Research Letter

Comparison of the Solid Solution Properties of Mg-RE (Gd, Dy, Y) Alloys with Atomistic Simulation

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Molecular dynamic simulations have been performed to study the solid solution mechanism of Mg_{100-x}RE_x (RE = Gd, Dy, Y, $x = 0.5, 1, 2, 3, 4$ at.%). The obtained results reveal that the additions of Gd, Dy and Y increase the lattice constants of Mg-RE alloys. Also the axis ratio c/a remains unchanged with increase in temperature, restraining the occurrence of nonbasal slip and twinning. Furthermore, it is confirmed that bulk modulus of Mg alloys can be increased remarkably by adding the Gd, Dy, Y, especially Gd, because the solid solubility of Gd in Mg decrease sharply with temperature in comparison with Dy and Y. Consequently, the addition of the RE can enhance the strength of Mg-based alloys, which is in agreement with the experimental results.

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1. INTRODUCTION

Magnesium alloys are becoming increasingly important due to potential weight saving in comparison with aluminum-based alloys. However, the mechanical properties of magnesium alloys in some respects are inferior to those of aluminum alloys which are also light-weight materials. Recently, it was reported that the addition of rare earth elements (REs), such as Gd, Dy, Y [1–6], especially Gd [7], can remarkably improve the mechanical properties of magnesium at room and high temperatures [1–4, 8]. The effects of RE have been explained by two mechanisms. One is solution-hardening and the other is precipitation-hardening.

Experimentally, the equilibrium solid solubility of Dy, Y, and Gd in magnesium is relatively high. Their values are 3.5, 3.75, and 4.53 at.%, respectively. The solid solubility decreases sharply with temperature, especially Gd. For example, the maximum solid solubility of Gd in Mg is relatively high (4.53 at.% at 821 K) and decreases exponentially with temperature (to 0.61 at.% at 573 K). It has been reported that the addition of Gd, Dy, and Y is effective for improving strength and creep resistance of magnesium alloys at elevated temperature [1–3, 9]. So the aim of this work is to investigate the solid solution properties of the Mg-RE alloy by the addition of different atomic fraction of Gd, Dy, and Y at

room temperature and elevated temperature (500 K) using the modified analytical-embedded atom method (EAM) [10], which has been successfully applied in the calculations of some Mg-rare earth alloys [11–13].

2. SIMULATION PROCEDURE

The interactions between Mg, Gd, Dy, Y atoms are described by an analytical-embedded atom method (EAM) potential [11–13].

In the simulation runs, simulations were performed for 10944 atoms based on HCP unit cell, which comprise pure Mg, and Mg_{100-x}-Gd_x, Mg_{100-x}-Dy_x, and Mg_{100-x}-Y_x ($x = 0.5, 1, 2, 3, 4$ at.%) alloys. The periodic boundary conditions were applied on the fundamental directions of molecular dynamic (MD) cell. Molecular dynamics calculations are carried out in two successive ensembles. The lattice constants for simulation systems are determined from the constant temperature-constant pressure (NPT) ensemble simulations. And then the constant volume-constant temperature (NVT) ensemble is used to compute the elastic constants of the systems. In integration of the classic equations of motion, we used a fourth-order gear predictor-corrector algorithm with a time step of 3 femtoseconds [14]. The simulation

FIGURE 1: The lattice parameter as a function of the temperature for Mg-RE alloys by the use of Gd and Dy additions.

systems are relaxed by 50 000 time steps at room and elevated temperature, and all of the statistical data are collected from further 50 000 MD time steps.

3. RESULTS AND DISCUSSION

3.1. Effect of Gd, Dy, and Y on lattice parameters in Mg

Magnesium with hexagonal close-packed crystal structure has three slip systems: a basal slip system of $(0001)\langle 11\bar{2}0 \rangle$, a prismatic slip system, such as $\{10\bar{1}0\}\langle 11\bar{2}0 \rangle$, and the pyramidal slip system, such as $\{10\bar{1}\bar{1}\}\langle 11\bar{2}0 \rangle$ and $\{11\bar{2}2\}\langle 11\bar{2}3 \rangle$. The latter two slip systems act together in many cases and are called the nonbasal slip system versus the basal slip

system. Magnesium is plastic-deformed by the basal slip and twinning mainly at relatively low temperature. The critical resolved shear stress for the basal slip in pure magnesium is very low, approximately 0.60–0.7 MPa, at room temperature. It is also independent of temperature. In contrast, the critical shear stress for the nonbasal slip is over 40 MPa at low temperature, which is two orders of magnitude higher than that for the basal slip, and drastically decreases to 2–3 MPa with increasing temperature [16].

