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Modeling Brittle and Ductile Behavior of α-Fe

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1. Introduction

A stacking fault plays an important role in dislocation behavior. In particular, the ratio of an unstable stacking fault (USF) energy and a free surface (FS) energy is an important parameter to describe the brittle versus ductile behavior of materials[1,2]. The sacking fault energy problem has been extensively studied for a long time, however, the energy values calculated with different empirical potentials are scattered over a wide range depending on the selected potentials[3,4]. Especially, materials involving α-Fe show the largest discrepancies in the results for the USF energy. In this study, we calculated the USF energy and the FS energy of α-Fe which is used for nuclear reactor vessel materials, by using quantum mechanical *ab initio* methods.

2. Methods and Results

2.1 Calculation details

Ab initio study has no parameter dependence, thus the calculations give accurate and reliable data. In this study, we used the generalized gradient approximation (GGA) [5] based on density functional theory. To describe the electron-ion interaction, the PAW potential [6] was employed. We tested the convergence of total energy to choose a theoretical lattice constant, suitable plane-wave cut-off energy, and k-point grid in Brillioun zone (BZ). The calculated lattice constant was obtained by fitting the Birch's equation of state as shown in Fig. 1. Table 1 summarizes the calculated results for structural and magnetic properties. The present results agree well with experimental data.

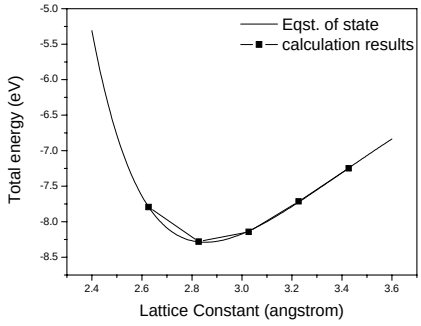

Figure 1 Calculated lattice constant of Fe

Plane waves with the kinetic energy of 300 eV are used to expand the wave functions, and the charge density is obtained by using 12 × 12 × 12 k-point grid in Brillouin zone.

Table 1 Structural and magnetic parameters of Fe

Potentials	This work	Exp.
Lattice constant (Å)	2.84	2.87
Bulk modulus (GPa)	180	172
Magnetic moment (μ_B)	2.22	2.22

2.2 Supercell Method

We calculate the USF energy of Fe to the slip system $[111](110)$, because $\{110\}$ planes are the most densely packed planes and the most common planes of crystallographic slip in bcc materials. We use a 1 × 1 × 12 supercell containing 24 atoms as shown in Fig. 2

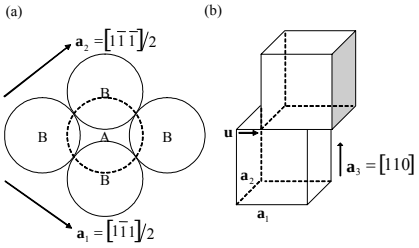

Figure 2 1 × 1 × 12 supercell to calculate the USF and the FS energy of Fe

The maximum displacement energy is obtained at $u = 1/2\,a_1$, and is identified as the USF energy. The FS energy is obtained by slicing the perfect crystal along a defined crystallographic plane and removing the upper part. The USF energy is obtained from the total energy difference between supercells of the stacking fault vector $\vec{u} = 0$ and $\vec{u} \neq 0$ as following

$$E_{USF} = \frac{E^{DFT}_{u\neq 0} - E^{DFT}_{u=0}}{A} \qquad (1)$$

where A is the area of (110) plane. Ionic relaxation between planes to the stacking fault has to be taken into account, because the force acting ions is not zero any more by breaking of atomic bond. All calculations wear performed by VASP code [7,8,9].

2.3 Results and Discussion

We summarize the calculated USF energies in Table 2. As for the results obtained by relaxing to the a_3-axis

and volume, the energy differences are as much as about 22 %. The calculation of the force acting on all ions was carried out until 0.01 eV/Å. It is clear from Table 2 that atomic relaxation must be considered in the USF energy calculation.

Table 2 Calculated USF energies

Atomic relaxation	E_{USF} (J/m^2)
no	1.161
a_3-axis	0.995
a_3-axis & volume	0.904

We compare the present results with the previous studies as indicated in Table 3. It is found that theoretical values of E_{USF} largely depend on various kinds of empirical potentials.

Table 3 Comparison the present USF energy with previous results derived from empirical potentials.

	Potentials	E_{USF} (J/m^2)
Farkas[3]	Simoneli *et al.*	0.737
Farkas[3]	Johnson *et al.*	0.900
Farkas[3]	Harrison *et al.*	0.358
Sun[4]	Harrison *et al.*	0.438
This work	PAW-GGA	0.904

We expect that the energy values calculated with an *ab initio* method of PAW-GGA will be used fundamental data to understand mechanical property of Fe. In near future, we will also calculate the FS energy of Fe. The brittle and ductile behavior depends on the ratio of two energies E_{USF} and E_{FS}. Brittle behavior is the consequence of the condition of $2E_{FS}$ being satisfied before the condition of αE_{USF} (α is a constant which depends of the geometry of the crack tip); if the converse is true, the material will be ductile [2]. We will calculate the ratio of E_{USF}/E_{FS} and compare it the experimental results.

3. Summary

We calculated the USF energy using PAW-GGA method which is one of quantum mechanical ab initio methods. We checked the effect of atomic relaxation and found that the USF energy is lowered about 22% by calculating force acting ions. We compared the results with previous theoretical data derived from various empirical potentials. In near future, we expect to obtain the ratio of E_{USF}/E_{FS} and analysis the experimental results for brittle and ductile behavior of α-Fe.

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