Effect of deformation conditions on compression phase transformation of AZ31

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Abstract: In this article, the compression simulation of AZ31 magnesium alloy is simulated by the molecular dynamics method. The effects of loading mode, temperature, and strain rate on the compression behavior are analyzed. The lattice distortion, mechanical behavior, structural evolution, and dislocation evolution in the compression process are deeply analyzed, and the results of different loading modes are obtained. The hexagonal close-packed (HCP) → face-centered cubic (FCC) phase transformation mechanism of AZ31 magnesium alloy during compression at temperature and strain rate, which is related to the mechanical behavior, has been studied completely. This article perfects the research on the compression behavior of magnesium alloys, excavates the application potential of magnesium alloys, and provides a new idea for improving the processing technology and developing high-performance magnesium alloys.

Keywords: plane strain compression, uniaxial compression, temperature, strain rate, phase transformation

1 Introduction

Magnesium and magnesium alloys have excellent physical and mechanical properties, high specific strength, good thermal conductivity, and some more properties. They are important and excellent materials for automotive and aerospace industry structures [1–9]. Mg–Al–Zn magnesium alloy is currently one of the most widely used magnesium alloy series [10], of which the most representative is AZ31 wrought magnesium alloy. However, the large-scale commercial application of Mg-based alloys still faces some obstacles [11–13]. To further improve the strength of magnesium alloy, it is necessary to fully understand the influence of microstructure and dislocation evolution on the strength [14]. Magnesium alloys have a hexagonal closely packed structure [15], and its deformation mechanism is closely related to stress/strain state, temperature, and strain rate. Plastic deformation still plays a key role in the strengthening of the hexagonal close-packed (HCP) phase [16,17]. Grain refinement of magnesium alloys, especially magnesium–aluminum (Mg–Al) alloys, is the most effective method to improve strength [18].

Integrated computational material engineering has become a reliable tool to establish the relationship between structure, process, and properties, which will promote the development and the application of new magnesium alloys to a great extent [19–21]. Among them, molecular dynamics (MD) simulation, as an important method in the study of plastic deformation mechanism at micro- and nano-scale in metal materials [22–25], can predict the effects of grain size, grain boundaries, stacking faults, and dislocations on the deformation behavior of materials at the atomic level [26–37]. MD simulations show that grain boundaries are the origin of dislocations in nanomaterials [38]. The nucleation and diffusion of some Shockley dislocations are caused by grain boundary (GB) deformation, that is, the position migration under the action of atomic phase transformation and stress [39,40]. Therefore, the study of dislocation evolution mechanism and phase transformation mechanism is of great significance to the total plastic deformation [41].

Rajput and Paul [42] studied the effect of uniaxial and plane strain tensile deformation on the mechanical behavior of nanocrystalline copper and found that the yield of the material begins with the nucleation of Shockley partial dislocations, and the subsequent deformation leads to the increase of dislocation line length in the material. The nucleation and diffusion of dislocations and stacking faults jointly control the strain hardening behavior of
materials. The uneven distribution of atomic strain and dislocation was observed in uniaxial and plane strain tensile deformation. Higher GB migration was observed during uniaxial tensile deformation. Vlasova [43] investigated the deformation characteristics of nanocrystalline magnesium under high-speed deformation by MD simulation. Uniaxial compression and plane strain compression (PSC) of [0001]-nanocrystalline magnesium were carried out, and the effects of loading methods on the deformation and strength properties of [0001]-nanocrystalline magnesium were investigated. Paul et al. [44] studied the deformation mechanism and pore nucleation of nanocrystalline aluminum under uniaxial and plane strain loading. Compared with uniaxial loading, nanocavities nucleate earlier under plane strain loading. Zhang et al. [45] studied the micro-mechanical behavior of Cu/Ti laminated composites during uniaxial tension and PSC by the MD method and revealed the microdeformation mechanism of closely packed hexagonal metal laminated composites.

