Tensile properties of phase interfaces in Mg–Li alloy: A first principles study*

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Employing density functional theory, we study the tensile and fracture processes of the phase interfaces in Mg–Li binary alloy. The simulation presents the strain–stress relationships, the ideal tensile strengths, and the fracture processes of three phase interfaces. The results show that the α/α and α/β interfaces have larger tensile strength than that of β/β interface. The fractures of both α/α and β/β interfaces are ductile fractures, while the α/β fractures abruptly. Further analyses show that the fracture of the α/β occurs at the interface.

Keywords: density functional theory, interface, fracture, magnesium

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1. Introduction

With attention on environment protection and the energy crisis, Mg alloys, which have the lowest density of structural material, are commonly used in automobiles.[1–7] However, the applications of Mg alloys are limited due to their poor plasticity, for the crystal structure of Mg is hexagonally close-packed. The hexagonal close-packed structure (hcp) would transform into a body-centered cubic structure (bcc) with the addition of Li in Mg alloys, thus the plasticity of the Mg alloys could be improved and their density could be further reduced. According to the equilibrium Mg–Li phase diagram, Mg alloys with the addition of about 5.7 wt%–10.3 wt% Li exhibit a two-phase eutectic microstructure, which consists of Mg-rich α-phase (hcp) and Li-rich β-phase (bcc).[8] Kral *et al.*[9] studied the crystallography of the bcc/hcp transformation in an Mg–8Li binary alloy and found that the precipitate phase α and matrix phases β are parallel. i.e., $(0\,0\,0\,1)_\alpha \,\|(0\,\bar{1}\,1)_\beta$, $(\bar{1}\,1\,0\,0)_\alpha \,\|(2\,\bar{1}\,1)_\beta$. Yang *et al.*[10] investigated the tensile mechanical properties and failure behavior of Mg–Li–Al–Zn alloys and found that at deformation temperatures higher than 100 °C, the dominant failure behaviors occurred at the α/β interfaces.[10] There have been some other experiments on the tensile and fracture behavior of Mg–Li binary alloys, but little or no work on the tensile and fracture process of the phase interfaces in these alloys from the atomic and electronic point of view has been done so far.

Density functional theory (DFT) can be used to explore the interface properties in alloys by calculating the energy and work of adhesion and by analyzing the electronic structure of the interface.[11,12] Sun *et al.*[13] studied the atomic structure and bonding of the interface between Al and precipitation in an Al–Cu–Mg–Ag alloy. Chen and Wang[14] investigated the partitioning behaviors and alloying effects of Re and Ru in Co-based superalloys with the Co/Co_3 (Al, W) interface model. DFT also highlights clearly and presents understanding of the deformation, ideal strength, and variation of electronic properties under the external stress.[15] In this work, we carefully investigate the tensile and fracture processes of phase interfaces in Mg–Li binary alloys.

2. Method

The Cambridge serial total energy package (CASTEP)[16] is applied to this study, which adopts a first-principles pseudopotential plane-wave method based on DFT. The exchange–correlation energy is described by the self-consistent local density approximation (LDA)[17] for surface and interface models, by the generalized gradient approximation of Perdew and Wang (GGA-PW91)[18] for bulk models. $E_{\rm cut}$ is set at 340 eV and the k-point meshes for Brillouin zone sampling are constructed using the Monkhorst–Pack scheme. The $9\times9\times6$ and $8\times8\times8$ k-point meshes are used for Mg and Li bulks, respectively, and a $5\times5\times1$ k-point mesh is used for all slabs. This set of parameters assures a total energy convergence of 5.0×10^{-7} eV/atom, maximum displacement of 1.0×10^{-5} Å and a maximum force of 0.001 eV/Å.

To make the validation for the method and to avoid errors on later results, the lattice constants of Mg and Li primitive cells are calculated. For Mg, our calculated result for

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the lattice constant ($a = b = 3.213$ Å, $c = 5.164$ Å) is in good agreement with the experimental result ($a = b = 3.21$ Å, $c = 5.213$ Å);[19] meanwhile, the lattice constant ($a = b = c = 3.560$ Å) of Li is also in excellent agreement with the experimental result ($a = b = c = 3.510$ Å),[20] thereby validating the applicability of the method to study the interfacial properties.