The variation of lattice parameters with temperature in pure Mg, $\text{Mg}_{100-x}\text{-Gd}_x$, and $\text{Mg}_{100-x}\text{-Dy}_x$ ($x = 0.5, 1, 2, 3, 4$ at.%) alloys is shown in Figure 1, along with the experimental data [17]. The temperature dependence of the lattice parameters for $\text{Mg}_{100-x}\text{-Y}_x$ alloys is similar to those

FIGURE 2: Bulk modulus of Mg as function of Gd content at room and high temperature, as well as the experimental data [15].

of $\text{Mg}_{100-x}\text{-Gd}_x$ and $\text{Mg}_{100-x}\text{-Dy}_x$ alloys. By adding the Gd and Dy, the lattice parameters a and the axis ratio (c/a) become larger. The lattice parameters in the pure Mg, $\text{Mg}_{100-x}\text{-Gd}_x$ and $\text{Mg}_{100-x}\text{-Dy}_x$ alloys increase linearly with temperature increasing. We can also see that the values from EAM calculations are larger than experimental values. As an example of Mg-0.5Gd, as shown in Figure 1(c), the c/a in Mg-0.5Gd alloy almost keeps a constant with increasing temperature, whereas pure metal Mg does not exhibit this behavior. Thus, the RE metals (Gd, Dy, and Y) give rise to the variation of lattice parameters, whereas the c/a remains unchanged with increasing temperature, which indicates that the temperature-independent c/a restrains the occurrence of nonbasal slip and twinning. Because the slip and twinning in HCP metals may be related to the axis ratio, c/a . Nonbasal slip hardly occurs when the c/a is large, whereas at high temperature, where the c/a becomes lower, the nonbasal slip can occur [18, 19]. This phenomenon has been reported in Mg-Y alloys [19].

3.2. Comparison of the solid strength of Mg-RE alloys

As discussed above, the addition of RE metals can vary the lattice parameter for Mg-Gd, Mg-Dy, and Mg-Y alloys. The larger the rare earth metal content, the larger the lattice parameters for Mg-RE alloys. At the same time, the addition of rare earth metals also varies the solid strength for Mg-rare earth alloys. As an example of Mg-Gd alloys, the bulk modulus of pure Mg and $\text{Mg}_{100-x}\text{-Gd}_x$ alloys at room and high temperature are presented in Figure 2, along with the experimental data [15]. It can be noted that the addition of Gd gives rise to the sudden increase of bulk modulus of Mg at room and high temperature. The Mg-Dy and Mg-Y alloys exhibit a similar solid strength behavior. This behavior

FIGURE 3: Comparison of the bulk modulus for Mg-RE alloys with different rare earth content at room temperature.

indicates that the addition of Gd, Dy, and Y can enhance strength of Mg, which is in agreement with experiments [1–3, 20, 21]. Furthermore, the bulk modulus of Mg increases with increasing the content of Gd, Dy, and Y.

The comparison of the bulk modulus for Mg-RE alloys with various rare earth metal compositions at room temperature is shown in Figure 3. The magnitude of the bulk modulus of Mg-Gd is the largest one among the three Mg-RE alloys, which demonstrate that the addition of Gd can further improve the strength of Mg-RE alloys [8]. This behavior may be explained in terms of the equilibrium solid solubility of Gd in Mg decreasing sharply with temperature in comparison with Dy and Y. For example, the maximum solid solubility of Gd in Mg is 4.53 at.% at 821 K and decreases exponentially with temperature, to 0.61 at.% at 573 K.

4. CONCLUSIONS

In this paper, the solid solution properties of Mg-RE (RE = Gd, Dy, Y) alloys with different RE contents have been investigated in terms of molecular dynamic simulation using an analytical-embedded atom method. It has been found that the lattice parameters of magnesium alloys containing Gd, Dy, and Y increase. However, the axis ratio c/a almost keeps a constant with increasing temperature, which restrains the occurrence of nonbasal slip and twinning. Furthermore, the addition of the RE also gives rise to the variation of bulk modulus, which indicates that the strength of Mg alloys can be improved by Gd, Dy, and Y, especially Gd. This behavior may be interpreted by the idea that the equilibrium solid solubility of Gd in Mg decreasing more sharply with temperature in comparison with Dy and Y.

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