Computational Materials Science 152 (2018) 113–117

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Tailoring the stability of $\{10\bar{1}2\}$ twins in magnesium with solute segregation at the twin boundary and strain path control

Heyu Zhu[a], Shan Liu[a], Ziran Liu[a,b,*], Dongyang Li[c]

[a] Key Laboratory of Low-dimensional Quantum Structures and Quantum Control of Ministry of Education, School of Physics and Electronics, Hunan Normal University, Changsha 410081, PR China

[b] Synergetic Innovation Center for Quantum Effects and Applications, Hunan Normal University, Changsha 410081, PR China

[c] Department of Chemical and Materials Engineering, University of Alberta, Edmonton, AB T6G 1H9, Canada

ARTICLE INFO

Keywords:
Magnesium alloys
First-principles calculation
Twinning
Work function

ABSTRACT

$\{10\bar{1}2\}\langle10\bar{1}1\rangle$ twins in magnesium is commonly activated at the room temperature under mechanical loading to accommodate arbitrary deformation. The effect of solute segregation at twin boundary on the stability of $\{10\bar{1}2\}$ twins was investigated by employing first-principles calculations. A definition of twinning energy under external stress is proposed to predict the stability of twin with solid solutes at twin boundary under strains. The calculations reveal that the stability of $\{10\bar{1}2\}$ twins, which is dependent on the strain path could be tailored by applying external stress with or without solid solutes at boundary. The modeling well matches the previous experimental results qualitatively. Effective solute could be selected based on the electron work function (EWF) to substitute Mg atoms in certain positions along the $\{10\bar{1}2\}$ twin boundary in order to stabilize the twin.

1. Introduction

Magnesium alloys have attracted considerable interest due to their potential applications as lightweight structural materials in automotive and aerospace industry [1,2]. Mg has a hexagonal close-packed (HCP) structure with two basal and two prismatic independent slip systems altogether, which do not satisfy the von-Mises criterion (at least five) [3]. Thus, single crystalline Mg has poor room-temperature ductility and produces anisotropic deformation. To this regard, twins play an important role in accommodating deformation of Mg alloys by providing additional deformation systems to satisfy the criterion. Several types of deformation twinning have been reported in previous work [4–9], among which the $\{10\bar{1}2\}$ twins are the most easily and frequently observed one. It is recognized that the $\{10\bar{1}2\}$ twins are possible to form in the process plane (rolling plane) by compression along the process direction. Because majority of wrought Mg alloys have a strong basal texture understood as most basal planes aligned parallel to the process direction. However, this intense basal texture can be weakened by changing the rolling process [10–12] or adding rare earth element [13,14]. These suggest that the formation of $\{10\bar{1}2\}$ twins is achieved not only through one strain path, i.e., compression perpendicular to the c-axis, but also other strain paths such as applying tensile strain parallel to the c-axis. Recent work has further proved that the $\{10\bar{1}2\}$ twins are likely to form in two strain paths, i.e., tension parallel to c-axis or compression perpendicular to c-axis of the HCP lattice of Mg, experimentally [7,8,13].

The migration of $\{10\bar{1}2\}$ twins could also be pinned by periodic segregation of solute atoms at twin boundary [14], which known as complexions [15,16]. Meanwhile, the stability of the twin could also be tailored by the segregation of solute atoms [17,18], especially one rare earth element and one metal element together, such as Gd and Zn. It was demonstrated that superior physical properties can be achieved by stress, including excellent mechanical properties of metallic alloys in high-pressure physics [19]. Experimental work showed that under 5% of deformation, Mg alloys with solute atoms such as La, Ca, Gd, Al, and Sn show promoted formation of $\{10\bar{1}2\}$ twins [20]. Hence, the stability of the twins with solid solute atoms under strain is crucial for understanding the arbitrary deformation at finite temperature under mechanical loading.

In this study, the stabilities of $\{10\bar{1}2\}$ twins with and without solid solutes in different strain paths, i.e., $[10\bar{1}2]$, $[\bar{1}011]$, and $[1\bar{2}10]$ are investigated by employing first-principles calculations. The effect of applied strain on the twinning energy was studied. Detailed calculation shows that the quantitative effect of external strain on the stability of $\{10\bar{1}2\}$ twins could be precisely calculated, and the prediction well agrees with the reported experimental work.

