Molecular dynamics simulation of pore-containing single crystal magnesium stretching along different crystalline orientations

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Abstract. The uniaxial stretching process of single crystal magnesium containing holes was simulated by molecular dynamics method, and the influence of the stretching crystal orientation on the growth and deformation of the holes was studied. Tensile simulations of different crystal orientations show that the microscopic mechanism of void growth and deformation in single crystal magnesium was different. For the orientation of the \([1\bar{2}10]\) crystal, there will be small holes in the crystal at first, and with the process of loading, the polymerization of large and small holes will make the holes grow and then lead to the failure of the material. For the \([0001]\) crystal orientation, the deformation mechanism was different from the former. In the early stage, it was caused by dislocation movement and stacking fault deformation, while in the later stage, it was mainly caused by twin nucleation and growth.

1. Introduction
The nucleation, growth and coalescence of pores are the main reasons for the fracture of metallic materials (such as metallic aluminum and magnesium) [1-4]. Once the hole nucleates from the nonmetallic inclusion or at the interface between the particle and the matrix, subsequent failure continues through the growth and coalescence of the hole [2]. Therefore, it is of great scientific significance to study the microplastic deformation mechanism of hole-containing metals. Aghababaei R et al. [5] used molecular dynamics simulation method to simulate the magnesium single crystal with initial ideal defect structure. The analysis shows that the extension along the C axis of the defective crystal produces incomplete slip on the cone surface, followed by twinned crystals and base dislocation. Zu Q et al. [6] Molecular dynamics simulation is employed to study the tension and compression deformation behaviors of magnesium single crystals with different orientations. The simulation results show that the initial defects usually nucleate on the free surface, but the initial plastic deformation and subsequent microstructure evolution are different due to different loading directions. Poeimiche G P [7] conducted molecular dynamics studies on the growth and aggregation of pores in single crystal nickel, and analyzed the influence of material length on the destruction process of single crystal nickel. The results showed that the specimen length scale changes the dislocation pattern Tang et al. [8] studied the void growth and void aggregation in single crystal magnesium, and the results showed that the model size and temperature have a significant effect on void deformation.

In summary, molecular dynamics method has been used to study the microscopic plastic deformation mechanism of materials, and fruitful results have been achieved. However, most researchers have studied only one crystal orientation or heterogeneous crystal orientation. And there
are few studies on low symmetry crystal structure with HCP. In order to understand the microplastic deformation mechanism of materials more comprehensively, this paper simulates the tightly arranged hexagonal single crystal magnesium, stretches the model in different crystal orientations, and studies its microplastic deformation mechanism in detail.

2. Molecular dynamics calculation method
Molecular dynamics is a method of simulating the interaction between microscopic particles to determine the trajectory of particles based on Newton's law of motion. The research object of molecular dynamics is an atomic system. The movement of each particle in the system obeys Newton's three laws, and the interaction between particles will satisfy the superposition principle. The trajectory of particles in the system is calculated using Newton's equation of motion, which can represent the position and velocity of particles that change with time.

2.1. Forces between atoms
Potential function is needed in molecular dynamics simulation to determine the interaction between atoms. Therefore, the correct selection of the potential function is the first step in the simulation. Embedded Atomic Method (EAM) is a commonly used potential function. This article uses the EAM potential function developed by Sun., and its expression is as follows

\[ E = \sum_i G_i \left[ \sum_{j \neq i} \rho_{ij}^{\alpha} (r_{ij}) \right] + \frac{1}{2} \sum_{i,j} U_{ij} (r_{ij}) \]  

Where \( G_i \) is the function density of the embedded energy and the local electron; \( \rho_{ij}^{\alpha} \) is the average atomic electron density on the sphere; \( U_{ij} \) is the pair potential; \( r_{ij} \) is the distance between the atom \( i \) and \( j \). In molecular dynamics, energy is used to determine the force acting on each atom. At each atom, the dipole force \( \beta_{im}^i \) is given by:

\[ \beta_{im}^i = \frac{1}{\Omega_i} \sum_{j \neq i} f_{ij} (r_{ij}) r_{im}^j \]  

