



Simulation on microstructure evolution and mechanical properties of Mg–Y alloys: Effect of trace Y

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Received 31 March 2021; accepted 28 October 2021

Abstract: The influence of trace Y on the microstructure evolution and mechanical properties of $\text{Mg}_{100-x}\text{Y}_x$ ($x=0.25, 0.75, 1.5, 3, 4, 5$, at.%) alloys during solidification process was investigated via molecular dynamics (MD) simulations. The results show that the $\text{Mg}_{100-x}\text{Y}_x$ alloys are mainly characterized by a face-centered cubic (FCC) crystal structure; this is different from pure metal Mg, which exhibits a hexagonal close packed (HCP) structure at room temperature. Among these alloys, $\text{Mg}_{99.25}\text{Y}_{0.75}$ has a larger proportion of FCC cluster structures, with the highest fraction reaching 56.65%. As the content of the Y increases up to 5 at.% (Mg_{95}Y_5 alloy), the amount of amorphous structures increases. The mechanical properties of the $\text{Mg}_{100-x}\text{Y}_x$ alloys are closely related to their microstructures. The $\text{Mg}_{99.25}\text{Y}_{0.75}$ and Mg_{97}Y_3 alloys exhibit the highest yield strengths of 1.86 and 1.90 GPa, respectively. The deformation mechanism of the Mg–Y alloys is described at the atomic level, and it is found that a difference in the FCC proportion caused by different Y contents leads to distinct deformation mechanisms.

Key words: Mg–Y alloy; molecular dynamics; microstructure evolution; mechanical properties; deformation mechanism

1 Introduction

Magnesium (Mg) and its alloys have attracted much attention owing to their low density, high specific strength, and high stiffness [1–3]. Because of their suitable mechanical properties, Mg-based alloys can be used for implants in biomedical applications. More specifically, the elastic modulus of Mg-based alloys is close to that of human bones, which is believed to diminish the “stress-shielding effect” when implanted in the human body [4,5].

There are three requirements for biomedical Mg alloys [6–8]. Firstly, Mg alloys should exhibit appropriate mechanical properties, either as bone substitutes or scaffold materials, which ensure the stability and functionality over time after the implantation. Secondly, Mg alloys should have a suitable degradation performance, as a high degradation rate of Mg implants will result in a premature loss of the mechanical properties, numerous hydrogen bubbles, and alkalization in the vicinity of the implant. Thirdly, Mg alloys should be biocompatible or nonbiotoxic.

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DOI: 10.1016/S1003-6326(22)65835-7

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Two problems should be considered when using Mg alloys as biomaterials. On the one hand, the mechanical and degradation properties of Mg alloys are often improved by alloying suitable elements [9]. On the other hand, the content of heavy metals and rare-earth elements (REEs) in the human body gradually increases with the implant degradation. For example, REEs tend to accumulate in the bones and kidneys [10], posing a threat to human health. Therefore, the chemical composition of biomedical Mg alloys should be as simple as possible, and the additional metal content should be as small as possible (dealloying or micro-alloying) [3,11]. It is a big challenge to decrease the content of added heavy metals while maintain satisfactory mechanical properties and a sufficiently low degradation rate in the design of Mg alloys.

Mg has low ductility and poor formability at room temperature because its hexagonal close packed (HCP) structure has few slip systems and specific $\langle c+a \rangle$ dislocation slip characteristics [12]. Element alloying is one of the effective methods to improve the material properties, such as mechanical properties, degradation and anticorrosion performance [13,14]. At present, commonly used alloy elements for biomedical Mg alloys include Al, Ca, Li, Zn, Zr, Sr, Mn and REEs [15,16]. Among them, REEs have attracted more attention because of their ability to greatly enhance the ductility of Mg alloys [17]. Moreover, adding trace amounts of REEs can significantly improve the mechanical strength of alloys. STANFORD et al [18] demonstrated that adding 0.1 wt.% of REEs could improve the ductility by weakening the texture of Mg alloys. Yttrium (Y) is a typical REE that has been demonstrated to be able to significantly improve the comprehensive performance of Mg alloys [19,20]. SANDLÖBES et al [21] found that a high proportion of pyramidal $\langle c+a \rangle$ slips appeared during the tensile deformation of a cold-rolled Mg–3wt.%Y alloy at room temperature, and the addition of Y could improve the plasticity of the Mg alloy by nearly a factor of five, compared with that of pure Mg, without loss of strength.

Although the effects of the addition of trace elements on the structure and properties of the alloy is well known, the mechanisms behind these effects have not been systematically investigated; however, this information is important for the development of new Mg alloys. With the increased computing

ability of giant computers, it has become easier to study the microscopic structure of alloys and, in particular, its evolution during deformation process. The molecular dynamic (MD) simulations [22,23] were performed to reveal the evolution mechanisms of the microstructure and the mechanical properties of the alloys during the solidification processes, and some analytical tools were used to better present the results from the MD simulations. In this work, MD simulations were used to study the influence of the Y content on the Mg alloys.

In order to investigate the effect of trace amounts of Y on the microstructure and mechanical behavior of Mg–Y alloys during solidification, the solidification processes of the $\text{Mg}_{100-x}\text{Y}_x$ ($x=0.25, 0.75, 1.5, 3, 4, 5$, at.%) alloys were studied via MD simulations at a cooling rate of 0.01 K/ps. The structure evolution and mechanical properties were analyzed in terms of the system energy, pair distribution function (PDF $g(r)$), cluster-type index method (CTIM), and visualization analysis at the atomic level. These results will provide a deep understanding of the relationship between the microstructure and the mechanical properties of Mg–Y alloys.