3. Interface and tensile test

3.1. Interface model

In this study, α is constructed by lithium atoms with the content of about 5 wt% substituting for magnesium atoms in a magnesium 2×2 supercell, which is equivalent to lithium dissolved in magnesium; likewise, β is constructed by magnesium atoms with a content of about 91 wt% substituting for lithium atoms in a lithium 2×2 supercell, which is equivalent to magnesium dissolved in lithium. Based on the experimental observations,[7] the $(0\,0\,0\,1)_\alpha \,\|(0\,\bar{1}\,1)_\beta$ interface model is built in our calculations with the 5% misfit. The lattice constants, which are parallel to the interface of α and β, are 6.426 Å and 6.082 Å, respectively; the effect of lattice mismatch on the calculation results is negligible in later discussions. To make sure that both sides of the slabs are thick enough to show the bulk-like characteristic interiors, we build 10 layers in which each of both sides has 5 layers for α and β, respectively. The interface models used in the tensile test with the direction of the strain are shown in Fig. 1.

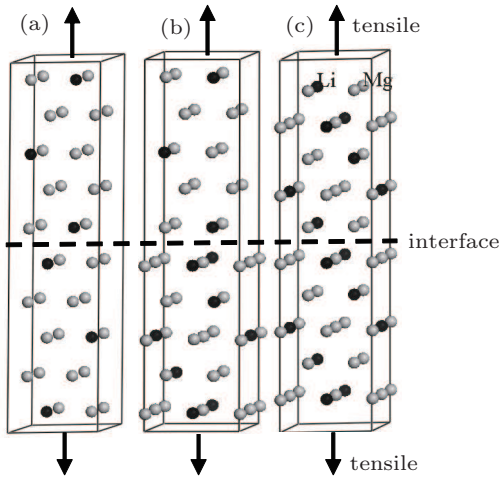


Fig. 1. Supercell models used in the tensile test with the direction of the strain, (a) α/α, (b) α/β, (c) β/β. Atoms in black color and in gray color denote Li and Mg, respectively.

3.2. Tensile test on α/α, α/β, and β/β interfaces

Generally speaking, alloys often fracture at the interface. To find out the potential rupture area in Mg–Li binary alloys, such interfaces between the matrix and the precipitation phase as α/α, α/β, and β/β are selected, and the tensile tests are performed on them in this work.

In the tensile simulation, uniaxial strain is introduced into the interface model. The tensile test is simulated by gradually increasing the dimension along the direction perpendicular to the interface. The atomic positions of the whole system readjust according to the new dimension; the atomic positions of the new configuration are fully relaxed at each strain stage. The next strain configuration starts from the former relaxed configuration. This process simulates a real tensile process with no defects in a material at zero temperature, in which the plastic deformation is not considered.

Tensile stresses of α/α, α/β, and β/β interfaces, each as a function of strain, are shown in Fig. 2. The variation of tensile stress of the α/α interface with the strain is similar to that of the β/β interface, while the variation of tensile stress of the α/β interface is different from those of the two interfaces. At the first stage of the tensile simulation, the stress rises with the increase of strain. Further, we find that there is a "kink" on the strain–stress curve of the β/β interface; it indicates that the β/β interface is at the elastic plastic deformation stage (yield stage) near the "kink". Then there are the maximum values at around 25% strain, 17.5% strain and 32.5% strain for α/α, α/β, and β/β interfaces, respectively. The values of maximum stress are about 6.77 GPa, 6.64 GPa, and 6.33 GPa, respectively, which are the ideal tensile strengths of the α/α, α/β, and β/β interfaces. Why are the maximum stresses of three interfaces different? One possible reason is that α and β are a dense-hexagonal structure and a body-centered cubic structure, respectively; accordingly, the coordination numbers are twelve and eight, when the element types and the distributions of atoms are similar, the larger the number of nearest atoms, the stronger the interaction among atoms is; therefore, the values of the tensile strength of the α/α and α/β interface are greater than the tensile strength of the β/β interface.

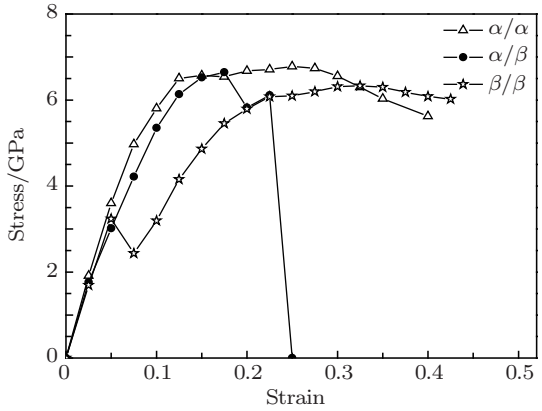


Fig. 2. Relationship of strain–stress through the tensile simulation.

