Effects of the Rare Earth Y on the Structural and Tensile Properties of Mg-based Alloy: A First-Principles Study

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Abstract: In order to investigate the effect of the rare earth element Y on the strengthening potency of magnesium alloys and its strengthening mechanism under tension. In this paper, the solid solution structures with Y atom content of 1.8 at.% and 3.7 at.% were built, respectively, and their cohesive energies and stress-strain curve were calculated in the strain range of 0–20%. The calculation results of the cohesive energies showed that the structure of element Y is more stable with the increase of strains. The calculation results of stress and strain showed that Y element can improve the yield strength and tensile strength of the Mg-based alloy, and the strengthening effect is better when the Y content is 3.7 at.%.

Keywords: Mg-based alloy; first principles; structural properties; tensile properties

1. Introduction

In recent years, magnesium alloys have been widely used in aerospace, the automotive industry, computers, the chemical industry and national defense and military industries due to their excellent properties, such as low density, light weight and high specific strength [1–3]. However, the defects of magnesium alloys are also very obvious [4]. The mechanical properties of ordinary magnesium alloys in high temperature environments are not good, which seriously restricts their further development and application [5].

Alloying is the most commonly used among a variety of magnesium alloy strengthening methods [6]. A new type of composite magnesium alloy is formed by adding alloying elements to make it a high-strength, high-toughness, high-performance magnesium alloy [7,8]. Among the many alloying elements of magnesium alloys, rare earth elements perform best [9]. Rare earth elements have the functions of deoxidizing by removing hydrogen and improving casting performance, and also have the ability to enhance alloy strength and high temperature creep resistance [10,11]. In addition, the large size of the rare earth atoms can prevent the α-Mg crystal grains from becoming larger, and help to refine the crystal grains, reduce the tendency of hot cracking due to the looseness of the microstructure, and improve the casting and welding performance of magnesium alloys [12]. Therefore, in recent years, rare-earth magnesium alloys have gradually become a hot spot for development.

The element Y is a widely used rare earth element in heat-resistant magnesium alloys, and it has the same hexagonal close-packed crystal structure as Mg atoms [13]. Magnesium alloy containing Y has the characteristics of high temperature resistance, high plastic toughness and high strength [14]. After the high melting point Y element is added to the magnesium alloy, on the one hand, it can increase the nucleation rate of the alloy and play the role of grain refinement [15], on the other hand, dispersed second-phase particles can be precipitated in the magnesium alloy, which can effectively hinder the movement of dislocations and grain boundary slip. It can improve the creep resistance of magnesium.
alloy at high temperature and achieve the purpose of enhancing the strength of magnesium alloy [16,17].

The first-principles tensile test method can calculate the stress value of a crystal structure under different stresses (the stress-strain relationship). The theoretical tensile strength of the crystal structure can be predicted by analyzing the stress value at the yield or fracture of the crystal structure. Wang et al. [18] calculated the stress-strain curves of solid solution structures Mg$_{53}$Al and Mg$_{51}$Al$_3$. It was found that the strong covalent bond between Al and Mg and the rearrangement of the electron charge density could improve the tensile strength of the Mg-based alloy, and the Mg$_{51}$Al$_3$ unit cell could increase the tensile strength of the Mg$_{54}$ unit cell by 9.4%. Zhang et al. [19] calculated and studied the tensile strength of the Al unit cell. The calculation results showed that the theoretical tensile strength of the Al grain boundary was 9.5 GPa at the strain of 16%. Wang et al. [20] calculated the influence of the distribution of Al and Zn atoms on the strength of Mg alloys. It was found that the structure with uniform distribution of alloying elements has greater ideal tensile strength than the structure with separate distribution of alloying elements. Luo et al. [21] calculated the stress-strain curve of Mg-based alloy solid solution in which Al, Zn and Y atoms were dissolved. It was found that the Al, Zn and Y atoms all have a solid solution strengthening effect on the Mg-based alloy, and the Y atom has the best solid solution strengthening effect, which conforms to the experimental rules.

The ideal tensile strength of the crystal structure is an important index parameter to measure material properties and evaluate material quality [22,23]. Therefore, the first-principles tensile calculation method can be used to study the solid solution strengthening effect of alloying elements on Mg-based alloy, and which has an important guiding value for the development and application of magnesium alloys. Considering that the solid solubility of Y atoms in the magnesium alloy does not exceed 3.75 at.%. In this research, Mg$_{53}$Y$_1$ and Mg$_{52}$Y$_2$ with Y atom solid solubility of 1.8% at.% and 3.7 at.% were used as the research object. The stress-strain curves and electronic structure changes of the Mg$_{54}$, Mg$_{53}$Y$_1$ and Mg$_{52}$Y$_2$ structures under 0–20% strains were calculated, and the improvement of the yield strength and tensile strength of the Mg-based alloy by the element Y and the strengthening mechanism were analyzed.