To sum up, the compression simulation of AZ31 magnesium alloy is simulated by the MD method, the effects of loading mode, temperature, and strain rate on the compression behavior are analyzed, the lattice distortion, mechanical behavior, structural evolution, and dislocation evolution in the compression process are deeply analyzed, and different loading modes are obtained. The HCP $\rightarrow$ face-centered cubic (FCC) phase transformation mechanism of AZ31 magnesium alloy during compression at temperature and strain rate, which is related to the mechanical behavior, has been studied completely. This article studies the compression behavior of magnesium alloys, excavates the application potential of magnesium alloys, and provides a new idea for improving the processing technology and developing high-performance magnesium alloys.

2 Simulation method

The potential function is a mathematical function that describes the total energy $E$ and particle coordinates ($r$) of the model particles in the study of MD [46–49]. The modified embedded atomic method potential function can be used to calculate the pairwise interactions of various materials, which is more suitable for the calculation of metals and alloys with FCC, body-centered cubic (BCC), HCP, and diamond structures [50–56]. Eq. (1) for modified embedded atom method is given as follows:

$$E = \sum_{i} \left[ F_i(\rho_i) + \frac{1}{2} \sum_{i \neq j} \phi_{ij}(\rho_i \rho_j) \right].$$  \hspace{1cm} (1)

In Eq. (1), $E$ is the total energy of atom $i$, $F_i$ is the embedded energy and is the function of atomic electron density $\rho$, $\rho$ is the atomic electron density, $\gamma$ and $\phi$ is a pair of potential interactions, and $a$ and $b$ is the element type of atoms $i$ and $j$.

The model of AZ31 magnesium alloy was established by Atomsk [57], and the X-axis, Y-axis, and Z-axis were set to correspond to [1210], [0010], and [0001], respectively. The model is imported into large-scale atomic/molecular massively parallel simulator (LAMMPS) [58] for MD simulation. The potential function developed by Stukowski [59] can be used to study the deformation and recrystallization characteristics of Mg–Al–Zn alloy in the whole processing temperature range, and so this potential function is used for calculation. $X$, $Y$, and $Z$ are all periodic boundary conditions, constant-pressure, constant-temperature (NPT) ensemble is adopted, and the time step is 0.001 ps. The NPT ensemble and the nose-hoover thermostat maintain the stability of the entire system at constant pressure and temperature. The conjugate gradient algorithm is used to minimize the model energy to obtain the equilibrium structure at a given temperature in the NPT ensemble. Therefore, the model is first relaxed 10 ps under constant temperature and pressure, and then different deformation conditions are imposed, the deformation time is 20 ps, and the final deformation of magnesium alloy reaches 20%. The deformation Eq. (2) is expressed as follows:

$$\varepsilon = \frac{L_2 - L_1}{L_1} \times 100\%. \hspace{1cm} (2)$$

In Eq. (2), $\varepsilon$ is strain; $L_1$ is the initial length of the model in [0001] crystal direction; and $L_2$ is the length of the model compressed along the [0001] crystal direction.

The results are imported into the visualization software OVITO for analysis. Common neighbor analysis (CNA) can observe the face-centered cubic, body-centered cubic, closely packed hexagonal (HCP) structure, and other structure (GB atoms) in the metal. DXA (dislocation analysis) can determine the Burgers vector of each dislocation and identify the dislocation junction. Grain segmentation can observe the grain changes in the simulation process. Construct surface mesh can identify the cavity and calculate the cavity area [60–65].

3 Results and analysis

3.1 Influence of compression mode on phase transition

The model of AZ31 magnesium alloy with a size of 192.6 Å $\times$ 222.395 Å $\times$ 208.4 Å is established, in which
96% are Mg atoms, 3% are Al atoms, and 1% are Zn atoms. The model contains 20 grains, and the X-axis, Y-axis, and Z-axis are set to correspond to the crystal directions of $[\overline{1}2$10], [010], and [0001], respectively. Import the model into LAMMPS and then assign the potential function developed by Hyo-Sun Jang to the model. X, Y, and Z are all periodic boundary conditions, and the time step is 0.001 ps. The model energy is minimized and 10 ps is relaxed at 300 K. The change of temperature during the relaxation process is shown in Figure 1a. Keeping the size of the Y-axis model unchanged, the model is uniformly compressed 20 ps along the Z-axis ([0001] direction) at the strain rate of 0.01 ps$^{-1}$ at 300 K, and the PSC simulation is realized. The process diagram is shown in Figure 2b.