2 Simulation conditions and methods

MD simulations of the $\text{Mg}_{100-x}\text{Y}_x$ ($x=0.25, 0.75, 1.5, 3, 4, 5$, at.%) alloys were performed by employing large-scale atomic/molecular massively parallel simulator (LAMMPS) [24]. The embedded-atom model (EAM) potential was adopted to describe the interaction among atoms; this potential was developed by PEI et al [25], and its accuracy and efficiency have been proven in extensive published work [26,27]. The potential can be written as [25]

$$E_{\text{tot}} = \sum_{i,j} \phi(r_{ij}) + \sum_i F(n_i) \quad (1)$$

where $n_i = \sum_j \rho(r_{ij})$, and $\phi(r)$, $\rho(r)$ and $F(n_i)$ are the pair, density and embedding functions, respectively. The simulation was performed using three-dimensional (3D) periodic boundary conditions (PBCs) with a time step of 1 fs and isothermal isobaric (NPT) ensemble [28]. After 80000 atoms (e.g, the $\text{Mg}_{99.75}\text{Y}_{0.25}$ alloy contains 79800 Mg atoms and 200 Y atoms) were randomly generated

in a cubic box at a pressure of 0 GPa, the system was isothermally relaxed for 2 ns at 1400 K to obtain an equilibrium liquid. The system was then cooled down to 100 K at a cooling rate of 0.01 K/ps under the NPT ensembles. At each selected temperature, all the relevant information was recorded for each atom.

In order to investigate the mechanical behavior of the Mg–Y alloys, the uniaxial tension in the alloys was simulated at a constant strain rate of $1.0 \times 10^8 \text{ s}^{-1}$ along the z -axis at a temperature of 100 K for each solidified sample. Furthermore, the relevant information for each atom in the system was recorded at each selected strain.

3 Results and discussion

3.1 Microstructure evolution

3.1.1 Energy–temperature curve analysis

For a cooling system, the energy versus temperature (E – T) curve can describe the evolution of the microstructure. An abrupt decrease in the E – T curve indicates a phase transition, whereas a smooth transition corresponds to a vitrifying process.

From the E – T curves of the six alloys with different compositions (Fig. 1), it can be seen that three alloys ($\text{Mg}_{99.75}\text{Y}_{0.25}$, $\text{Mg}_{99.25}\text{Y}_{0.75}$, and $\text{Mg}_{98.5}\text{Y}_{1.5}$) exhibit a sudden decrease in E at almost the same temperature (around 450 K). This is the typical indicator of the occurrence of crystallization in metals, which denotes an important structural change or a phase transition. For the Mg_{97}Y_3 and Mg_{96}Y_4 alloys, E – T curve exhibits a continuously

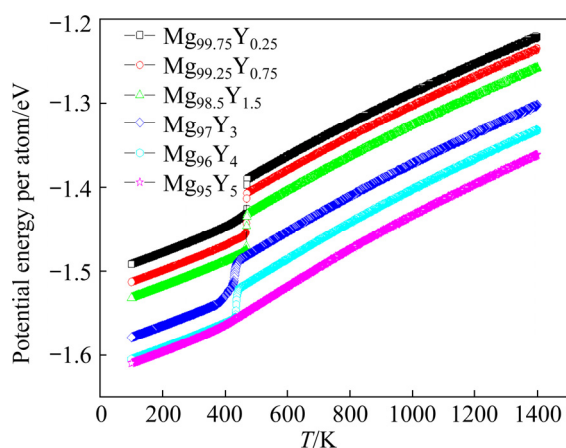


Fig. 1 Potential energy as function of temperature (E – T curve) for six alloys with different compositions during solidification

decreasing trend over a certain range, which means that the phase transition lasts longer. Additionally, for the alloy containing 5.0 at.% Y atoms, the continuous transition indicates that this alloy is mainly transformed into amorphous structures during solidification.

3.1.2 PDF analysis

It is well known that the structure factor $S(q)$ can be obtained from the X-ray diffraction patterns, and the PDF ($g(r)$) can be obtained from $S(q)$. Both $S(q)$ and $g(r)$ are usually used to validate the simulation results.

Both crystalline and amorphous structures can be identified by analyzing the shape and position of the peaks on the $g(r)$ curve. For example, a set of sharp and intense peaks indicate the formation of a crystalline structure, while a split second peak on the $g(r)$ curve is the characteristic of an amorphous structure. The PDF curves of the six alloys are shown in Fig. 2 in the temperature range from 1400 to 100 K with a data point interval of 100 K.

It can be seen from Fig. 2 that, with the decrease in temperature, all the first peaks on the $g(r)$ curve become sharper and more intense, indicating that the probability of forming ordered structures has increased. In the higher-temperature region of 1400–500 K, the metal alloys are in a liquid state, the $g(r)$ curves (which are shown in blue in Fig. 2) show wider 1st and 2nd peaks and valleys, and the intensity of each peak changes slightly. In the lower-temperature region of 400–100 K, the $g(r)$ curves (which are shown in black in Fig. 2) exhibit the features typical of crystallization for $\text{Mg}_{100-x}\text{Y}_x$ ($x=0.25, 0.75, 1.5, 3, 4$, at.%) or vitrification for Mg_{95}Y_5 . For the first five $g(r)$ curves at 100 K, the positions and intensities of the peaks are very similar, which means that their final crystal structures are also analogous. Additionally, for the Mg_{95}Y_5 alloy, only the second peak of the $g(r)$ curve is split into two, indicating that an amorphous structure is formed at 100 K.

3.1.3 CTIM analysis

Though the $g(r)$ curves can be used to accurately analyze the one-dimensional structures, they cannot describe and discern 3D cluster structures. To deeply understand the crystallization of Mg–Y alloys at the atomic level, the CTIM-3 was employed; this method was proposed by LIU et al [29–31] based on the work of QI and WANG [32]. This method can be used to

quantitatively describe almost all types of local clusters formed in the simulation system. In the CTIM-3, the cluster is composed of a central atom and its surrounding bonded atoms, and it is represented by nine integer indices ($N, n_{1441}, n_{1551}, n_{1661}, n_{1421}, n_{1422}, n_{1541}, n_{1431}, n_{1321}$), where N is the coordination number of the central atom, and the following eight integers denote in turn the numbers

of the 1441, 1551, 1661, 1421, 1422, 1541, 1431 and 1321 H—A bond-types, through which the surrounding atoms are bonded to the central atom [33].