2. Computational Methods

The research content in this paper was assembled using the CASTEP software, which is based on the first-principles density functional theory [24,25]. Tensile tests were performed by applying stress to the c-axis direction of the crystal structures of Mg$_{54}$, Mg$_{53}$Y$_1$ and Mg$_{52}$Y$_2$, with a 2% strain increment. In order to obtain accurate stress and strain conditions, the strain interval is 1% between 6% and 10% strain, and the upper limit of the applied strain is 20%. The crystal structure must be geometrically optimized after each strain is applied. The optimize cell option was not checked during the relaxation process, therefore, the lattice constant was not optimized, and only the atomic coordinates in the supercell were optimized. After geometric optimization, the energy, stress and strain values and electronic structure of the supercell structure were calculated.

The CASTEP software parameter setting includes the following contents: Considering that the number of atoms in the unit cell is relatively large, in order not to affect the calculation speed exchange correlation, the function option selects the PW91 functional in the approximate form of GGA. In the convergence setting of the optimized crystal structure, the convergence value of the total energy is 1.0 × 10$^{-5}$ eV/atom. The convergence value of the force between atoms is 0.03 eV/Å, the maximum internal stress is 0.05 GPa, and the tolerance offset value is set 0.001 Å. In the electronic setting, the cut-off energy is 340 eV, and the number of K points is 3 × 3 × 1. The correlation between particles is set to Ultrasoft super soft pseudopotential. The SCF self-consistent iteration tolerance value is 1.0 × 10$^{-6}$ eV/atom, the number of convergence steps for geometric mechanism optimization and electronic properties calculation is 150, and the electronic minimizer is set to the default density mixing method and Pulay correction.
3. Results and Discussion
3.1. Structure Properties

As shown in Figure 1a the unit cell of pure magnesium with two Mg atoms has a close-packed hexagonal structure, which space group is P63/MMC, and the lattice constants are \( a = b = 0.3209 \) nm, and \( c = 0.5211 \) nm. Based on the pure magnesium unit cell and considering factors such as calculation time and accuracy, a \( 3 \times 3 \times 3 \) supercell is built as shown in Figure 1b. The cell contains 54 Mg atoms, and is therefore hereinafter referred to as Mg\(_{54}\), and the corresponding supercell lattice constants are \( a = b = 0.9628 \) nm, \( c = 1.5632 \) nm. Replacing the magnesium atom at coordinates \( x = 0.5556, y = 0.4444, z = 0.5833 \) with an Y atom we obtain the Mg\(_{53}\)Y\(_1\) crystal structure, that is, a Mg-based alloy solid solution structure with a Y atom content of 1.8 at.%. This structure is shown in Figure 1c. By replacing the magnesium atoms at coordinates \( x = 0.5556, y = 0.4444, z = 0.5833 \) and \( x = 0.5556, y = 0.4444, z = 0.2500 \) with Y atoms, as shown in Figure 1d, the crystal structure of Mg\(_{52}\)Y\(_2\) can be obtained, that is, a Mg-based alloy solid solution structure with a Y atoms content of 3.7 at.%.
In this formula, $\sigma_{\alpha\beta}$ is the average stress acting on the unit cell, $\Omega$ is the unit cell volume, $E_{\text{tot}}$ is the total energy of the unit cell, and $\varepsilon_{\alpha\beta}$ is the strain tensor. A tensile strain is applied in the direction of the C axis of the unit cell:

$$\varepsilon = \frac{(l_e - l_0)}{l_0} \times 100\% \tag{2}$$

In Equation (2), $l_0$ is the initial cell c-axis length when no strain is applied, and $l_e$ is the c-axis length of the cell corresponding to the applied strain. It is worth noting that in order to save calculation time, the simulation calculation in this section does not consider the influence of Poisson effect, that is, ignores the influence of tensile strain on the other two axial lattice constants, and considers its value to be fixed.

The stability of the crystal structure depends on its cohesive energy. The definition of binding energy is: if the crystal is split into single free atoms, the work done by the outside world is the cohesive energy of the compound. The cohesive energy of a stably existing compound is negative, and the lower the cohesive energy value, the more stable the crystal structure of the compound. The calculation formula of cohesive energy is as follows [27]:

$$E_{\text{coh}} = \frac{E_{\text{AB}}^{\text{tot}} - N_A E_{\text{A}}^{\text{atom}} - N_B E_{\text{B}}^{\text{atom}}}{N_A + N_B} \tag{3}$$

In the above formula, $E_{\text{coh}}$ is the cohesive energy of the intermetallic compound, $E_{\text{tot}}$ is the total energy of the compound, $E_{\text{A}}^{\text{atom}}$ and $E_{\text{B}}^{\text{atom}}$ are the energies of the A and B atoms in the free state, respectively. The free state atomic energies of Mg and Y are $-972.5822$ eV/atom and $-188.5729$ eV/atom, respectively; $N_A$ and $N_B$ are the corresponding numbers of atoms in the unit cell.