Figure 1 shows the grain change, Figure 3a shows the grain number curve, Figure 3b shows the grains at different strains under PSC, and Figure 3c shows the grains at different strains under UC. It can be seen that under PSC, the grain number is more, the grain volume is smaller, the grain refinement is more obvious, and the grain refinement occurs earlier.

Figure 2 shows parameter changes during compression. Figure 4a shows the stress–strain curve. The yield stress under PSC is 2.85 GPa, and the yield stress under UC is 1.92 GPa, which increases by 48.43%. The yield
strain under PSC is 10.2%, and the yield strain under UC is 9.6%, with an increase of 6.25%. The elastic modulus of PSC is larger, which means that PSC can improve the plasticity of AZ31 magnesium alloy. Figure 4b shows the dislocation density curve. The dislocation occurs earlier, and the dislocation density is higher in AZ31 magnesium alloy under PSC.

Figure 5 shows cavity evolution. Figure 5a shows the curve of the cavity area, Figure 5b shows the evolution of the cavity under PSC, and Figure 5c shows the evolution of the cavity under UC. It can be found that cavity appears earlier in magnesium alloys under PSC, the time of cavity appearing is almost consistent with the time of dislocation increase, and the cavity area formed under PSC is larger. Therefore, in the PSC process, because the $Y$ direction is fixed, the atomic position changes faster, forming dislocations and cavity, and at the same time, the yield stress of magnesium alloy increases.

Figure 6 shows GB evolution. Figure 6a shows the atomic fraction curve within the grain, and Figure 6b shows the atomic fraction curve of the GB. The GB diffusion of magnesium alloy occurs earlier under PSC, and the rate and degree of diffusion are higher than that of UC. Figure 6c and d are CNA diagrams of PSC and UC, respectively, in which the red atom is the HCP structure, the green atom is FCC structure, and the white atom is GB atom. It is obvious that with the increase in compression, the number of atoms in the GB increases, the GB diffuses, and the atoms of the FCC structure increase gradually, and the FCC stacking faults increase. The FCC stacking
Figure 5: Cavity evolution: (a) cavity area curve, (b) cavity evolution under PSC, and (c) cavity evolution under UC.

Figure 6: Grain boundary evolution: (a) fraction curve of GI atoms, (b) fraction curve of GB atoms (c) figure of CNA under PSC and (d) figure of CNA in UC.
fault first forms at the GB and then expands into the grain. The formation principle is as follows: due to the compression, the position of the HCP structure atom changes and becomes the GB atom. With the increase in the squeezing amount, the GB atom forms an FCC stacking fault.

Figure 7 shows structural evolution. Figure 7a–c shows the fractional curve of HCP, FCC, and BCC structure, respectively. It can be seen that the change of grain internal (GI) atoms curve is mainly caused by HCP structure and FCC structure, while the proportion of the BCC structure is very small. The structural change of PSC is earlier than that of UC, and the number of BCC atoms in PSC is slightly more than that of UC. The changes of HCP structure and FCC structure are earlier than the occurrence of plastic deformation. In the process of compression, the atoms of the HCP structure first become GB atoms. With the increase in the amount of compression, the position of GB atoms continues to change, and some atoms form FCC stacking faults. Figure 7d–f shows the evolution diagram of each structure under PSC, and Figure 7g–i shows the evolution diagram of each structure under UC. It can be seen that under PSC, the occurrence of FCC stacking fault is earlier than that of UC and the occurrence of the BCC structure is earlier than that of UC. The FCC stacking fault occurs between the HCP structure and the GB, so that the phase structure transformation of HCP → GB → FCC occurs during compression.