Using the CTIM-3, several important basic clusters are obtained, as presented in Fig. 3. The face-centered cubic (FCC), body-centered cubic (BCC), and icosahedron (ICO) basic clusters could

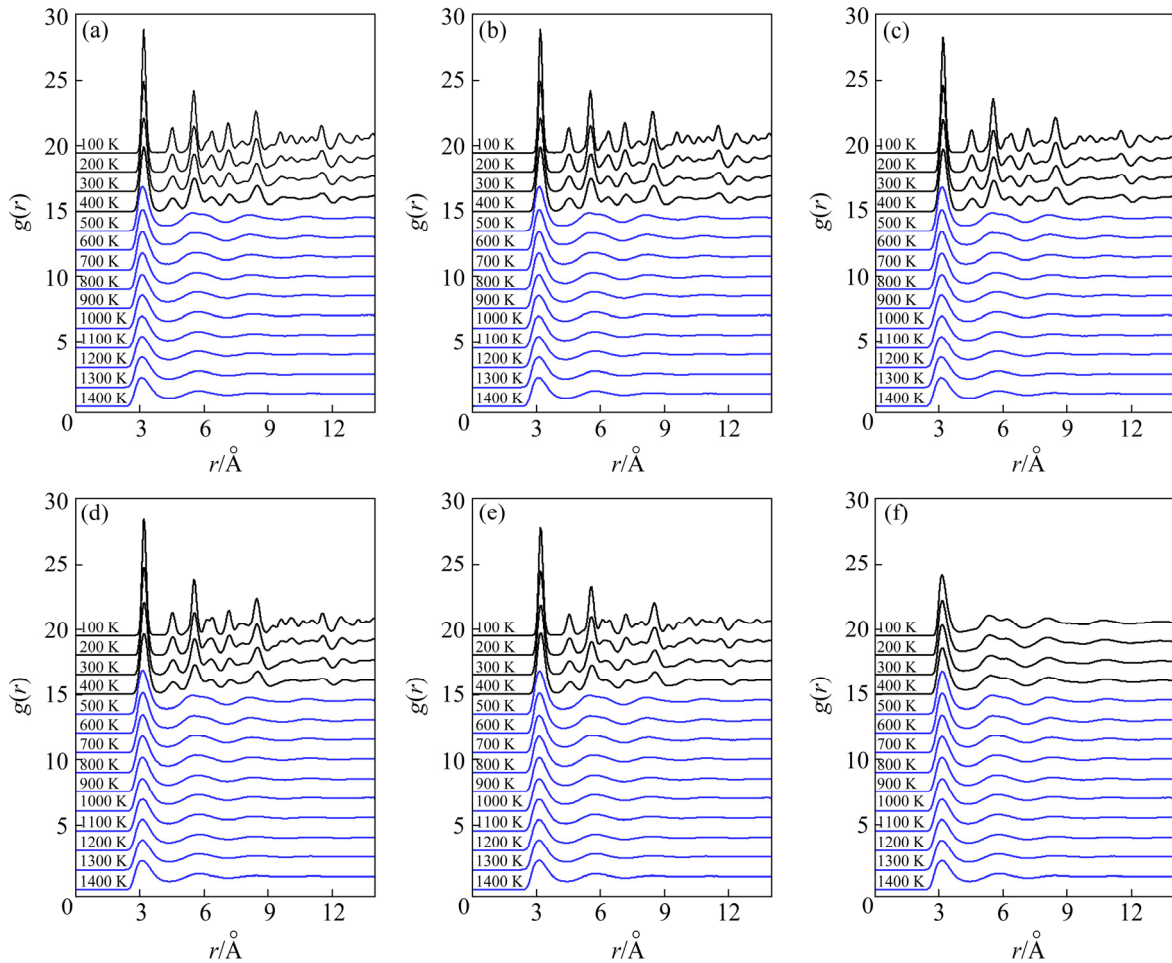


Fig. 2 $g(r)$ curves at several selected temperatures for six Mg–Y alloys: (a) $\text{Mg}_{99.75}\text{Y}_{0.25}$; (b) $\text{Mg}_{99.25}\text{Y}_{0.75}$; (c) $\text{Mg}_{98.5}\text{Y}_{1.5}$; (d) Mg_{97}Y_3 ; (e) Mg_{96}Y_4 ; (f) Mg_{95}Y_5

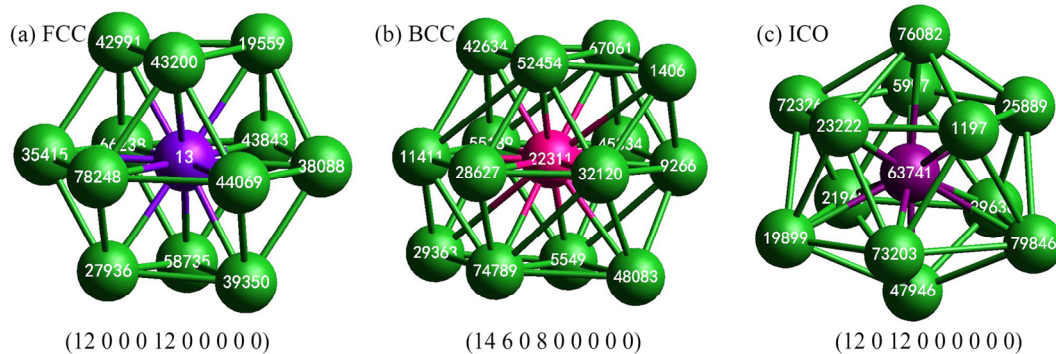


Fig. 3 Three basic clusters in system: (a) FCC basic cluster (12 0 0 0 12 0 0 0 0) with center atom represented by 13; (b) BCC basic cluster (14 6 0 8 0 0 0 0 0) with center atom represented by 22311; (c) ICO basic cluster (12 0 12 0 0 0 0 0 0) with center atom represented by 63741

be represented by (12 0 0 0 12 0 0 0 0), (14 6 0 8 0 0 0 0 0), and (12 0 12 0 0 0 0 0 0) respectively, as shown in Figs. 3(a–c).