The cohesive energy of Mg$_{54}$, Mg$_{53}$Y$_1$, and Mg$_{52}$Y$_2$ at 0–20% strains were calculated, as shown in Table 1. First, the cohesive energy of the three structures are all negative at zero strain, indicating that the three structures can exist stably. Further analysis found that in the range of 0–20% strains, the cohesive energy of the three structures all increase with the increase of strain. Since the larger the absolute value of the cohesive energy, the more stable the structure, so it can be determined that the stability of the three structures decreases with the increase of strain. The reason why the structures become unstable may be the weakening of the chemical bonds between atoms due to stretching. It is worth noting that although the stability of the three structures has decreased, but the cohesive energy values are always negative, indicating that the three structures can still remain stable within the range of 0–20% strains. In addition, it can also be found that the stability of the Mg$_{53}$Y$_1$, and Mg$_{52}$Y$_2$ structures are stronger than that of Mg$_{54}$, and the Mg$_{52}$Y$_2$ structure is the most stable.

Table 1. The cohesive energy of Mg$_{54}$, Mg$_{53}$Y$_1$ and Mg$_{52}$Y$_2$ under different strains.

| Strain (%) | $E_{\text{coh}}$, kJ·mol$^{-1}$ | Mg$_{54}$ | Mg$_{53}$Y$_1$ | Mg$_{52}$Y$_2$ |
|------------|-------------------------------|-----------|----------------|----------------|
| 0          | $-193.46$                     | $-199.66$ | $-205.63$      |
| 2          | $-193.01$                     | $-199.40$ | $-205.52$      |
| 4          | $-192.44$                     | $-198.95$ | $-205.15$      |
| 6          | $-191.70$                     | $-198.28$ | $-204.49$      |
| 7          | $-191.41$                     | $-197.97$ | $-204.33$      |
| 8          | $-191.37$                     | $-197.74$ | $-204.08$      |
| 9          | $-190.90$                     | $-197.43$ | $-203.77$      |
| 10         | $-190.47$                     | $-196.97$ | $-203.32$      |
| 12         | $-189.77$                     | $-196.15$ | $-202.43$      |
| 14         | $-188.75$                     | $-195.08$ | $-201.29$      |
| 16         | $-187.46$                     | $-193.77$ | $-199.92$      |
| 18         | $-186.00$                     | $-192.32$ | $-198.84$      |
| 20         | $-184.60$                     | $-190.84$ | $-197.64$      |
3.2. Tensile Properties

In production applications, structural parts often fail due to excessive plastic deformation. For components with strict requirements, plastic deformation is generally not allowed. For components with less stringent requirements, materials are often selected based on the yield strength value \( \sigma_y \). Under 0–20% strains, the stress values of \( \text{Mg}_{54} \), \( \text{Mg}_{53}Y_1 \), and \( \text{Mg}_{52}Y_2 \) solid solution structure are listed in Table 2, and the stress-strain curve is drawn at the same time, as shown in Figure 2. The abscissa represents the applied strains, and the ordinate represents the stress values corresponding to the strains.

Table 2. The Stress values of \( \text{Mg}_{54} \), \( \text{Mg}_{53}Y_1 \), \( \text{Mg}_{53}Y_2 \) under different strains.

| Strains (%) | \( \text{Mg}_{54} \) | \( \text{Mg}_{53}Y_1 \) | \( \text{Mg}_{52}Y_2 \) |
|-------------|----------------|----------------|----------------|
| 0           | 0.00           | 0.00           | 0.00           |
| 2           | 1.74           | 1.23           | 0.75           |
| 4           | 2.35           | 1.94           | 1.83           |
| 6           | 2.69           | 2.67           | 2.63           |
| 7           | 1.21           | 1.49           | 1.57           |
| 8           | 1.85           | 1.99           | 2.04           |
| 9           | 2.22           | 2.36           | 2.40           |
| 10          | 2.47           | 2.76           | 2.92           |
| 12          | 3.11           | 3.39           | 3.65           |
| 14          | 4.15           | 4.25           | 4.47           |
| 16          | 4.97           | 4.93           | 5.15           |
| 18          | 5.15           | 5.24           | 5.63           |
| 20          | 5.02           | 5.37           | 4.22           |

Figure 2. Stress-strain curve of \( \text{Y Mg}_{54} \), \( \text{Mg}_{53}Y_1 \), and \( \text{Mg}_{53}Y_2 \).

