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AB INITIO STUDY OF GENERALIZED STACKING FAULT ENERGIES IN MAGNESIUM

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ABSTRACT

The light weight and high specific strength magnesium alloys are important as structural materials. However, magnesium and magnesium alloys have low plastic formability and occur brittle fracture at room temperature, because their active slip systems are not sufficient. In the behaviors of slip deformation and dislocation motions, the critical and effective parameter is the generalized stacking fault (GSF) energy. The GSF energy is identified with the energy necessary to ideal slip, and shear strength of real materials should increase as the GSF energy increases. In HCP metals including magnesium, $\{0001\}<11\bar{2}0>$ basal slip and $\{10\bar{1}0\}<11\bar{2}0>$ prismatic slip with $1/3<11\bar{2}0>$ ***a*** dislocations are well known and basal slip is active and dominant in magnesium. We employ *ab initio* pseudopotential method for magnesium to study accurate the GSF energies on basal and prismatic plane and discuss the difference between basal and prismatic slip. It is also investigated from the GSF energy that the dissociation with stable stacking fault of ***a*** dislocations on prismatic plane is not so clear. The calculated GSF energy on basal plane is much lower than that on prismatic plane. This result agrees with that the observed main slip system is basal slip in real magnesium.

KEYWORDS

ab initio, pseudopotential, basal plane, prismatic plane, generalized stacking fault, stable stacking fault, dislocation, magnesium

INTRODUCTION

Recently the usage of magnesium alloys are increasing as light weight and high specific strength structural materials in automotive and aerospace industries. However, it is large problem that magnesium alloys have low plastic formability. The cause is that the active slip systems of magnesium are not sufficient near room temperature, and so it becomes low ductility. The ductility greatly depends on slip deformations and it is important to understand the deformation mechanism associated with the slip.

In HCP metals including magnesium, $\{0001\}<11\bar{2}0>$ basal slip with the dislocations along the shortest Burgers vector ***a***$=1/3<11\bar{2}0>$ (so called ***a*** dislocations) is the most commonly known plastic deformation mode and this slip system is active and dominant in magnesium. For a general loading, it is not only basal slip but also other independent slip systems are needed to deform the polycrystalline materials. It has been

reported that $\{10\bar{1}0\}<11\bar{2}0>$ prismatic slip, $\{10\bar{1}1\}<11\bar{2}0>$ first order pyramidal slip and $\{11\bar{2}2\}<\bar{1}\bar{1}23>$ second order pyramidal slip are also activated in magnesium at high temperature [1,2]. These slip systems are shown in Figure 1. Additionally, it is interesting that the dominant slip mode is different in HCP metals. For example, slip occurs preferentially on basal plane in Mg, Be, Cd and Zn, but prismatic slip is preferred in Ti, Y, Hf and Zr.

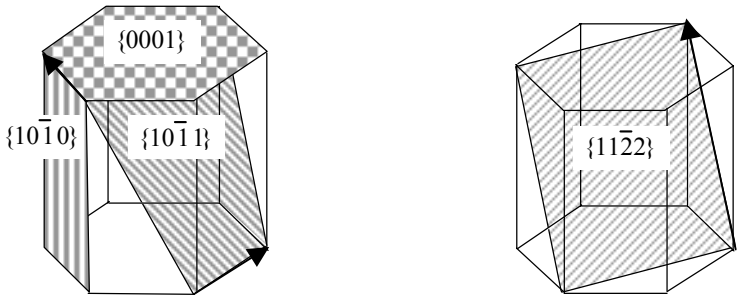

Figure 1: Slip systems in magnesium.

In slip deformations, the critical parameter is a property of the generalized stacking fault (GSF) energy which is also called γ-surface [3]. The GSF energy is defined as follows; a crystal is cut into two halves along the slip plane and one half is displaced relative to the other by the vector **t**. As this vector is varied, the energy changes and traces out the GSF energy $\gamma(\mathbf{t})$, which is normally defined as energy differences from bulk crystal. If this vector are varied along with Burgers vector, the GSF energy is identified with the potential energy necessary to ideal slip. So shear strength of real materials should increase as the GSF energy increases. There exists a relationship between the GSF energy and the dislocation density or Peierl's stress [4]. Especially, the stable stacking fault energy which is the minimum of the GSF energy play a major role in the behavior of dislocation core.