The evolution of the major clusters in the six alloy systems is shown in Fig. 4, including all clusters with content exceeding 1% during the process. It can be seen that a few clusters are still present in the six systems at the initial temperature of 1400 K. As the temperature decreases, the numbers of ICO and defect-ICO (13 1 10 2 0 0 0 0 0) (12 0 8 0 0 0 2 2 0) (14 2 8 4 0 0 0 0 0) clusters increase slightly. As the temperature drops to the transition temperature T_c , for all Mg–Y alloys

except for the Mg_{95}Y_5 alloy, the numbers of both the HCP and FCC crystal clusters increase remarkably, accompanied by the appearance of defect-FCC (11 0 0 0 7 0 0 0 4) (12 0 0 0 9 1 0 0 2) or defect-HCP (12 0 0 0 4 4 2 2 0) clusters. At the same time, the numbers of ICO and defect-ICO clusters start to decrease. Among the different systems, the FCC clusters reach the maximum content of 56.65% in the $\text{Mg}_{99.25}\text{Y}_{0.75}$ alloy at 100 K. In the Mg_{95}Y_5 alloy, the numbers of the main clusters decrease below T_g , and their content becomes relatively low. Few crystal structures are found in the Mg_{95}Y_5 alloy, which means that a

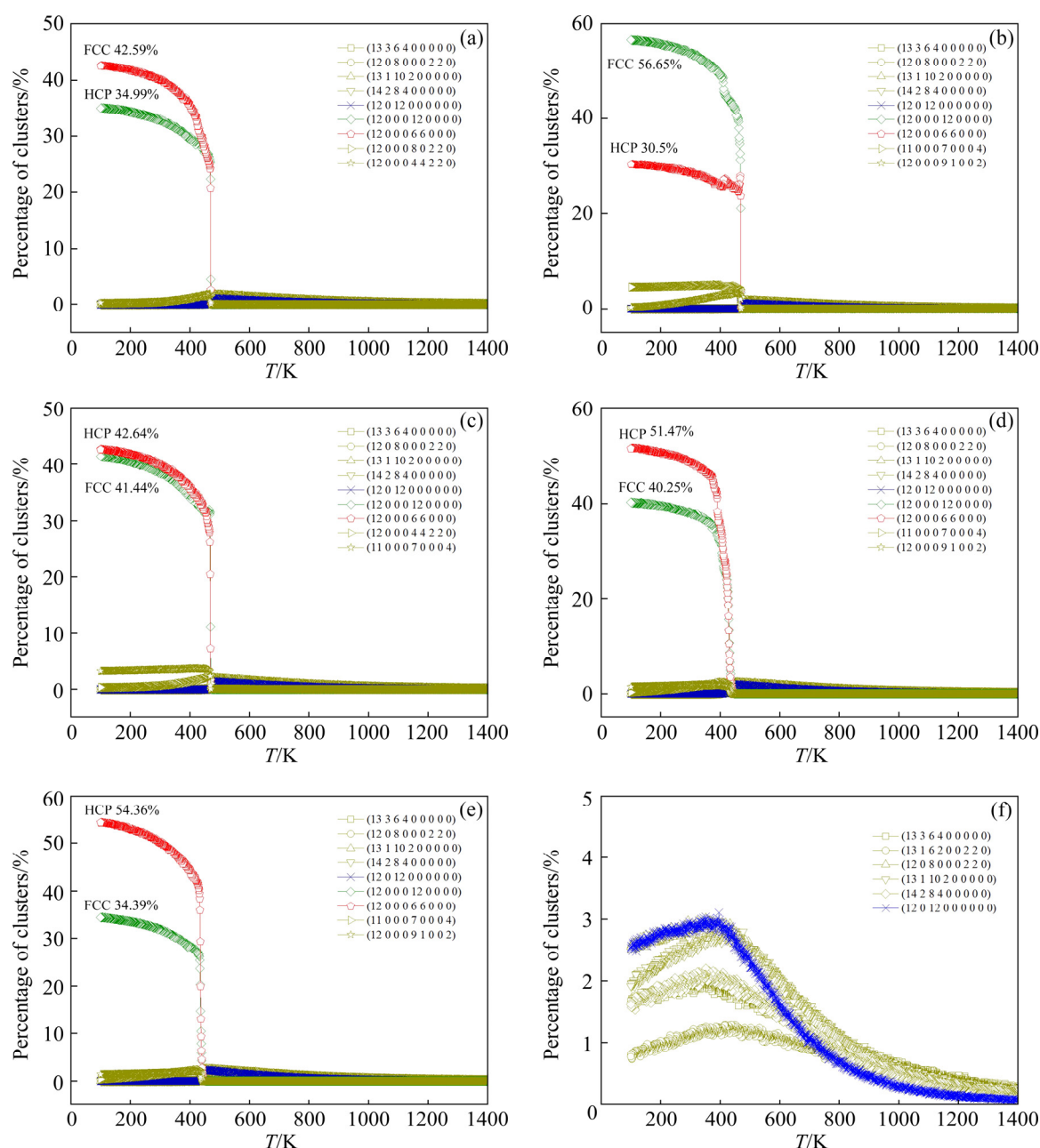


Fig. 4 Content of main basic clusters during solidification process: (a) $\text{Mg}_{99.75}\text{Y}_{0.25}$; (b) $\text{Mg}_{99.25}\text{Y}_{0.75}$; (c) $\text{Mg}_{98.5}\text{Y}_{1.5}$; (d) Mg_{97}Y_3 ; (e) Mg_{96}Y_4 ; (f) Mg_{95}Y_5

long-range order structure is not formed. That is to say, the Mg_{95}Y_5 alloy has an amorphous structure. These results are consistent with the $g(r)$ curves. Furthermore, it can be seen from Fig. 5 that the Y atoms are evenly distributed in the matrix in all Mg–Y alloys.

3.1.4 Visualization analysis

To directly visualize the spatial distribution of the clusters in the system, the microstructure distribution is shown in Fig. 6.

