AB INITIO STUDY OF $\{10\bar{1}2\}$ TWINNING TRANSITION IN MAGNESIUM

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Abstract

Twinning is an important deformation mode in materials with the hexagonal close-packed (hcp) structures. The shear deformation combined with shuffling of atomic planes can lead to a transition between the Mg hcp structure and a twinned hcp structure. Studying such a transition by means of ab initio methods should bring more insight into the twinning mechanism in magnesium where the $\{10\bar{1}2\}$ planes are the twinning planes. Comparison of ab initio results with those obtained using the semi-empirical embedded atom method is provided. It can help improve the fitted parameters of the embedded atom method.

Keywords: Twinning, magnesium, shuffling, shear deformation, ab initio

1. INTRODUCTION

Twinning is an important deformation mechanism that operates in metals with hexagonal structure [1-3]. Generally, a *twin* involves two different orientations of the crystal meeting at the twinning plane such that the positions of atoms in the two parts of the crystal can be related either by a reflection through some plane or by rotation by an angle about some axis [4]. Apart from experimental observations of twins in metals [5, 6], theoretical modeling is employed in order to explain the displacement of atoms during twinning. There are more twinning modes that are in operation within the deformation [7]. However, in spite of a decades long research, some of the aspects of the twinning mechanism are still not clear.

Recently, $\{10\bar{1}2\}$ twin boundaries in Co with mutual orientation 86 degrees [8] have been experimentally observed and theoretically modeled using the embedded atom method (EAM). A possible mechanism of formation of $\{10\bar{1}2\}$ twins in Mg with mutual orientation 86 degrees has been suggested and theoretically modeled (within EAM) in Refs. [9-11]. They introduce the so called hcp–hcp path. This model balances both "shear-dominated" and "shuffling-dominated" mechanisms of twinning [12].

Our ab initio calculations focus on the reproducing the total energy profiles along the hcp–hcp path in Mg [11] that were obtained using the Liu [13] and Sun [14] semi-empirical interatomic potentials. Comparison of the ab initio results with those results obtained by EAM is useful for further development of the semi-empirical potentials, namely for fitting their adjustable parameters.

2. THE HCP-HCP TRANSITION PATH

A basic sketch of the hcp–hcp path is shown in **Figure 1**. 2/3 of the area of a bottom (dashed) hexagon forms a bottom face of our employed orthorhombic unit cell. The orthorhombic lattice parameters corresponding to the bottom face are a and $b = a\sqrt{3}$ where a was the lattice parameter a of the original hcp structure. The lattice parameter of that side of the orthorhombic unit cell that is perpendicular to its bottom face is c. It corresponds to the c lattice parameter of the original hcp structure. At the beginning, the employed orthorhombic unit cell is base centered, but during the transition, the symmetry of the unit cell is lowered by atomic shuffling that is depicted in green color in **Figure 1**.

The transition itself is realized by several shifts of atoms that happen at the same moment. They are as follows. First, the atom in the middle of the bottom face of the unit cell is shifted by the length of *c*/6 down. (The same shift happens with the periodically repeated atom in the top face of the unit cell). Second, the atom that is found in the proximity to the front face of the orthorhombic unit cell shifts by *b*/6 in the direction of *b* in order to hit the middle of the front face of the unit cell. In this way, an atomic layer *A* with a six-fold symmetry (hexagon) is formed and this hexagonal layer is perpendicular to the (dashed) original bottom hexagon. As the hcp structure consists of two hexagonal layers with the *AB* stacking, one needs to displace the remaining two atoms in the unit cell (one of them represents only a periodical repeating of the other) in such a way that they should form the second hcp layer *B*. This can be done, if they are shifted by *b*/6 in the direction of *b* and (at the same time) by *c*/6 down.

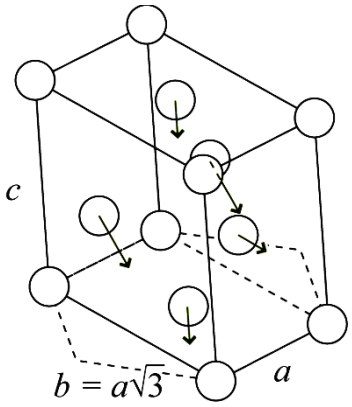

Figure 1 The shuffling mechanism of the hcp–hcp path

However, the described shuffling (shifts of the atoms in the unit cell) are not able to ensure a six-fold symmetry for the newly formed hcp layers *A* and *B*. In order to accomplish this, one needs to modify the ratio *c*/*b* of the orthorhombic unit cell. The ratio of hexagonal lattice parameters *c*/*a* for Mg is 1.624. The same ratio *c*/*a* applies for the orthorhombic unit cell. Further, the ratio $b/a = \sqrt{3}$. These two ratios should be exchanged so that $c/a = \sqrt{3}$ and *b*/*a* = 1.624. During this modification, the atomic volume and the orthorhombic lattice parameter *a* should be kept fixed. Such a modification of the orthorhombic lattice parameters corresponds to a shear deformation in the $(10\bar{1}2)$ atomic plane. The whole hcp-hcp transition includes both this shear deformation and the aforementioned shuffling. The shuffling and the deformation act simultaneously.

