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Generalized-stacking-fault energy and surface properties for HCP metals: A first-principles study

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ABSTRACT

We present first-principles calculations on the generalized-stacking-fault (GSF) energies and surface properties for several HCP metals on Mg, Be, Ti, Zn, and Zr, employing density functional theory (DFT) within generalized-gradient-approximation (GGA) and spin-polarized GGA (SGGA) using the Vienna *ab initio* simulation package (VASP). Using a supercell approach, stacking fault energies for the $[1\,1\,\bar{2}\,0]$ and $[1\,0\,\bar{1}\,0]$ slip systems, and surface properties on basal plane (0 0 0 1) have been determined. Our results show that GSF energy is sensitive to the primitive cell volumes and the ratio c/a for HCP metals. A spin-polarized calculations should be considered for transition-metal Ti, Zn, and Zr. The results for Mg from this work are good with ones from the previous *ab initio* and the experiments.

1. Introduction

There is a long history of study on the mechanical properties in various HCP materials, especially for Mg. Magnesium alloys are being actively developed for structural applications due to their light weight and high strength, however they have low plastic formability [1]. The key dominant method on studying mechanical properties was captured in a more comprehensive approach by Vitek [2,3], who introduced the concept of the generalized-stacking-fault (GSF) energy surface. The GSF energy is crucial to describing accurately the dislocation core structure [4,5]. The GSF energies for Mg have always been studied by atomic potentials simulation [6,7], *ab initio* [8–13], and experiment methods [14,15], respectively. Unfortunately, the values of GSF for Mg in experiments are great disparity. In comparison with the experiments, the first-principles calculations are more reliable since the values of stable stacking fault energy of Mg are in the range of 16 and 37 mJ/m^2[9]. So the first-principle calculations is an effective method of obtaining the GSF energy values for study on the core properties of dislocations. Other HCP metals are also applied widely besides magnesium. For example, titanium and zirconium have been broadly structural applications, particularly in the automotive and aerospace industries due to their high strength, light weight, corrosion resistance, and so on [16]. The dislocation in zinc had been used to study the positron-trapping mechanism [17]. Furthermore, a detailed knowledge of the structure and energy of surfaces is important for the understanding of many surface phenomena such as adsorption, oxidation, corrosion, catalysis, crystal growth, etc. [18]. The surface energy of HCP metals by using the modified embedded atom method was calculated by Zhang et al. [19].

The purpose of this paper is to present the GSF energy surfaces of the HCP materials using the first-principles calculations by VASP, in order to further obtain the core structure of dislocations and understand the mechanical properties of HCP metals. Moreover, the surface properties are also obtained. In order to test the reliability of our model, we have calculated equilibrium lattice parameters of virous metals comparison with the experimental value. While, the stacking fault energy values and surface properties for Mg in our calculation are good agreement with the previous *ab initio*. The remainder of this paper is organized as follows: Section 2 describes the computational techniques used in our first-principles calculations. In Section 3, we present the results of the GSF energy surfaces for the basal plane (0 0 0 1) of HCP metals, while the different stacking fault energy values for virous HCP materials are analyzed qualitatively. Finally, the surface properties is presented in Section 4.

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Table 1
The equilibrium lattice parameters (a, c/a) for *hcp* metals are given by GGA, SGGA, and experimental value, respectively.

	Mg	Be	Ti	Zn	Zr
GGA	(3.21 Å, 1.62)	(2.28 Å,1.56)	(2.90 Å, 1.55)	(2.64 Å, 1.81)	(3.20 Å, 1.56)
SGGA	(3.21 Å, 1.62)	(2.29 Å, 1.56)	(2.94 Å, 1.58)	(2.67 Å, 1.87)	(3.23 Å, 1.58)
Experimental value	(3.209 Å, 1.623)	(2.286 Å, 1.568)	(2.951 Å, 1.588)	(2.665 Å, 1.856)	(3.232 Å, 1.593)
Primitive cell volume (V_{cell})	46.4	16.2	35.3	30.4	46.6

2. Computational methods and the simulation geometries

We carried out first-principles calculations on the density functional theory (DFT) level, using the “Vienna *ab initio* simulation package” (VASP 4.6) [20–22]. The Perdew–Wang [23] (PW91) exchange-correlation functional for the generalized-gradient-approximation (GGA) and spin-polarized GGA (SGGA) was used. A plane-wave basis set was employed within the framework of the projector augmented wave method [24,25]. The generalized-stacking-fault energies (GSFs) and surface energies for several types of HCP metals on Mg, Be, Ti, Zn, and Zr were optimized as follows.

In order to get accurate results, the plane-wave cut-off was set to a high value of 500 eV. To avoid any “wrap-around errors” a sufficiently large Fourier grid was used, including all wave-vectors up to twice the cut-off wavenumber. We have performed *k*-point convergence studies by use of a uniform Monkhorst-Pack scheme [26]. From these studies, we have determined that a grid consisting of 15 × 15 × 15 divisions in the Brillouin zone of the primitive unit cell of bulk HCP metals is adequate for good convergence. Calculations for bulk HCP Mg, Be, Ti, Zn, and Zr have been performed within the GGA and SGGA. In Table 1, we give the equilibrium lattice parameters (a, c/a) of Mg, Be, Ti, Zn, and Zr for the GGA, SGGA, and experimental value, respectively.

Obviously, the equilibrium lattice parameters for Mg and Be are in excellent agreement with the experimental value only using the GGA calculations, so the spin-polarized calculation need not to considered for Mg and Be. Meanwhile, Ti, Zn, and Zr are the transition-metals, therefore the spin-polarized calculation must be considered. In Fig. 1, we show the unit cell energy calculations for bulk Mg in relation to the lattice parameters a and c/a.