Among the five alloys with the main crystal structure, only the $\text{Mg}_{99.75}\text{Y}_{0.25}$ alloy (Fig. 6(a))

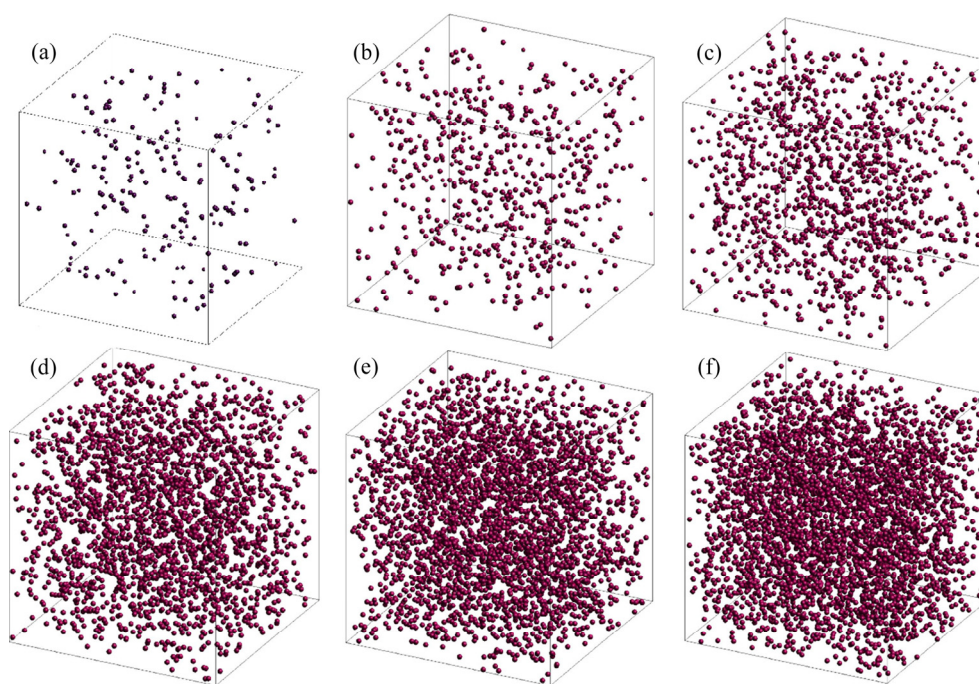


Fig. 5 Snapshots of Y atom distribution for six Mg–Y alloys at 100 K: (a) $\text{Mg}_{99.75}\text{Y}_{0.25}$; (b) $\text{Mg}_{99.25}\text{Y}_{0.75}$; (c) $\text{Mg}_{98.5}\text{Y}_{1.5}$; (d) Mg_{97}Y_3 ; (e) Mg_{96}Y_4 ; (f) Mg_{95}Y_5

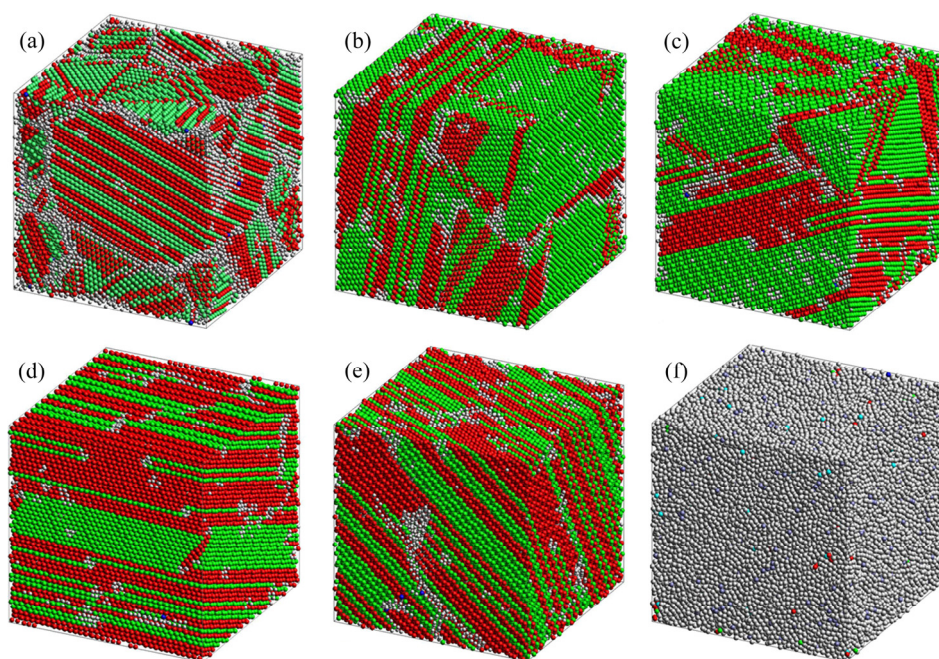


Fig. 6 3D atomic snapshots of six Mg–Y alloys at 100 K: (a) $\text{Mg}_{99.75}\text{Y}_{0.25}$; (b) $\text{Mg}_{99.25}\text{Y}_{0.75}$; (c) $\text{Mg}_{98.5}\text{Y}_{1.5}$; (d) Mg_{97}Y_3 ; (e) Mg_{96}Y_4 ; (f) Mg_{95}Y_5 (The red, green, blue, wathet blue, and gray balls denote the HCP, FCC, BCC, ICO, and other atoms, respectively)

exhibits a clear grain boundary (the continuously arranged gray atoms are grain boundary atoms). In the $\text{Mg}_{99.25}\text{Y}_{0.75}$ (Fig. 6(b)) and $\text{Mg}_{98.5}\text{Y}_{1.5}$ (Fig. 6(c)) alloys, most of the HCP cluster atoms are interspersed in the FCC structures, and layered structures are formed, which might be related to the higher content of the FCC structure in the matrix. In the Mg_{97}Y_3 (Fig. 6(d)) and Mg_{96}Y_4 (Fig. 6(e)) alloys, layers of HCP and FCC structures are formed and interlaced with each other, which might be due to the close content of the HCP and FCC structures. In the Mg_{95}Y_5 alloy (Fig. 6(f)), the atoms are randomly arranged and no continuous arrangement of the ICO atoms occurs, which is typical of amorphous crystals. The 3D atomic snapshots reveal that the microstructure of the six Mg–Y alloys is greatly affected by the Y content, and an amorphous structure is finally formed in the Mg_{95}Y_5 alloy at a cooling rate of 0.01 K/ps.