3. COMPUTATIONAL DETAILS

For the total-energy calculations, we employed the full-potential linearized augmented-plane wave (FLAPW) method [15] implemented in the *WIEN*2k code [16]. For exchange-correlation energy, we used the generalized gradient approximation (GGA) [17]. The muffin-tin radii of Mg atoms were constantly 2.2. a.u. throughout the calculations. The number of *k*-points in the whole Brillouin zone was equal to 10 000 for the hcp structure of Mg and was doubly reduced for the structures containing four atoms that were needed to describe the mechanism of the hcp–hcp path. In this way, the same density of *k*-points was reached for all structures studied. The product of the muffin-tin radius and the maximum reciprocal space vector, $R_{MT}k_{max}$, was equal to 7.5, and the maximum value of ℓ for the waves inside the atomic spheres, ℓ_{max}, was set to 10. The largest reciprocal vector |**G**| in the charge Fourier expansion, G_{max}, was equal to 16. The energy convergence criterion was $2 \cdot 10^{-5}$ eV/atom and, on the basis of the convergence tests with respect to the number of k-points and the parameter $R_{MT}k_{max}$, the error in calculated total energies may be estimated to be less than $4 \cdot 10^{-3}$ eV/atom.

4. RESULTS AND DISCUSSION

Following the example of Ref. [11], we have calculated the total energy profile for the hcp–hcp path that contains both shuffling and shear deformation. In addition, we calculated the total energy profiles for the shuffling only and for the deformation only. The results are depicted in **Figure 2**.

The whole transformation has been sequenced in 20 steps where step 0 corresponds to the original hcp structure and step 20 corresponds to the twinned hcp structure. The height of the energy barrier between the two hcp structures is 17.8 meV/atom. This result is close to the value of about 20 meV/atom obtained in Ref. [11] for the Sun potential. On the other hand, the height of the hcp–hcp energy barrier obtained using the Liu potential is higher, more than 30 meV/atom. In the vicinity of step 18, there is a shallow minimum on the total

energy profile of the path consisting only in the shear deformation. We point out that this minimum was not reproduced by any of the semi-empirical potentials for Mg. This is promising for future development of those potentials.

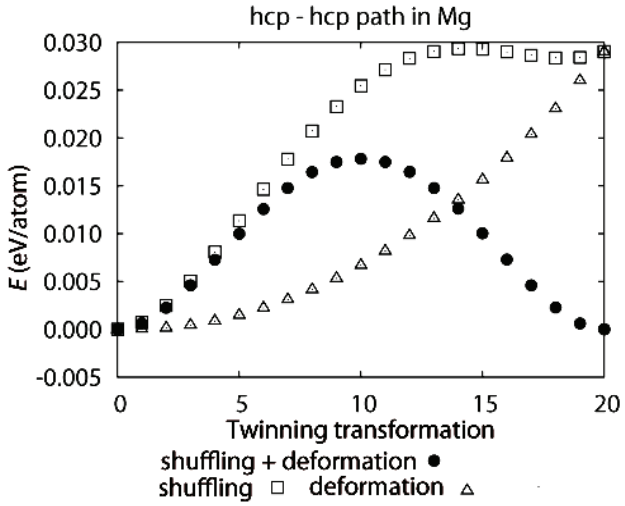

Figure 2 The total energy profile for the hcp–hcp path (shuffling + deformation) and two total energy profiles for the paths that includes only the shuffling or only the deformation

5. CONCLUSION

Using ab initio calculations, we have studied the hcp-hcp path in Mg that suggests a model for a formation of a twin on the microscopic scale. We have calculated the total energy profile along this hcp–hcp path as well as along two paths that contain (i) only shear deformation of the hcp structure in the $(10\bar{1}2)$ atomic plane and (ii) only atomic shuffling. The results of our calculations have been compared to former results obtained using the semi-empirical potentials within the embedded atom method. Concerning energy differences along the studied paths, it turned out that the Sun interatomic potential provides a more suitable description of Mg than the Liu potential. Our results can further develop the interatomic potential for Mg.

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