Legrand [5] calculated the GSF energy on basal and prismatic planes for various HCP metals including Mg using empirical pseudopotential method and tight-binding method. He found good agreements between the observed main slip system of various HCP metals and ratio of basal to prismatic stable stacking fault energy. It can be explained that the stable stacking fault energy is a dominant factor of the splitting width of the dislocation core and it is easy to slip as the energy is smaller. However, their calculations are based on the semi-empirical method and there is hardly quantitative and accurate investigations. Thus, in the present work we employ *ab initio* pseudopotential method for magnesium to study accurate GSF energy on basal and prismatic plane.

METHODS

All calculations presented in this paper were performed using Cambridge Serial Total-Energy Package (CASTEP). CASTEP is an *ab initio* pseudopotential method code for the solution of the electronic ground state of periodic systems with the wavefunctions expanded in plane wave basis using a technique based on density functional theory (DFT) [6,7]. The electronic exchange-correlation energy is given by the generalized gradient approximation (GGA) of Perdew and Wang [8] in the DFT. We use the norm-conserving pseudopotential of Troullier and Martins [9] in a reciprocal space. The pseudopotential is transformed to a separable form as suggested by Kleinman-Bylander [10]. The partial core correction [11] is also included in this pseudopotential. The electronic ground state is efficiently obtained using the conjugate-gradient technique [12]. The cutoff energy for the plane-wave basis is 4.36×10^{-17}J (20Ry) which is sufficient for all our purposes. The stable atomic configurations are obtained through relaxation according to the Hellmann-Feynman forces.

The supercells containing 10 basal atomic layers and 12 prismatic atomic layers are used for the calculation of the GSF energies on basal and prismatic plane, respectively (see Figure 2). For basal and prismatic supercells, Brillouin zone integration over k points are performed using $12\times12\times2$ and $11\times7\times3$ regular divisions of each axis in reciprocal space, respectively.

The slip deformation occurs with dislocations along Burgers vector, but dislocations are dissociated to

partial dislocations with stacking fault. Hence, it is important the GSF energy displaced by dissociated Burgers vector of partial dislocations, not simple Burgers vector of dislocations. We calculate the GSF energies displaced by vector **t** that changes continuously 0 to $\boldsymbol{b}_p$. The $\boldsymbol{b}_p$ is dissociated Burgers vector of partial dislocations. The atomic layers are cut into two half halves parallel to basal or prismatic plane and one half is displaced by displacement vector **t**. The GSF energy $\gamma(\mathbf{t})$ defined as

$$\gamma(\mathbf{t}) = \frac{E_{\text{fault}}(\mathbf{t}) - E_{\text{bulk}}}{2\mathbf{A}}, \tag{1}$$

where E_{bulk} is the total energy of supercell of magnesium bulk, $E_{\text{fault}}(\mathbf{t})$ is the total energy of supercell containing two generalized stacking faults displaced by vector **t** and **A** is the area of stacking fault per a supercell.

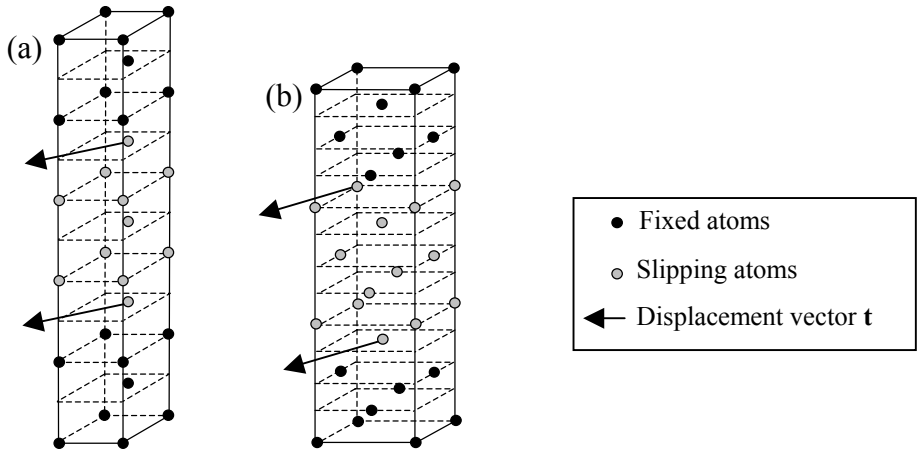

Figure 2: (a) Supercell for basal slip and (b) supercell for prismatic slip.