It is well known that the stable structure of both Mg and Y at room temperature is the HCP structure. In addition, long-period stacking ordered (LPSO) structures have been experimentally found in Mg–REE–TM (where TM represents a transition metal) alloy systems [34,35]. Depending on the tacking morphology, the LPSO structures are named 6H, 10H, 14H, 18R, 24H, and so on. In LPSO structures, atomic lattices are layered following the arrangement of the HCP and FCC structures. As an example, the intact stacking sequence of the 14H LPSO structure is shown in Fig. 7. It can be seen that the 14H structure consists of five layers of HCP atoms separated by two layers of FCC atoms. Most LPSO structures are composed of a metastable phase, which in some cases may be formed directly during the solidification process of casting, while in other cases is precipitated from the matrix via solid-phase transformation through high-temperature heat treatment or hot extrusion [36,37]. Several studies have shown that rapid solidification is beneficial for the generation of LPSO

structures [38]. In the simulations, the cooling rate is fast, and the scale is not sufficiently large to clearly show grains and grain boundaries. Therefore, there exist many FCC fault structures, but a complete LPSO structure is not observed. Besides, adding Y elements to pure Mg results in a change in the local lattice energy, which promotes the formation of the FCC stacking fault structure [39]. At present, no LPSO structure has been found in binary Mg alloys. Additionally, upon addition of a small Y content, a large proportion of FCC cluster atoms appear in the Mg–Y alloys during rapid solidification. It is believed that the rapid solidification process might lead to the formation of LPSO structures in binary Mg alloys; this topic deserves future studies.

3.2 Mechanical properties

3.2.1 Stress–strain curve analysis

In order to investigate the effect of the Y element on the mechanical properties of the Mg–Y alloys, uniaxial tensile deformation tests were performed after solidification. Figure 8 shows the stress–strain curves of the six Mg–Y alloys under a uniaxial tensile deformation at 100 K with a constant strain rate of $1.0 \times 10^8 \text{ s}^{-1}$. It can be seen that the first five alloys ($\text{Mg}_{100-x}\text{Y}_x$ ($x=0.25, 0.75, 1.5, 3, 4, \text{at.}\%$)) display similar behaviors. Firstly, they pass through the elastic and plastic stages and reach the yield limit. Then, they exhibit noticeable serrated fluctuations on the stress–strain curves. The elastic deformation phase usually corresponds to dislocation nucleation and growth in the material; on the other hand, the plastic deformation phase corresponds to dislocation diffusion or slip in the material. The turning point of each peak and valley on the curve often corresponds to a structural change in the material. Among the six alloys, for a strain (ε) of 0.058, both the $\text{Mg}_{99.25}\text{Y}_{0.75}$ and Mg_{97}Y_3 alloys reach the yield limit (1.86 and 1.90 GPa, respectively). Additionally, the yield strength (YS)

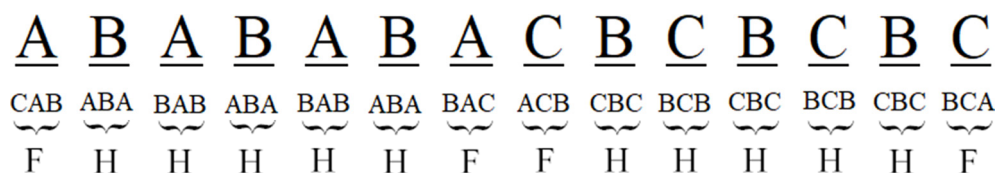


Fig. 7 Stacking sequence of 14H lattice (A, B, and C denote different atomic layers, while F and H denote the FCC and HCP structures, respectively; According to convention, the perfect FCC lattice structure is described by the three-layer atoms sequence ABCABC..., while the perfect HCP lattice structure lattice is described by the two-layer atoms sequence ABAB...)

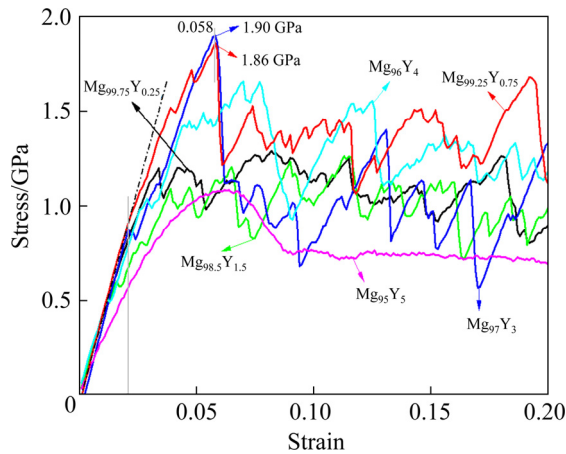


Fig. 8 Stress-strain curves of six Mg-Y alloys under uniaxial tensile deformation at 100 K with constant strain rate of $1.0 \times 10^8 \text{ s}^{-1}$

of $\text{Mg}_{99.75}\text{Y}_{0.25}$ and $\text{Mg}_{98.5}\text{Y}_{1.5}$ alloys is relatively low, which might be attributed to the presence of more defect structures. For the Mg_{95}Y_5 alloy, the stress-strain curve is slightly different, and no change is observed after reaching the yield limit, which is typical of a standard amorphous curve. Moreover, the amorphous structure is isotropic, and no noticeable grain boundary or dislocation is found; thus, the simulated stress-strain curve is relatively smooth and accompanied by a shear zone. The elastic modulus of Mg-Y alloys can be calculated from the slope of the elastic deformation state on the stress-strain curves. The elastic moduli of the six $\text{Mg}_{100-x}\text{Y}_x$ ($x=0.25, 0.75, 1.5, 3, 4, 5$, at.%) alloys are found to be 39.88, 46.94, 45.91, 47.90, 39.03, and 25.49 GPa, respectively. It is noted that the $\text{Mg}_{99.25}\text{Y}_{0.75}$ and Mg_{97}Y_3 alloys have a higher elastic modulus.

3.2.2 Evolution of main clusters under strain

Figures 9 and 10 show the structure evolution with strain and the atomic snapshots, respectively, of the FCC and HCP clusters in the $\text{Mg}_{99.25}\text{Y}_{0.75}$ and Mg_{97}Y_3 alloys at different strains during uniaxial tensile deformation.

