Molecular dynamics study on the deformation of void single crystal magnesium under uniaxial stress

Jinqi Tang* and Junping Yao

School of Aeronautical Manufacture Engineering, Nanchang Hangkong University, Nanchang 330063, China

*Email: 690970298@qq.com

Abstract. The uniaxial tension and compression process of single crystal magnesium model with voids along [0001] direction was simulated by using embedded atom potential and molecular dynamics method, and the micro plastic deformation mechanism of voids under tension and compression was studied. The results show that the elastic modulus of the single crystal magnesium model under compression is greater than the elastic modulus under tension, indicating that compression deformation is more difficult; In the process of plastic deformation, the dislocation, stacking fault and twin will be produced in the single crystal magnesium model under tension and compression, but the emission mechanism of dislocation is different. Tension will make the dislocation slip to the edge of the model along the direction of 45° and produce four symmetrical slip bands, while compression will produce an annular defect band near the cavity; In addition, the stacking fault area and twin type produced are also different. This asymmetry is mainly caused by the different initial deformation mechanisms under the two loading conditions.

1. Introduction

Magnesium and magnesium alloys are typical metal structural materials. With a series of advantages such as low density and high specific strength, it is widely used in aerospace, automotive and electronic consumer products and other fields [1-2]. However, there are usually complex micro defects (such as point defects, micro holes and micro cracks) in the internal microstructure of materials, and the macro failure of materials is caused by the propagation, initiation and penetration of these micro defects [3-4]. Therefore, it is very important to study the deformation propagation and failure mechanism of internal micro defects under external load. In recent years, With the rapid increase of computer operating speed and storage space, computer simulation technology has developed rapidly. Molecular dynamics simulation can observe some micro-deformation details that are difficult to obtain in experiments. These micro-deformation details can help to better understand and master the change
law of the macroscopic morphology of matter. Therefore, molecular dynamics methods are often used when studying the physical and chemical properties of substances. [5].

So far, scholars at home and abroad have conducted a large number of studies on the effect of voids on the properties of different materials using molecular dynamics methods. Poeimiche G P [6] conducted a molecular dynamics study on the growth and aggregation of single crystal nickel voids, and analyzed the influence of material length on the destruction process of single crystal nickel. The results showed that the length dimension of the sample changed the dislocation mode. Tang et al. [7] studied the pore growth and pore aggregation in single crystal magnesium, and the results showed that the model size and temperature have a significant effect on the deformation of the pores. Zhao [8] established a single crystal copper model with columnar cavities using molecular dynamics methods to simulate the growth and evolution of columnar cavities. The results show that for a given porosity, the cell size has a significant effect on the initial yield strength. Mi et al. [9] simulated aluminum alloy materials with multiple voids and found that the distribution of large voids into small voids would increase the load-bearing capacity of the sample; No obvious dependence of void fraction evolution on void coalescence is observed.

In summary, domestic and foreign researchers have used molecular dynamics methods to study metal materials containing voids and have achieved many valuable results. However, most researchers only study materials in tension or compression. There are few comparative studies on the effects of tension and compression on the plastic deformation of crystals, and there is no report on the mechanism of tension and compression plastic deformation of single crystal magnesium containing voids. In order to understand the microscopic plastic deformation mechanism of metal materials more comprehensively, this paper takes the hexagonal close-packed single crystal magnesium as the research object to study the influence of tension and compression on its microplastic deformation mechanism.

2. Atomic model and calculation method

2.1 establish atomic model

Figure 1 shows the tensile and compressive stress-strain curves of the single crystal magnesium model along the [0001] crystal direction, a cubic single crystal magnesium model with side length of L = 20 nm was established for uniaxial tension and compression simulation. At the same time, a sphere with radius of 2.5nm is deleted from the center of the cube to form a void defect, forming a single crystal magnesium model with void defects. As shown in Fig 1, the total number of atoms in the system is about 350000, and the two dark parts of the model are simplified spherical voids. The xyz coordinate axes are [1120], [1100] and [0001] respectively. Considering the influence of boundary effect on the simulation, the periodic (PPP) boundary conditions are adopted in the xyz direction of the model. The simulation time step is 1 fs. In order to make the results of the stretching simulation closer to the actual situation, before the uniaxial stretching simulation, the conjugate gradient method is used to minimize the system energy, relax 50,000 steps, and then perform an isothermal and isostatic system on the single crystal magnesium model with voids Comprehensive (NPT) stretch. The model was simulated with an average strain rate of 2×10^9s^-1 and a temperature of 100K.
2.2 Calculation method
In order to study the tensile and compressive deformation mechanism of the single-crystal magnesium model with voids, the large-scale molecular dynamics simulation software Lammps was used. The interaction between the metal mg atoms was described by the embedded atomic potential (EAM) developed by Sun et al. [10] The total potential energy $E$ of the entire system composed of atoms is expressed as follows:

$$E = \sum_i G_i \left( \sum_{j \neq i} \rho_j^0 (r_{ij}) \right) + \frac{1}{2} \sum_{ij} U_{ij}(r_{ij})$$  \hspace{1cm} (1)

In the formula, $G_i$ is the function density of the local electron; $\rho_j^0$ is the electron density; $U_{ij}$ is the pair potential; $r_{ij}$ is the distance between the $i$ atom and the $j$ atom. At the atom, the dipole force $\beta_{km}^i$ is as follows:

$$\beta_{km}^i = \frac{1}{\Omega^i} \sum_{j \neq i} f_k^i (r_{ij}) \cdot \vec{r}_{ij}$$  \hspace{1cm} (2)

In the formula, $f_k^i$ is the force between atoms; $\vec{r}_{ij}$ is the displacement between atom $i$ and atom $j$; $N$ is the number of nearest neighbor atoms; $\Omega^i$ is the atomic volume. The stress tensor is determined as the volume average of the entire material block:

$$\sigma_{mk} = \frac{1}{N^*} \sum_i N^* \beta_{mk}^i$$  \hspace{1cm} (3)

In the formula, $N^*$ is the number of active atoms, indicating the directional component.