* Corresponding author at: Key Laboratory of Low-dimensional Quantum Structures and Quantum Control of Ministry of Education, School of Physics and Electronics, Hunan Normal University, Changsha 410081, PR China.
E-mail address: zrliu@hunnu.edu.cn (Z. Liu).

https://doi.org/10.1016/j.commatsci.2018.05.035
Received 24 November 2017; Received in revised form 16 May 2018; Accepted 18 May 2018
0927-0256/ © 2018 Elsevier B.V. All rights reserved.

2. Method

First-principles calculations were based on DFT implemented in the Vienna Ab initio Simulation Package (VASP) [21–23] with projector-augmented wave (PAW) potential [24]. The generalized gradient approximation (GGA) with the exchange-correlation functional of Perdew-Burke-Ernzerhof (PBE) [25] was employed. Convergence tests indicated that 360 eV was a sufficient cutoff (higher than 1.3* maximum default cutoff energy) for PAW potential to achieve high precision in calculations on the supercell containing twin. The k-point grid of $7 \times 3 \times 1$ was selected for structure relaxations and that of $13 \times 5 \times 1$ for static energy calculations. The global break condition for the electronic self-consistency is chosen as 10^{-5} eV per supercell. Due to the ferromagnetic nature of Fe, Co, and Ni, related calculations were performed using spin-polarized approximation unless otherwise noted. For rare earth elements, the potentials in which the valence *f*-elements were treated as core electrons (appended with _3 in VASP potentials).

3. Result and discussion

3.1. The anisotropic property of single crystalline Mg under hydrostatic pressure

First, we investigate the behavior of anisotropic single crystalline Mg under the hydrostatic pressure. The result may help understanding the deformation behavior of Mg at finite pressures or under shock loading conditions. The ratio of c/a is one of critical quantities closely related to the activation of slip systems in Mg. The ratio could be tailored by adding solid solute atoms, which is critical to the operation of slip systems in hexagonal closed-packed metals [17]. For example, the preferred slip plane of Mg is basal and it's c/a ratio is 1.623. Similarly, the preferred slip plane of Zn is also basal and corresponding c/a ratio is 1.856. While the preferred slip plane for Zr is prism with corresponding c/a ratio equal to 1.593, which is smaller than that of Mg [26]. The above information suggets that the smaller c/a may introduce non-basal slip systems and improve the ductility of hcp metals. The ratio of c/a versus hydrostatic pressure of single crystal Mg is shown in Fig. 1. In the calculations, the relative energy is the energy of certain crystal structure under pressure relative to the energy of the same structure without pressure. The relative energy between high and low pressures is very different. This is also the reason why we should subtract the energy of single crystalline Mg under pressure in the definition of the twinning energy, as being discussed in the following sections. Besides, the calculations show that the c/a ratio decreases with increasing the external pressure, indicating that the c direction is easier for Mg to be deformed

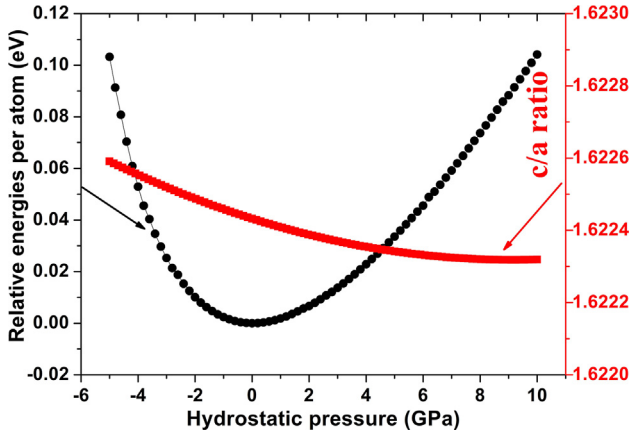

Fig. 1. The black circle doted curve and red square doted curve are the relative energies and c/a ratio as a function of external hydrostatic pressure, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

