacancies and interstitials [8–10]. With the rapid development of the cosmic space and nuclear industries, many devices made of aluminum alloys may serve under the condition of irradiation damage. Dislocation loops may be generated easily owing to the creation of interstitials and vacancies by the irradiation of energetic particles (such as electrons, neutrons and other high energy particles) [11–13]. In addition, the vacancies and interstitials may be produced in aluminum materials during quenching from high temperature to low temperature, or through a high temperature plastic deformation process [14–16]. Dislocation loops are generated after those point defects aggregating and collapsing, i.e., forming disks of interstitial and vacancy SFs in the Al lattice. Hence the study of crystal defects has long been a serious subject in order to better understand the structure–property relations of Al materials.

The stacking fault energy (SFE) has been used to describe the ease with which a metal plastically deforms by twinning in competing with dislocation-medicated slip. Al is such a metal in which twins rarely form due to its high SFE, hence twins in Al are only associated under specific conditions. Molecular dynamics simulations predicted deformation twinning and twin boundary migration in nanocrystalline (nc) Al [17,18]. Furthermore, twinning has been observed by experimental observation in nc Al and its alloys [19,20]. This has generated a great interest in the SF and twinning mechanism for the plastic deformation of Al. Recently, twins and SFs were successfully introduced into nc Al through the template method [21]. Additionally, the stress concentration near a crack tip can lead to deformation twinning in pure polycrystalline Al, and these twins reverse as the stress relaxes [22]. Nonetheless, the introduction of twins into a bulk Al material remains a major scientific challenge.

One approach to fundamentally altering the slip behavior in Al is to reduce its SFE by adding alloy elements in the lattice. If the added alloying atoms can lower the SFE greatly, deformation twinning may occur in high strength Al alloys. Regarding Al-based alloys, a few first-principles calculations have analyzed the SFEs and the generalized stacking fault energy (GSFE) curves affected by alloying elements. For instance, Lu et al. [23] reported the H impurities can significantly reduce the GSFE. Qi et al. [24]

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investigated the SFE in binary and ternary alloys of Al with common alloying elements. Muzyk et al. [25] discussed the effects of 5 alloying elements (Cu, Ga, Mg, Si and Zn) on the GSFE. However, these studies were usually done by substituting solute atoms in a fault plane, in which the actual concentrations of solute atoms were not considered. Effectively, the interactions between solute atoms and the SF can reach far up to several layers near to the fault plane, and simultaneously cause the redistribution of solute atoms. In addition, most previous studies about the effects of alloying atoms on the SFEs of Al were performed at the temperature of 0 K. It is interesting to know how actual concentration of impurities and temperature may affect the SFEs of Al. Therefore, a more systematic study is needed about the effects of solute atoms on the SFE of Al solid solutions. Recently, Fan et al. [26] have proposed a new model to investigate the effect of solute atoms on the SFE in Mg–X (X = Li, Cu, Zn, Al, Y and Zr) solid solution. By considering the interaction between solutes and SF, the contribution of solute concentration and temperature to the SFE of Mg–X solid solutions has been investigated, obtaining the results consistent with experimental ones.

The present work aims to investigate how the SFEs of Al solid solutions are affected by intrinsic defects, substitutional and interstitial solute atoms. To be more adequate to the real situation, we took into account the effects of both temperature and impurity concentration on the SFE. Furthermore, from a microscopic view we analyzed the electronic structures of the related systems to reveal the reasons why the SFE can vary. Our results suggest that at circumstances the possibilities to introduce twins in Al materials can be increased drastically, since their SFEs can be lowered to values smaller than 45 mJ/m^2.

2. Theoretical model and computational method

2.1. Theoretical model

The simple (1 1 1) SF of face centered cubic (fcc) metals can be described by a sequence of planes labeled by A, B, and C in the usual notation corresponding to the three possible atomic positions in a (1 1 1) plane. The stacking sequence of the unfaulted fcc structure is described as $\cdots ABCABCABC\cdots$, the intrinsic stacking fault (ISF) is as $\cdots CAB\dot{C}\dot{B}CABC\cdots$, and the extrinsic stacking fault (ESF) as $\cdots ABC\dot{A}\dot{C}\dot{B}CABC\cdots$, where one (1 1 1) atomic plane is missing or being inserted in the normal stacking sequence respectively. For convenience of description, we define the up-dotted planes $\dot{C}$ and $\dot{B}$ as the layer 1 for ISF, whereas the up-dotted plane $\dot{C}$ as the layer 1 for ESF. It should be noticed that due to the structure symmetry, the chemical environment of the layer above the layer 1 is equal to that of the one below because of their equal distance to the SF plane. Then the planes nearest to the layer 1 are defined as the layer 2 in both the ISF and ESF structures, and so are the other planes, respectively, named as the layer 3, 4, ..., n, according to their distances to the SF plane.