Figure 8 shows dislocation evolution. Figure 8a and b shows the dislocation evolution diagrams under PSC and UC, respectively. With the increase in the amount of squeezing, the atomic position changes, and the dislocation density increases. Figure 8c and d shows the dislocation density curves under PSC and UC, respectively. It is found that the dislocations in the model are mainly other dislocations and \( \{1100\} \) dislocations. Under PSC, the dislocation density in magnesium alloy is significantly higher than that in UC. This is because the Y-axis is fixed, and the atom can only move to the X-axis, resulting in more \( \{1100\} \) dislocations and other dislocations, resulting in more FCC stacking faults. The change of other dislocation density is almost the same as that of GB atom, and the change of \( \{1100\} \) dislocation is almost the same as that of FCC stacking fault. Table 1 presents the Bergson markings of common dislocations in closely

![Figure 7: Structural evolution: (a) HCP structure fraction curve, (b) FCC structure fraction curve, (c) BCC structure fraction curve, (d)–(f) structural evolution diagram under PSC, and (g)–(i) structural evolution diagram under UC.](image)
packed hexagonal crystals. Among them, $\overrightarrow{AB} \left( \frac{1}{3} \langle 1120 \rangle \right)$ is the basal complete dislocation, $\overrightarrow{TS} \langle 0001 \rangle$ is the cylindrical complete dislocation, $\overrightarrow{SA}/\overrightarrow{TB} \left( \frac{1}{3} \langle 1123 \rangle \right)$ is the incomplete dislocation, and $\overrightarrow{A\sigma} \left( \frac{1}{3} \langle 1100 \rangle \right)$ is the Shockley incomplete dislocation [66]. The strain corresponding to the increase of dislocation density is consistent with that when the atomic fraction of FCC structure begins to increase, so that there is a positive correlation between Shockley partial dislocations and FCC stacking faults.

**Table 1:** Bergson marks of common dislocations in hexagonal close packed crystals [67]

| Mark | $\overrightarrow{AB}$ | $\overrightarrow{TS}$ | $\overrightarrow{SA}/\overrightarrow{TB}$ | $\overrightarrow{A\sigma}$ | $\overrightarrow{AS}$ |
|------|----------------------|----------------------|-------------------------------|----------------------|-------------------|
| $b$  | $\frac{1}{3} \langle 1120 \rangle$ | $\langle 0001 \rangle$ | $\frac{1}{3} \langle 1123 \rangle$ | $\frac{1}{3} \langle 1100 \rangle$ | $\frac{2}{3} \langle 0001 \rangle$ | $\frac{1}{2} \langle 2203 \rangle$ |

**Figure 8:** Dislocation evolution: (a) dislocation evolution diagram under PSC, (b) dislocation evolution diagram under UC, (c) dislocation density curve under PSC, and (d) dislocation density curve under UC.

**Figure 9:** Temperature change during relaxation.
3.2 Effect of temperature on phase transition under PSC

The AZ31 magnesium alloy model with a size of $200\,\text{Å} \times 200\,\text{Å} \times 200\,\text{Å}$ is imported into LAMMPS, then the potential function is assigned to the model, $X$, $Y$, and $Z$ are all set as periodic boundary conditions, NPT ensemble is adopted, the time step is 0.001 ps, and the 10 ps is relaxed under 300–700 K, respectively. The change of temperature during the relaxation process is shown in Figure 9. Then, keeping the size of the $Y$-axis model unchanged, the PSC is realized by uniformly compressing...

Figure 10: Grain evolution: (a) grain diagram and (b) grain number curve.

Figure 11: Force energy parameter curve: (a) stress–strain curve, (b) potential energy curve, (c) volume curve, and (d) total dislocation density curve.
20 ps along the Z-axis ([0001] direction) at the strain rate of 0.01 ps$^{-1}$.