Now we turn our attention to the calculations of GSF energies. The ideal *hcp* structures have the configuration . . . *ABAB* . . . stacking sequence of the atomic planes. In Fig. 2, we show the basic supercell used to calculate the GSF energies for the slips along the $[1\,0\,\bar{1}\,0]$ and $[1\,1\,\bar{2}\,0]$ directions on the basal plane $(0\,0\,0\,1)$. The supercell consists of twelve atomic layers in the $[0\,0\,0\,1]$ direction. We use a large vacuum gap of 15 Å between periodically repeated slabs. The GSF energies for the twelve-layer and fourteen-layer supercell are reasonably close. Furthermore, we found that the variations of calculated results for vacuum gap of 15 and 18 Å are less than 1%. So, the adequate convergence with respect to the supercell size consisting of twelve-layer and vacuum gap of 15 Å is indicated. Afterward, the same parameters and schematic representation of the geometry are used to calculate the surface energy values for HCP metals.

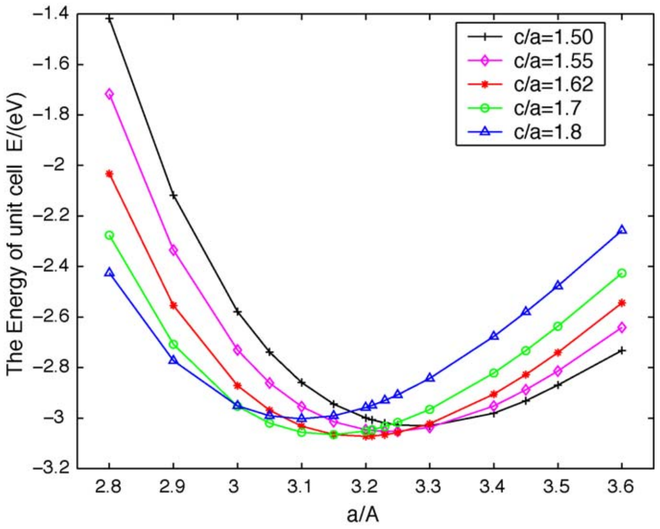

Fig. 1. Calculations for bulk Mg have been performed within GGA. The equilibrium lattice parameters a and c/a are 3.21 Å and 1.62, in good agreement with the corresponding experimental values of 3.209 Å and 1.623, respectively.

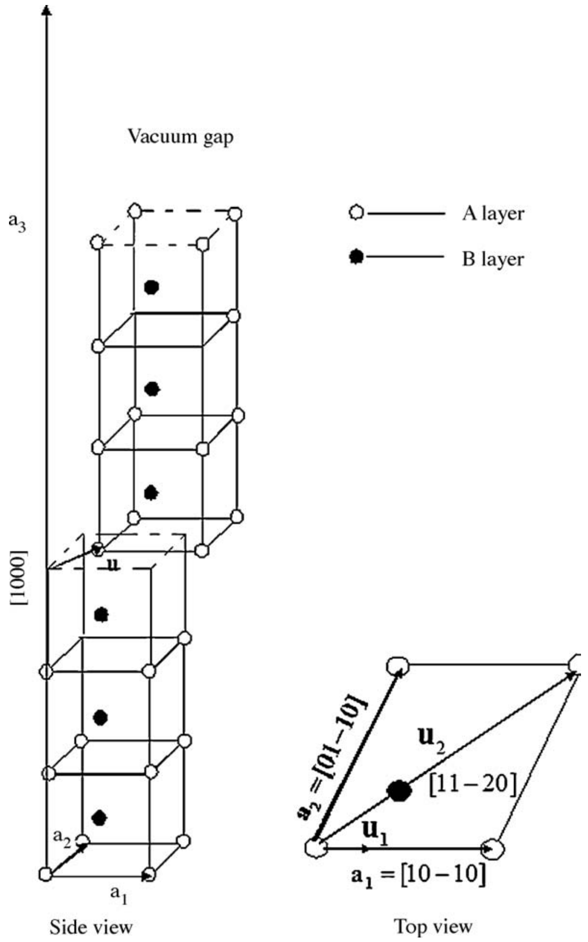

Fig. 2. A schematic representation of the geometry used in the total-energy calculations for the $[1\,0\,\bar{1}\,0]$ and $[1\,1\,\bar{2}\,0]$ in basal plane $(0\,0\,0\,1)$ slip systems. The basic supercell is shown in side and top views. The slab consists of twelve layers in the $[0\,0\,0\,1]$ direction and has repeat vectors on the basal plane equal to the ideal crystal primitive lattice vectors, denoted by $\mathbf{a}_1$, $\mathbf{a}_2$. The angular separation of $\mathbf{a}_1$ and $\mathbf{a}_2$ is 60°, and $|\mathbf{a}_1| = |\mathbf{a}_2| = a$. The third vector $\mathbf{a}_3$ is along the $[0\,0\,0\,1]$ direction in the undistorted cell, perpendicular to the plane ($\mathbf{a}_1$, $\mathbf{a}_2$). Furthermore, we used a large vacuum gap of 15 Å between periodically repeated slabs. Distortions of the cell in the direction $[1\,0\,\bar{1}\,0]$ (denoted by $\mathbf{u}_1$) or in the $[1\,1\,\bar{2}\,0]$ direction (denoted by $\mathbf{u}_2$), lead to configurations relevant to the generalized-stacking-fault energy for $[1\,0\,\bar{1}\,0]$ $(0\,0\,0\,1)$ or $[1\,1\,\bar{2}\,0]$ $(0\,0\,0\,1)$.