When the impurities are introduced to the Al solid solutions, the temperature-dependent SFE can be calculated by [26]:

$$\gamma(T) = \gamma_{Al}(T) + \sum_n c_{SF\text{-}n} E_{int\text{-}n}(T)/A, \tag{1}$$

where $\gamma_{Al}(T)$ is the SFE of pure Al at temperature T, A is the area of (1 1 1) plane in unit cell. $E_{int\text{-}n}(T)$ is the interaction energy between SF and impurities when they are located in the nth plane, and can be calculated by comparing the energy difference between two supercells: in one supercell the impurity atom is near the SF, whereas in another one it is sufficiently far away from the SF without any influence on each other. $c_{SF\text{-}n}$ is the concentration of impurities at the nth plane, which obeys the Fermi–Dirac distribution:

$$c_{SF\text{-}n} = \frac{1}{1+\exp\left[\left(E_{int\text{-}n} - kT\ln\frac{c_0}{1-c_0}\right)\Big/kT\right]}, \tag{2}$$

where c_0 is the concentration of impurities in a far plane with $E_{int} = 0$. Then, the increment of SFE caused by impurities can be described as:

$$\Delta\gamma(T) = \sum_n c_{SF\text{-}n} E_{int\text{-}n}(T)/A. \tag{3}$$

2.2. Computational details

The calculations have been performed using first-principles methods based on density functional theory (DFT) as implemented in the Vienna Ab initio Simulation Package (VASP) [27]. The Perdew–Wang 91 version of generalized gradient approximation (GGA-PW91) [28] is used for describing the exchange correlation energy. To avoid interactions between SFs, large $3\times3\times14$ and $3\times3\times13$ supercells are used for ISF and ESF, respectively. After a careful convergence test, the energy cutoff is chosen as 350 eV for all calculations. The K-point sampling employs Monkhorst–Pack [29] meshes in the Brillouin zone, and the size of the K-Point meshes for all the supercells are $9\times9\times1$. In optimization, the conjugate gradient algorithm is used to relax the structures until the Hellmann–Feyman force on all atomic sites was smaller than 0.02 eV/Å. In this way, the precision in total energy of convergent results is higher than 10^{-5} eV per unit-cell.

3. Results and discussions

3.1. SFEs of pure Al

The intrinsic stacking fault energy (ISFE) (γ_{IN}) and extrinsic stacking fault energy (ESFE) (γ_{EX}) for pure fcc Al were calculated at 0 K firstly, which are 123.8 mJ/m^2 and 110.5 mJ/m^2, respectively. The published calculated results for ISFE is in the range of 130–154 mJ/m^2, while 113–138 mJ/m^2 for ESFE [30–32]. It should be noted that there are some differences among these numbers, which may possibly be resulted from the different details used in calculation procedures, such as supercell size, atomic potential and exchange–correlation functional. Hence, our results agree quite well with the available data.

To estimate the temperature dependence of SFEs of pure Al, we assume that the change of SFE at finite temperatures is mainly caused by volume change, and the V–T relation of the SF structure is almost the same as the perfect structure. The calculation procedure originally proposed by Shang et al.[33] includes the following steps: (1) calculating the SFE as a function of volume; (2) establishing the V–T relation; (3) computing the temperature-dependence SFE through the SFE-volume–temperature (*SFE*-V–T) relation. Furthermore, Wang et al. [34] has compared the calculated values with the experimental data assessed by Touloukian et al. [35], showing only a minor difference exists at a high temperature (about 10% at 900 K). Fig. 1(a) shows the experimental results of the linear expansion coefficient of Al [35]. According to Fig. 1(a), we get the V–T relation in Fig. 1(b), compared with our calculated result using the method given by Shang[33], in which the volume at 300 K is normalized to be 1.

As can be seen, the experimental results are in good agreement with the theoretical results. The volume of Al increases with temperature, and reaches its maximum value about 1.05 at 900 K. The calculated volume-dependence SFEs curves (*SFE*-V) for Al are plotted in Fig. 1(c). The SFEs decrease linearly as the volume changes. Combining the relationships of V–T (experimental and theoretical results shown in Fig. 1(b)) and *SFE*-V, the

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