Figure 10 shows the grain evolution, Figure 10(a) shows the grain diagram, and Figure 10(b) shows the grain curve. It can be seen that the change in the number of grains is not very obvious with the change of temperature, and the number of grains at different temperatures is roughly the same. Therefore, it is speculated that temperature has little effect on grain refinement.

Figure 11 shows the force–energy parameter curve under PSC, and Figure 11a shows the stress–strain curve. With the increase in temperature, the initial stress increases, the yield stress decreases, and the elastic modulus decreases. In the PSC process, with the increase in temperature, the potential energy of AZ31 magnesium alloy increases and plastic deformation occurs more easily, so the yield stress and yield strain decrease with the increase in temperature. Figure 11b shows the potential energy curve. The higher the temperature is, the more energy is obtained and the greater the potential energy is. Figure 11c is a volume curve. With the increase in the amount of compression, the elastic deformation first occurs and the

Figure 12: Cavity evolution: (a) cavity diagram and (b) cavity curve.

Figure 13: Grain boundary evolution under PSC: (a) CNA diagram, (b) GI atomic curve, and (c) GB atomic curve.
volume decreases. When the strain reaches the yield strain, the volume begins to increase when the strain reaches the plastic stage. The higher the temperature is, the shorter the elastic stage is and the smaller the volume change is. Figure 11d shows the total dislocation density curve. With the increase in the amount of compression, the atomic position changes, and the total dislocation density increases.

Figure 12 shows the evolution of the cavity, Figure 12a shows the cavity, and Figure 12b shows the cavity curve. It can be seen that cavities appear at the same time as the yield time of magnesium alloy; so in the process of compression, cavities are generated with the change of atomic position, and at the end of elastic deformation, magnesium alloys begin to yield and enter the plastic stage, the number of cavity increases, and the area increases, increasing the overall volume of magnesium alloys.

Figure 13 shows the evolution of grain boundaries under PSC, and Figure 13a shows the diagram of CNA. It is obvious that with the increase in compression, the number of atoms in the FCC structure increases, and the number of atoms in grain boundaries increases. When $\epsilon = 10\%$, a large number of FCC stacking faults have occurred in the model. Figure 13b shows the GI atomic curve, and Figure 13c shows the GB atomic curve. It can be seen that the atomic fraction of GB decreases with the increase in compression, and the higher the temperature
is, the higher the atomic fraction of GB is. When the atomic fraction of GB increases, the strain is about 4.5% smaller than the yield strain, so the phase transformation of magnesium alloy is earlier than plastic deformation.

Figure 14 shows the structure evolution, Figure 14a shows the CNA diagram of HCP structure, Figure 14b shows the CNA diagram of the FCC structure, Figure 14c shows the CNA diagram of the BCC structure, Figure 14d shows the atomic curve of the HCP structure, Figure 14e shows the atomic curve of FCC structure, and Figure 14f shows the atomic curve of the BCC structure. It can be seen that the higher the temperature is, the earlier
the atomic fraction of HCP begins to change, and the smaller the atomic fraction of the BCC structure is. When $\varepsilon = 20\%$, the atomic fraction curve of the FCC structure tends to be smooth. The higher the temperature is, the greater the potential energy of magnesium alloy is, and the position of magnesium alloy is easier to change. The earlier the HCP structure decreases, so the higher the temperature is, the smaller the yield strength is.

Figure 15 shows the evolution of dislocations, Figure 15a shows the dislocation lines, and Figure 15b–f shows the dislocation density curves at different temperatures.

Figure 18: Force energy parameter curve: (a) stress–strain curve, (b) potential energy curve, (c) volume curve, and (d) total dislocation density curve.

Figure 19: Cavity evolution: (a) cavity diagram and (b) cavity curve.
With the increase in compression, the number of dislocation lines increases, the dislocation lines become longer, and the dislocation density increases. Among them, the dislocations with the highest dislocation densities are $\frac{1}{3}[1\bar{1}00]$ dislocations (Shockley partial dislocations) and other dislocations. With the increase in temperature, the densities of $\frac{1}{3}[1\bar{1}00]$ dislocations (Shockley partial dislocations) and other dislocations decrease. The strain corresponding to the increase of $\frac{1}{3}[1\bar{1}00]$ dislocation density is consistent with that when the atomic fraction of the FCC structure begins to increase, so that there is a positive correlation between Shockley partial dislocations and FCC stacking faults.