From Fig. 8, it can be clearly observed that the elastic deformation stages of the $\text{Mg}_{99.25}\text{Y}_{0.75}$ and Mg_{97}Y_3 alloys are very similar, and a straight-line section on the stress-strain curves can be found in both cases for $\varepsilon < 0.021$. The proportion of the main crystal clusters (FCC and HCP) is slightly changed. However, some defect structures appear in the alloys, marked by the blue ellipse in Figs. 10(a₁–a₃) and 10(b₁–b₃), indicating the nucleation and growth

of dislocations at the grain boundary in the alloys to counteract the strain. During the plastic deformation stage for $\varepsilon=0.021$ –0.058, the main changes in the alloy should involve dislocation diffusion and slip. It should be emphasized that the $\text{Mg}_{99.25}\text{Y}_{0.75}$ and Mg_{97}Y_3 alloys exhibit quite different deformation mechanisms. The FCC cluster is transformed into the HCP cluster in the $\text{Mg}_{99.25}\text{Y}_{0.75}$ alloy, whereas the HCP cluster is changed into the FCC in the Mg_{97}Y_3 alloy. The red HCP split-layer atoms, as shown in Figs. 10(a₃–a₅), demonstrate the occurrence of dislocation diffusion or slip. Additionally, Figs. 10(b₃–b₅) show that some red HCP split-layer atoms are transformed into green FCC atoms.

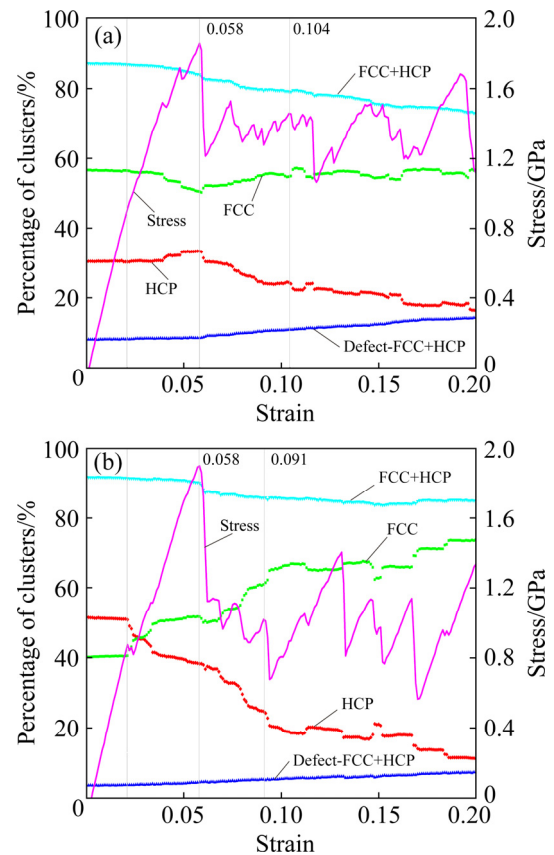


Fig. 9 Evolution of main clusters with strain during uniaxial tensile deformation: (a) $\text{Mg}_{99.25}\text{Y}_{0.75}$; (b) Mg_{97}Y_3

Nevertheless, the degree of structural change in the Mg_{97}Y_3 alloy is greater than that in the $\text{Mg}_{99.25}\text{Y}_{0.75}$ alloy. It is interesting to note that, at the yield limits ($\varepsilon=0.058$) of the two alloys, the contents of the FCC structures in the $\text{Mg}_{99.25}\text{Y}_{0.75}$ and Mg_{97}Y_3 alloys are very similar, namely 50.48% and 51.61%, respectively. For $\varepsilon > 0.058$, it can be seen that both the FCC and HCP contents increase

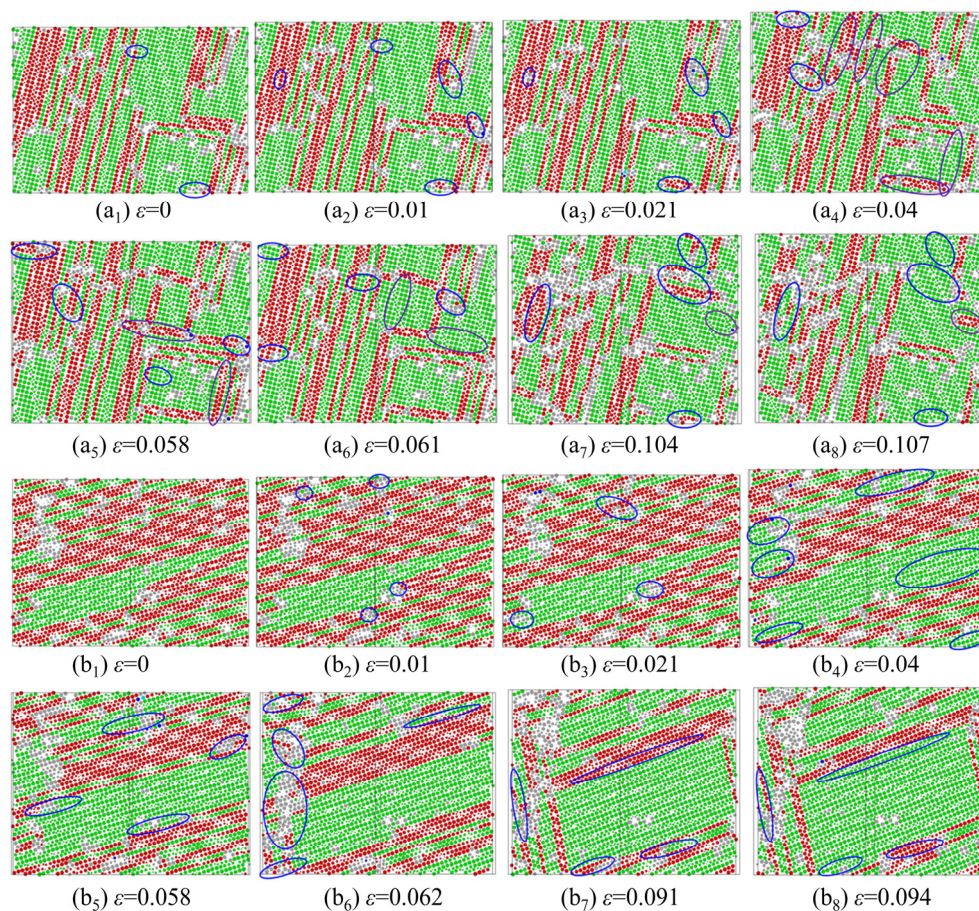


Fig. 10 Atomic snapshots of $\text{Mg}_{99.25}\text{Y}_{0.75}$ (a) and Mg_{97}Y_3 (b) alloys at different strains during uniaxial tensile deformation (The selected atomic cross section is the diagonal cut of a sample 4 Å wide along the z -axis, and the difference between the before and after photo is marked by circles; the red, green, blue, and gray balls denote the HCP, FCC, BCC, and other atoms, respectively)

and then decrease, while the proportion of defect structures increased slowly, and the total amount of the FCC+HCP structures decrease slowly.