RESULTS

When considering dislocation splitting in HCP metals, the situation is clear for ***a*** dislocations on basal plane which can always dissociate into Shockley-type partials. The dissociation of ***a*** dislocations is the splitting on basal planes according to the reaction

$$\frac{1}{3}<11\bar{2}0>=\frac{1}{3}<10\bar{1}0>+\frac{1}{3}<01\bar{1}0>, \tag{2}$$

with the I_2 stacking fault between the partial dislocations. However, the dissociation of ***a*** dislocations on prismatic plane is not so clear. Using a hard-sphere model, Tyson [13] proposed the splitting

$$\frac{1}{3}<11\bar{2}0>=\frac{1}{6}<11\bar{2}1>+\frac{1}{6}<11\bar{2}\bar{1}>. \tag{3}$$

Vitek and Igarashi [14] suggest from the γ-surface calculations of empirical many-body potentials that the same dislocations may also split on prismatic planes according to the reaction

$$\frac{1}{3}<11\bar{2}0>=\frac{1}{6}<11\bar{2}\mathbf{x}>+\frac{1}{6}<11\bar{2}\bar{\mathbf{x}}>, \tag{4}$$

where **x** varies from material to material.

We calculate the GSF energies displaced by the vector $\boldsymbol{b}_p = 1/6[11\bar{2}\mathbf{x}]$, **x** is from 0 to 1.2, in order to examine the stable stacking fault point on prismatic plane. The results are shown in Figure 3. We find lowest

energy stable stacking fault point $b_p=1/6[11\bar{2}\mathbf{x}]$, **x**=0.76. Vitek and Igarashi [14] calculated **x**=0.9 by empirical many-body potentials but their value is different from our value. This difference is based on the difference between the calculation methods. The stable stacking fault energy is 255.1 mJ/m^2 at **x**=0.76. From x=0.6 to x=0.9, this staking fault energy change little (~0.3 mJ/m^2) . The stable stacking fault on prismatic plane may exist in some extent range.

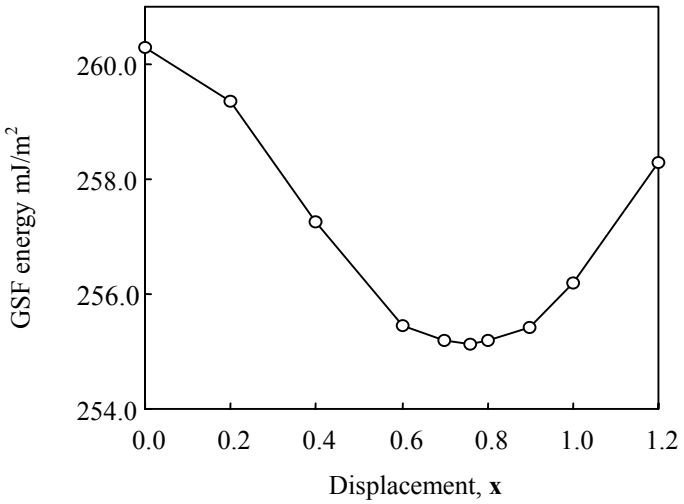

Figure 3: The stable stacking fault energy on prismatic plane.