3.3 Effect of strain rate on phase transformation under PSC

The AZ31 magnesium alloy model with a size of $200 \text{ Å} \times 200 \text{ Å} \times 200 \text{ Å}$ is imported into LAMMPS, and the potential function is assigned to the model. $X$, $Y$, and $Z$ are all periodic boundary conditions, using NPT ensemble, the time step is 0.001 ps, and the 10 ps is relaxed at 300 K. The change of temperature during the relaxation process is shown in Figure 16. Keeping the size of the $Y$-axis model unchanged, the model was uniformly compressed 20 ps along the $Z$-axis ($[0001]$ direction) at 300 K at the strain rate of 0.001–0.1 ps$^{-1}$ to achieve PSC.

Figure 17 shows the grain evolution, Figure 17a shows the grain diagram, and Figure 17b presents the grain curve. It can be seen that there is no obvious rule in the number of grains at different strain rates, so it is inferred that the strain rate has no significant effect on the grain refinement of magnesium alloys.

Figure 18 shows the force–energy parameter curve under PSC, and Figure 18a shows the stress–strain curve. When $\dot{\varepsilon} \leq 0.01 \text{ ps}^{-1}$, the yield stress and elastic modulus increase gradually with the increase in the strain rate. When $\dot{\varepsilon} > 0.01 \text{ ps}^{-1}$, the magnesium alloy no longer yielded. Figure 18b shows a potential energy curve. The higher the strain rate is, the greater the potential energy of magnesium alloy is, and the greater the rate of potential energy increase is. Figure 18c shows a volume curve. When $\dot{\varepsilon} \leq 0.01 \text{ ps}^{-1}$, as the number of compression increases, the elastic deformation first occurs and the volume decreases, and the larger the strain rate is, the greater the rate of volume reduction is. When the strain reaches yield strain, the volume begins to increase when the strain reaches the plastic stage. When $\dot{\varepsilon} > 0.01 \text{ ps}^{-1}$, the volume decreases all the time and the decreasing rate increases with the increase in the strain rate. Figure 18d shows the curve of total dislocation density, which increases with the increase in compression. However, the change of total dislocation density of $\dot{\varepsilon} > 0.01 \text{ ps}^{-1}$ is different from that of $\dot{\varepsilon} \leq 0.01 \text{ ps}^{-1}$.

Figure 19 shows the evolution of cavities, Figure 19a shows cavities, and Figure 19b shows cavity curve. It can be seen that the time of appearance of the cavity is the
same as the yield time of magnesium alloy, and so in the process of compression, with the change of atomic position, cavity is produced, at the end of elastic deformation, magnesium alloys begin to yield and enter the plastic stage, the number of cavity increases, and the volume increases, increasing the overall volume of magnesium alloys. With the increase in the strain rate, the cavity area decreases, and when \( \dot{\varepsilon} = 0.1 \text{ ps}^{-1} \), there will be no more cavity in the model.

Figure 20 shows the evolution of the GB, and Figure 20a shows the CNA diagram. It is obvious that with the increase in the amount of compression, the number of atoms in the FCC structure increases, and the number of atoms in the GB increases. With the increase in the strain rate, the FCC stacking fault occurs later. Figure 20b shows the GI atomic curve, and Figure 20c shows the GB atomic curve. It can be seen that the fraction of GB atoms increases with the increase in compression. The higher the strain rate, the later the growth of GB atoms and the greater the growth rate, so the strain rate affects the time and degree of phase transformation. The higher the rate is, the later the phase transformation is, and the greater the degree of phase transformation is.