It can be found from Figure 2 that the three types of structures are all elastic-uneven plastic-uniform plastic deformation types. When the structure is subjected to elastic deformation, obvious upper and lower yield points appear. In the initial stage, when the stress is small, the elongation of the structure changes in proportion to the stress. At this time, the material undergoes elastic deformation after stress, and the material can return to its original length when there is no stress. It can be seen from Figure 2 that the linear variation range of \( \text{Mg}_{54} \), \( \text{Mg}_{53}Y_1 \), and \( \text{Mg}_{52}Y_2 \) is very small.

As the stress increases, the tensile strains experienced by the material continues to increase. At this time, both elastic deformation and plastic deformation occur, and it is difficult for the material to fully recover to its original length after the stress is unloaded. When the strain reaches 6%, the upper yield points of the three structures appear at the same time. The upper yield strengths of \( \text{Mg}_{54} \), \( \text{Mg}_{53}Y_1 \), and \( \text{Mg}_{52}Y_2 \) are 2.69 GPa, 2.67 GPa and 2.63 GPa, respectively. At the same time, with the application of stress, the lower yield point appears at 7% strain. The lower yield strengths of \( \text{Mg}_{54} \), \( \text{Mg}_{53}Y_1 \), and \( \text{Mg}_{52}Y_2 \) are 1.21 GPa, 1.49 GPa, and 1.57 GPa, respectively. For structures with upper and lower yield
points, the lower yield strength is usually selected as the yield strength of the material structure, which is generally expressed by $\sigma_s$ [28]. The yield strength is a unique strength index for materials with yield phenomena. The yield strengths of $\text{Mg}_{53}\text{Y}_1$, and $\text{Mg}_{52}\text{Y}_2$ are higher than that of $\text{Mg}_{54}$, and are increased by 23.14% and 29.75%, respectively, compared to $\text{Mg}_{54}$. It shows that the rare earth element Y can increase the yield strength of Mg-based alloy alloys, and the strengthening effect on Mg-based alloy alloys is stronger when the Y content is 3.7 at.%. After the material is stretched to the yield stage, there will be a plastic deformation interval, and the resistance of the material against external force stretching will increase with the growth of the plastic deformation, until the stress reaches the tensile strength $\sigma_b$ [29]. Tensile strength is the ability of a material to resist damage under the action of external force. After reaching the tensile strength, the stress values will decrease as the strains increases. At this time, the deformation strengthening effect of the material structure can no longer compensate for the reduced load-bearing capacity due to the reduction of the cross-section. The tensile strength represents the maximum stress value that a material can withstand under tensile deformation, which is an important indicator of the material’s resistance to tensile deformation. It can be seen from Figure 2 that when the yield strength is reached, several structures begin to undergo plastic deformation. With the gradual increase of strains, the stress values of several structures increase rapidly until the tensile strength is reached. The tensile strength values of $\text{Mg}_{54}$, $\text{Mg}_{53}\text{Y}_1$, and $\text{Mg}_{52}\text{Y}_2$ are 5.15 GPa, 5.37 GPa and 5.63 GPa, respectively. It shows that the rare earth Y element can improve the tensile strength of Mg-based alloy alloys, and the enhancement effect is best when the Y content is 3.7 at.%. Based on the above analysis, it can be found that the Y element can enhance the strength of the Mg-based alloys. When the Y atom content is 3.7 at.%, the strengthening effect is greater than 1.8 at.%. This conclusion is consistent with the experimental results [30]. It was found that the Y element can increases the tensile strength of magnesium alloys, but the plasticity will be decreased. Therefore, although the addition of Y reduces the elastic deformability of the Mg-based alloy. However, both the yield strength and the tensile strength are improved, and the strengthening effect becomes stronger as the solid solubility increases.

4. Conclusions

The first-principles method is used to investigate the effect of rare earth Y element on the tensile properties of Mg-based alloys. Under the strains of 0–20%, the crystal structures of $\text{Mg}_{54}$, $\text{Mg}_{53}\text{Y}_1$, and $\text{Mg}_{52}\text{Y}_2$ can all remain stable. The structure of $\text{Mg}_{52}\text{Y}_2$ is more stable than that of $\text{Mg}_{54}$ and $\text{Mg}_{53}\text{Y}_1$, indicating that rare earth element Y can enhance the stability of Mg-based alloya. When the Y atoms are dissolved in the Mg-based alloy at a content of 1.8 at.% and 3.7 at.%, the yield strength and tensile strength of the Mg-based alloy can be promoted. The theoretical tensile strength values of $\text{Mg}_{54}$, $\text{Mg}_{53}\text{Y}_1$, and $\text{Mg}_{52}\text{Y}_2$ are 5.15 GPa, 5.37 GPa and 5.63 GPa, respectively. When the Y atom content is 3.7 at.%, the enhancement effect on the Mg-based alloy is better than 1.8 at.%.

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