Then, we calculate the GSF energies displaced by $\mathbf{t}=1/6[10\bar{1}0]u$, with u from 0 to 1 on basal plane, and the GSF energies displaced by $\mathbf{t}=1/6[11\bar{2}\mathbf{x}]u$, **x** = 0.76, with u from 0 to 1 on prismatic plane. These are calculated by using the three different relaxation methods of atoms. First, the atomic relaxation perpendicular to the slip plane is allowed but parallel is not allowed at all. Second, the atoms of two layers constituting stacking fault are relaxed only perpendicular to the slip plane, while other atoms move freely in all directions. Third, the atoms of two layers constituting stacking fault are relaxed in all directions, while other atoms are relaxed only perpendicular to the slip plane. On both basal and prismatic plane, the GSF energies do not change very much by different three relaxation scheme. The results by third relaxation method are shown in Figure 4. The calculated GSF energy on basal plane is much lower than that of prismatic plane. This results agree with that the observed main slip system is basal slip in real magnesium.

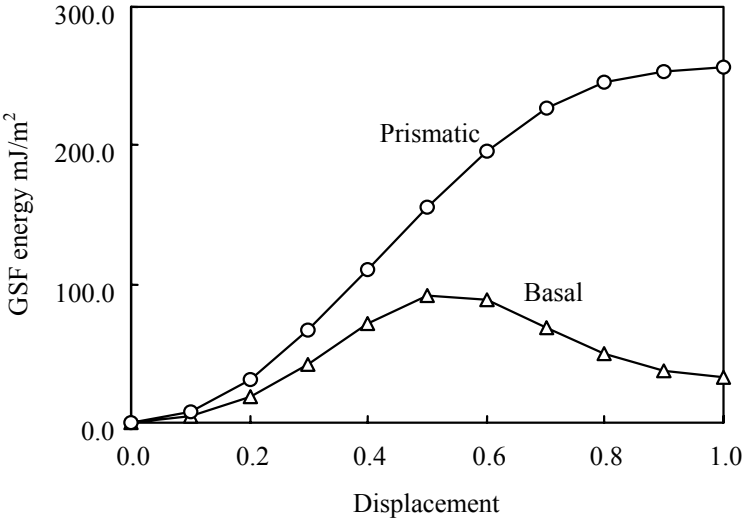

Figure 4: The GSF energies on basal and prismatic slip.

The stable stacking fault energy on basal plane, which is the minimum of the GSF energy path, is 32.4 mJ/m^2. On prismatic plane, it is different from basal plane, and stable staking fault point is the peak of the GSF energy path. We summarize the stable stacking fault energies in Table 1, which also includes other theoretical values.

TABLE 1
THE STABLE STACKING FAULT ENERGIES ON BASAL AND PRISMATIC PLANE

BASAL (mJ/m^2)	PRISMATIC (mJ/m^2)
32.4	255.1
44[a] [15]	
30[b] [5]	125[b] [5]

[a] *Ab initio* pseudopotential method [b] Empirical pseudopotential method

The result on basal plane is in good agreement with other theoretical values 30 mJ/m^2 by empirical pseudopotential method of Legrand [5] and 44 mJ/m^2 by *ab initio* pseudopotential method of Chetty and Weinert [15], while Chetty and Weinert calculated only the stable stacking fault energy, and not the GSF energies. However, the stable stacking fault energy on prismatic plane is 255.1 mJ/m^2, and it is much different from 125 mJ/m^2 by empirical pseudopotential method of Legrand [5]. In order to obtain accurate GSF or stable stacking fault energies, the precision is not sufficient by semi-empirical method, and so *ab initio* method is effective.

SUMMARY

The GSF energies on basal and prismatic plane in magnesium has been studied by *ab initio* pseudopotential method. It is also investigated that the dissociation with the stable stacking fault of ***a*** dislocations on prismatic plane is not so clear. We find the lowest energy stable stacking fault point $1/6[11\bar{2}\mathbf{x}]$, $\mathbf{x}$=0.76. The calculated GSF energy on basal plane is much lower than that on prismatic plane. This result agrees with that the observed main slip system is basal slip in real magnesium. The stable stacking fault energy, which is the minimum of the GSF energy, is 32.4 mJ/m^2 on basal plane and 255.1 mJ/m^2 on prismatic plane. In order to obtain accurate GSF or stable stacking fault energies, the precision is not sufficient by semi-empirical method, and so *ab initio* method is effective. In the future, much knowledge about slip systems will be obtained, if the similar calculations are performed on other slip planes or in other HCP metals.

ACKNOWLEDGMENTS

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