Figure 21 is the structure evolution under PSC, Figure 21a shows the CNA diagram of the HCP structure, Figure 21b shows the CNA diagram of the FCC structure, Figure 21c shows the CNA diagram of the BCC structure, Figure 21d shows the atomic curve of HCP structure, Figure 21e shows the atomic curve of FCC structure, and Figure 21f shows the atomic curve of BCC structure.
shows the CNA diagram of the BCC structure, Figure 21d shows the atomic curve of the HCP structure, Figure 21e shows the atomic curve of the FCC structure, and Figure 21f shows the atomic curve of the BCC structure. It can be seen that the higher the strain rate is, the later the atomic fraction of HCP begins to change. This is because the larger the strain rate is, the smaller the potential energy is, the less the atom is, and the position of the atom is not easy to change. The smaller the pore area is, the higher the strain rate is, the greater the yield strain is, and the greater the yield strength is. With the increase in the strain rate, the atomic fraction curves of the HCP structure and the FCC structure change later, while the strain phase of the BCC structure changes. The atomic fraction of the BCC structure increases with the increase in the strain rate. Therefore, the strain rate mainly affects the phase transition time and the degree of phase transformation.

Figure 22 shows the evolution of dislocations, Figure 22a shows the dislocation lines, and Figure 22b–f shows the dislocation density curves at different temperatures. It can be seen that the dislocation densities at all strain rates increase with the increase in compression. In the process of compression, the dislocations with the highest dislocation density are still $\frac{1}{3}(1100)$ dislocations (Shockley partial dislocations) and other dislocations. The strain corresponding to the increase of $\frac{1}{3}(1100)$ dislocation density is still the same as that when the atomic fraction of the FCC structure begins to increase, so there is still a strong correlation between HCP transition FCC phase transition and Shockley partial dislocations.

**4 Conclusion**

In this article, the compression simulation of AZ31 magnesium alloy is simulated by the MD method. The effects of loading mode, temperature, and strain rate on the compression behavior are analyzed. The lattice distortion, mechanical behavior, structural evolution, and dislocation evolution in the compression process are deeply analyzed, and the results of different loading modes are obtained. The HCP → FCC phase transformation mechanism of AZ31 magnesium alloy during compression at temperature and strain rate, which is related to the mechanical behavior, has been studied completely. The main results are as follows:

1) PSC can improve the plasticity of AZ31 magnesium alloy and produce more severe grain refinement, GB diffusion, and phase transformation earlier, and the dislocation density is significantly higher than that of UC.

2) The plastic deformation mechanism of magnesium alloy changes into GB diffusion due to the increase of temperature, which has no obvious effect on grain refinement and dislocation evolution. With the increase
in temperature, the potential energy of magnesium alloy increases and plastic deformation occurs more easily, so the yield stress and yield strain decrease.

3) The strain rate affects the time and degree of phase transformation. The higher the strain rate is, the later the phase transformation is, and the greater the degree of phase transformation is, the greater the yield strength and yield strain are.

4) The phase transformation of HCP $\rightarrow$ GB $\rightarrow$ FCC occurs in AZ31 magnesium alloy during compression. With the increase in compression amount, the number of atoms in GB increases, the number of atoms in GB diffuses, the number of atoms in the FCC structure increases gradually, and the number of FCC stacking faults increases. Due to the compression, the position of the HCP structure atom changes and becomes the GB atom, resulting in Shockley partial dislocations. As the squeezing continues to increase, the GB atom becomes an FCC stacking fault.

5) The phase transformation is before the specific plastic deformation in the compression process of magnesium alloy, and the yield occurs during the formation of the cavity. With the increase in the amount of compression, the elastic deformation of magnesium alloy occurs at first, the volume decreases, the atomic position changes gradually, and the phase transformation occurs. When a cavity occurs in the magnesium alloy, it begins to yield and enters the plastic stage, and the volume begins to increase.

6) There is a strong correlation between Shockley partial dislocations and FCC stacking faults. The corresponding strain when the density of Shockley partial dislocations increases is consistent with that when the atomic fraction of FCC structure begins to increase.

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