3. Simulation results and analysis

3.1 Stress-strain curve analysis
Fig 2 shows the tensile and compressive stress-strain curves of the single crystal magnesium model along the [0001] crystal direction. It can be seen from the figure that the overall stress change trend of the two curves is roughly the same, but the slope of the curve and the highest point of the curve are
different. There are differences between the two curves in the elastic deformation stage, and the slope of the curve along the z-axis compression is larger, which indicates that the compressive elastic modulus of the single crystal magnesium model is greater than the tensile elastic modulus along the z-axis compression, which also indicates that the single crystal magnesium model is more difficult to deform than the tensile model along the z-axis compression.

![Stress-strain curves](image)

**Fig 2** Stress-strain curves of single crystal magnesium model in tension and compression

### 3.2 Atomic configuration

The change trend of stress-strain curve mainly depends on the microstructure evolution of the crystal. In order to better understand the micro deformation mechanism in the process of void tension and compression, the microstructure evolution process of the crystal during uniaxial tension was analyzed combined with the stress-strain curve.

Fig 3 shows the dislocation analysis diagram when the single crystal magnesium model is stretched along the z-axis. Fig 3(a) shows the microstructure when the crystal is in the elastic deformation stage, that is, the corresponding strain $\varepsilon \leq 0.052$ stage. In addition to the structural changes of the atoms on the surface of the cavity, the atoms in the other crystals still belong to the perfect hexagonal close packed structure, and there are no dislocation, slip and other defects, but the distance between the atoms has a slight change, and the model can still return to the original shape when unloading. Fig 3(b)-(e) shows that the model has undergone plastic deformation. In Fig 3(b), the strain $\varepsilon=0.054$, the crystal reaches the yield strength. Due to the effect of stress concentration, the stress reaches the dislocation emission condition, and the dislocation begins to nucleate near the cavity. As the strain increases, it is observed that the dislocation starts to be emitted along the direction of about 45° from the horizontal plane of the cavity. A large number of dislocation emission is the main reason for the decrease of the stress-strain curve, and with the emission of dislocations, defect atoms (white atoms) continue to increase. In the stress-strain curve, it can be seen that there is a plateau period of stress in a-b segment. This is because at this stage, the slip band expands to the crystal surface, and the dislocation emission reaches the edge of the model, as shown in Fig 3(c). At this time, the strain $\varepsilon=0.060$, resulting in dislocation accumulation, which causes the overall stress to remain unchanged temporarily. After reaching b, the accumulated dislocations continue to emit, and the stress begins to
decrease. Moreover, in the figure, it is also found that stacking faults lead to the hcp (red atom) → fcc (green atom) phase transition, but the phase transition accounts for a small proportion relative to the dislocation, which indicates that the dislocation is easier than the phase transition in the tensile process of single crystal magnesium along the [0001] direction. When the strain reaches $\varepsilon=0.068$ in Fig 3(d), it can be observed that twins appear in the model, and then the twins continue to grow; when the strain is $\varepsilon=0.120$ in Fig 3(e), most of the crystals are occupied by twins.

Fig 3 Dislocation analysis diagram of single crystal magnesium model when stretched

Fig 4 shows the dislocation analysis of the single crystal magnesium model when compressed along the $z$-axis. In Fig 4(a) $\varepsilon \leq 0.056$ shows the microstructure of the crystal in the elastic deformation stage. Similar to the elastic deformation stage of tension, the distance between atoms only changes slightly, and the model can still return to its original shape when unloading. But the difference between the two is: the effect of stretching the single crystal magnesium model is to make the cavity elongate in the stretching direction, while compression makes the size of the cavity elongate in the vertical compression direction. Similarly, Fig 4(b)-(h) shows that the model has undergone plastic deformation. In Fig 4(b), the strain $\varepsilon=0.060$, the model reaches the yield strength. Due to the effect of stress concentration, the stress reaches the dislocation emission condition, and the dislocation begins to nucleate near the cavity; However, there is no dislocation extending to the edge of the model around the cavity, but a ring-shaped defect region (white atom) appears around the cavity, as shown in Fig 4(e), which is observed along the $z$-axis. Moreover, there is also a phase transition from hcp (red atom) → fcc (green atom) caused by atomic stacking faults. In Fig 4(c) $\varepsilon=0.065$, the ring defect atom has developed to the edge of the model, the single crystal magnesium model reaches the strength limit, and the stress begins to decrease. With the increase of strain, the stacking fault area caused by compression increases gradually, and is much larger than that caused by tension. As shown in Fig 4(d), the stacking...
Fault area reaches the maximum, and the thickness of stacking fault development at the edge of the model can be observed in Fig 4(f). Further compression, twins can be observed at the edge of the model, as shown in Fig 4(g). After that, the twins grow up, but they do not extend to the cavity and only expand at the edge of the model, as shown in Fig 4(h). From the dislocation analysis at the end of tension and compression, Fig 3(e) and Fig 4(h) can clearly see that the twin types produced by the single crystal magnesium model are different.

Fig 4 Dislocation analysis diagram of single crystal magnesium model during compression

4 Conclusion
1) In the process of tension and compression of single crystal magnesium, the change trend of the stress-strain curve is similar, but the elastic modulus and yield stress of the model during compression are greater than the elastic modulus and yield limit during tension, indicating that compression deformation is more difficult. 2) The yield stress of the material in compression is much greater than that in tension. This asymmetry is mainly caused by the different initial deformation mechanisms under the two loading conditions.
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