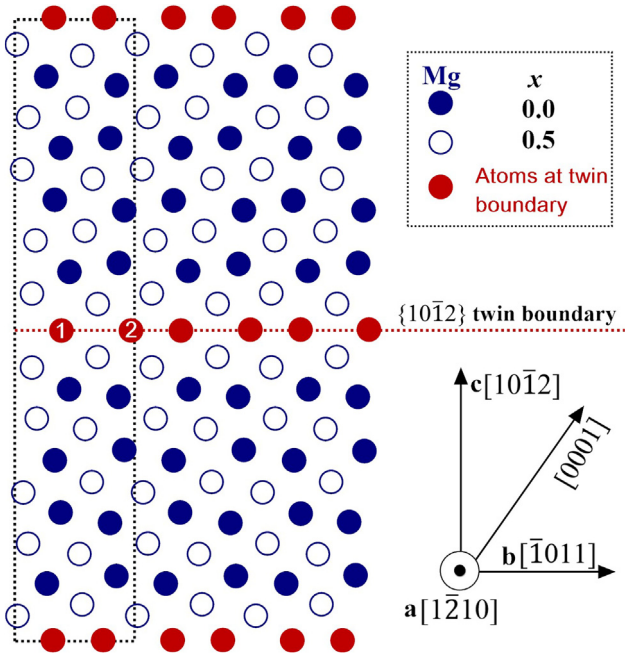

Fig. 2. Left panel is a $\{10\bar{1}2\}$ twin supercell model used in the calculations. In five strain paths, $[10\bar{1}2]$, $[\bar{1}011]$, and $[1\bar{2}10]$ are approximately orthogonal to each other. Strain along [0001] (the *c*-axis of single crystal Mg) path could be decomposed into two components along $[10\bar{1}2]$ and $[\bar{1}011]$, respectively. The atoms at twin boundary are marked in red, while the others are in navy. There are two different positions at the twin boundary labeled by white numbers 1 and 2.

than in other directions. The low ratio of c/a under high hydrostatic pressure may activate prismatic or even pyramidal slip planes. The anisotropic mechanical properties of single crystalline Mg would also result in an interesting dependence of twinning stability on the strain path.

3.2. The twinning energy versus strain paths

In order to quantify the dependence of $\{10\bar{1}2\}$ twins in Mg on the strain path, we define the twinning energy under certain path strain ε as:

$$\gamma(\varepsilon) = \frac{1}{2*A(\varepsilon)}[E_{twin}(\varepsilon) - E_{Mg}(\varepsilon)] \quad (1)$$

where $E_{twin}(\varepsilon)$ and $E_{Mg}(\varepsilon)$ represent the total energy of supercells under path strain ε with and without twin, respectively. $A(\varepsilon)$ is the cross area of the supercell under the strain ε. The number 2 means that there are two twins in one supercell. It is worth noting that the calculation of $E_{Mg}(\varepsilon)$ should also take account of applied strain, in order to eliminate the similar effect in the matrix of the supercell with twins. The twinning model used here is shown in Fig. 2. The reference systems were built from a crystalline hcp Mg with or without some of Mg atoms replaced by solutes, as shown in Fig. 3. It is unable to build an orthogonal supercell with *c* perpendicular to $\{10\bar{1}2\}$ plane with translational symmetry, but here the 20 layers of supercell is a relatively good choice. For the supercells with solute atoms at the twin boundary, we use the same method but replace the Mg atoms at twin boundary labeled as position-1 or position-2 with some solute atoms, as shown in Fig. 2. The strain path here refers to a specific crystal direction along which external strain is applied. The supercells with or without twins were built from a fully relaxed hcp Mg. The supercells were fully relaxed firstly, then only the coordinates of atoms were relaxed when the strain was applied.

The size of the supercells used for the calculations of twinning energy was carefully tested, as shown in Fig. 4(A) and (B). The tests show

Download English Version:

https://daneshyari.com/en/article/7957122

Download Persian Version:

https://daneshyari.com/article/7957122

Daneshyari.com