For the α/β interface, after the maximum stress at 17.5% strain, it is at the inhomogeneous plastic deformation stage and the stress decreases rapidly with the further increase of strain. Finally, the system breaks and the stress drops to nearly zero. While, for the α/α interface and β/β interface, after the max-

imum stress, the stress decreases slowly with a further increment of strain. This indicates that the fractures of both the α/α and β/β interfaces are ductile fractures, while the fracture of α/β is a brittle fracture. It should be noted that the plastic deformation is not considered in this tensile process and that the measured stress is bigger than the actual stress.

3.3. Local deformation analysis and charge density

In order to understand the micro-mechanism of deformation and the physical origin of the fracture of the α/β interface, the deformation of each interlayer, parallel to the interface, is systematically analyzed at some strain stage. The results are shown in Fig. 3. In this article, the assignments of α_1 and α_2 represent the α (0 0 0 1) interlayer, which are the first and second interlayers with respect to the interface. Similarly, β_1, and β_2 denote the β (0 $\bar{1}$ 1) interlayer, which are the first and second interlayers with respect to the interface, while α/β refers to the interface. In Fig. 3, the assignment of α denotes the parameter of the strain of the α interlayer; β means the strain of the β interlayer.

When stress is imposed on the system, the interlayer distance between the α and β layers and the interfacial bond both extend. The main feature of Fig. 3 is that the strain of each layer changes averagely under each strain before the system fractures. When the strain of the whole system is 25%, the strain of the α/β interface is about 200%, that is to say, the interface is the point of fracture of the the α/β interface system. It can be concluded that the α/β interface adhesion is much smaller than the tensile strengths of α and the β bulk, so the fracture occurs on the interface.

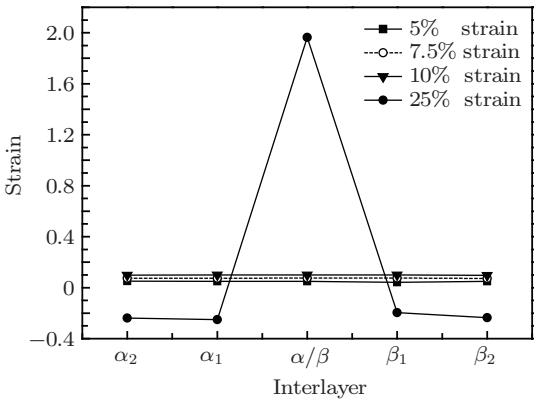


Fig. 3. Strains of the interlayer of the α/β system at different deformation stages of 5%, 7.5%, 10%, and 25%.

The tensile, and fracture processes of the interface, charge density of the relaxed atomic configure at some different strain stages are visually and vividly shown in Fig. 4. For α/β, before the strain reaches 20%, there is a large amount of charge density between the atoms near the interface, such as Mg and Li atoms. This means that α and β are combined strongly by the chemical bonds of Mg–Mg and Mg–Li. When the strain reaches 20%, the charge density becomes localized, when the strain reaches 25%, the interfacial bond breaks thoroughly and the interlayer bonds are combined strongly.

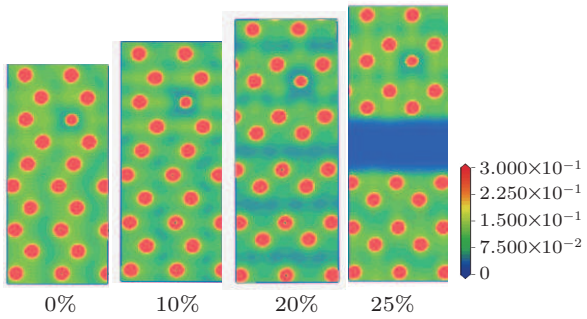


Fig. 4. (color online) Charge densities at different strain stages for α/β interface: 0.0%, 10%, 20%, and 25% strain.

4. Summary and conclusions

In this work, we performed a tensile simulation on the phase interface in the Mg–Li binary alloy. The stress–strain relationship is established and the ideal tensile strengths of the α/α, α/β, and β/β systems are obtained. As a result, the α/α, and α/β interfaces have larger tensile strengths than the β/β interface, the fractures of the α/α and β/β interfaces are both ductile fractures and the fracture of α/β is a brittle fracture. Furthermore, the micro-deformation of the α/β interface is investigated, the fracture of the α/β occurs on the interface.

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