Through the combined inspection of Figs. 9 and 10(a₅, a₆, b₅, b₆), it can be seen that the defect structure in the matrix increases suddenly as a consequence of a sudden drop in the stress. Furthermore, the conversion from HCP to FCC atomic layers is caused by dislocation slips. In the serrated fluctuation stage, the location of the turning point of each crest and trough on the stress-strain curve is often related to a structural change in the material. In this stage, the internal deformation of the alloy might involve mainly twinning and detwinning mechanisms [40] or dislocation slips and diffusion. As an example, in Figs. 10(a₇, a₈, b₇, b₈), the turning points in the $\text{Mg}_{99.25}\text{Y}_{0.75}$ and Mg_{97}Y_3 alloys are selected to show the structural change. Marked parts illustrate the presence of twinning and detwinning phenomena.

Moreover, it is worth noting that the overall content of the FCC structure in the Mg_{97}Y_3 alloy increases, and the final content reaches about 74%; on the other hand, the content of the FCC structure in the $\text{Mg}_{99.25}\text{Y}_{0.75}$ alloy does not significantly change before and after the deformation.

According to the characteristics of stress-strain curves and the atomic snapshots of the $\text{Mg}_{99.25}\text{Y}_{0.75}$ and Mg_{97}Y_3 alloys (Figs. 9 and 10), the difference in the FCC contents corresponding to different Y contents in the alloys is likely to be due to different deformation mechanisms. The YS and E values of the two alloys are close to each other, but the evolution mechanism of the main crystal clusters during the deformation process of the two alloys is different. After deformation, the FCC cluster becomes the main cluster in the Mg_{97}Y_3 alloy, while no similar change occurs in the Mg_{97}Y_3 alloy. WEI et al [41] found that the addition of Y into Mg alloys can lead to a decrease in the stacking

fault energy. From this point of view, more stacking faults in the Mg_{97}Y_3 alloy may be introduced during the deformation process because of the addition of more Y atoms. More FCC clusters and fewer defect structures are present in the final matrix of the Mg_{97}Y_3 alloy compared with the $\text{Mg}_{99.25}\text{Y}_{0.75}$ alloy. Moreover, the relaxation stress at the atomic level is a powerful driving force for structural transformations at the nanoscale [42,43]. The change in the stress relaxation at the atomic level caused by the different Y contents in the alloys might be one of the reasons behind these occurrences.

4 Conclusions

(1) The microstructure of the $\text{Mg}_{100-x}\text{Y}_x$ ($x=0.25, 0.75, 1.5, 3, 4, 5$, at.%) alloys is greatly affected by the Y content. The first five Mg–Y alloys have a high degree of crystallization; on the other hand, the FCC structure is the main cluster in the $\text{Mg}_{99.25}\text{Y}_{0.75}$ alloy, reaching the highest content of 56.65% in the final structure. However, the Mg_{95}Y_5 alloy possesses an amorphous structure. Y content for driving the amorphous transformation is in the range of 4–5 at.% at a cooling rate of 0.01 K/ps.

(2) The uniaxial tensile deformation tests show that, among the six alloys, the $\text{Mg}_{99.25}\text{Y}_{0.75}$ and Mg_{97}Y_3 alloys reach the highest yield strength of 1.86 and 1.90 GPa, respectively, and elastic moduli of 46.94 and 47.90 GPa, respectively, at a constant strain rate of $1.0 \times 10^8 \text{ s}^{-1}$ and under a strain of 0.058.

(3) The relations between the mechanical properties and the evolution of the microstructure analyzed at the atomic level indicate that the FCC structure plays a critical role in the solidification process of Mg–Y alloys. Furthermore, the difference in the FCC content caused by different Y contents leads to different deformation mechanisms.

Acknowledgments

We are grateful to the National Key Research and Development Program of China (No. 2017YFGX090043) and the Program for New Century Excellent Talents in University, China (No. NCET-12-0170) for supporting this work.

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微量钇添加对镁钇合金显微组织演化和力学性能影响的模拟

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摘 要: 采用分子动力学(MD)模拟方法研究微量 Y 添加对 $Mg_{100-x}Y_x$ ($x=0.25、0.75、1.5、3、4、5$, 摩尔分数, %) 合金凝固过程中显微组织和力学性能的影响。结果表明: $Mg_{100-x}Y_x$ 合金在室温下主要形成与单质 Mg 的 HCP 结构所不同的 FCC 晶体结构; $Mg_{99.25}Y_{0.75}$ 合金具有较多的 FCC 团簇结构, 含量最高可达 56.65%。当 Y 原子的含量增加到 5%(摩尔分数)时, 在 $Mg_{95}Y_5$ 合金中形成更多的非晶结构。 $Mg_{100-x}Y_x$ 合金的力学性能与其显微组织密切相关, $Mg_{99.25}Y_{0.75}$ 和 $Mg_{97}Y_3$ 合金具有最高的屈服强度, 分别为 1.86 GPa 和 1.90 GPa。从原子水平分析 $Mg_{100-x}Y_x$ 合金变形的机理, 发现不同 Y 含量引起的 FCC 含量的差异会导致合金不同的变形机制。

关键词: 镁钇合金; 分子动力学; 显微组织演变; 力学性能; 变形机理

(Edited by Bing YANG)