Where \( f_{ij} \) is the force vector between atoms; \( r_{im}^j \) is the displacement vector between \( i \) atoms and \( j \) atoms; \( N \) is the number of nearest neighbor atoms; \( \Omega_i \) is the atomic volume. Since the stress tensor can be determined as the volume average value on the material block, the similar formula is as follows

\[ \sigma_{mk} = N^v \sum_{i} \beta_{im}^i \]  

Where \( N^v \) is the number of active atoms that generate stress in the lattice and represents the orientational component. The average stress is used to determine the uniaxial stress-strain response.

2.2. Periodic boundary conditions
In the process of molecular dynamics simulation of actual crystals, the surface of the model will have an adverse effect on the movement of atoms in the structure. To avoid this effect, periodic boundary conditions are generally used. Periodic boundary conditions can eliminate surface effects, so it is suitable for systems with a large number of atoms. In addition, when the boundary atom moves away from the model, a new atom replaces the disappearing atom.

3. Establishment of calculation model
Single crystal magnesium is a hexagonal close-packed (hcp) crystal with a lattice constant \( a=b=0.321 \text{nm} \), \( c=0.521 \) and axial ratio \( c/a=1.62 \). The plastic deformation of single crystal magnesium is mainly slip, but due to the limited number of slip systems, twinning also plays an important role in the plastic deformation of single crystal magnesium [9].
In this paper, based on the LAMMPS molecular dynamics simulation method, the uniaxial tensile simulation of single crystal magnesium containing holes is carried out, and different influencing factors are studied. Figure 1 is a single crystal magnesium model with holes. It is a cube with a side length of 13, and the dark color in the middle is a spherical hole. The number of atoms in the entire model is about 10,000. Periodic boundary conditions (PPP) are used in all three orientations to eliminate surface effects. The intercalation potential is used to express the interaction between magnesium atoms.

![Figure 1. Single crystal magnesium model with holes.](image)

Before the uniaxial tensile loading simulation, the conjugate gradient method is used to relax the system to reach the minimum energy state (the ground state). The simulation time step is 1 fs, the average strain rate is \( 2 \times 10^{-9} \text{s}^{-1} \), and the temperature is 100 K. Uniaxial tensile loading is performed on the model. The simulated atomic trajectory information file is visualized by OVITO. Use dislocation analysis method (DXA) to observe defects such as dislocations, stacking faults, and slip bands in crystals.

4. Results and analysis

In order to study the effect of loading crystal orientation on the mechanical properties of single-crystal magnesium, this paper carried out uniaxial tensile loading on crystal orientation \( x-[\overline{1}2\overline{1}0] \) and the \( z-[0001] \) crystal orientation (\( x-[\overline{1}2\overline{1}0], y-[\overline{1}100], z-[0001] \)), and analyzed its stress-strain curve and atomic configuration.

Figure 2 shows the stress-strain curves of the two crystalline orientations. Due to the asymmetry of the structure of magnesium, the curves are quite different. It can be seen that the yield strength of \([0001]\) crystal orientation is 4.43 GPa (\( \varepsilon = 5.94\% \)) greater than that of the \([1\overline{2}10]\) crystal orientation 3.14 GPa (\( \varepsilon = 6.18\% \)). In addition, the initial slope of the \([0001]\) crystal orientation simulation is also greater than that of the \([1\overline{2}10]\) crystal orientation, that is, the elastic modulus of the \([0001]\) crystal orientation is greater than that of the \([1\overline{2}10]\) crystal orientation. It can be seen that the dislocation nucleation stress in the \([0001]\) crystal orientation is greater than the \([1\overline{2}10]\) crystal orientation.
Figure 2. Tensile loading stress-strain curves of two crystal directions.

Figures 3 and 4 are the dislocation analysis diagrams of the [1210] crystal orientation and [0001] crystal orientation model at several moments before and after plastic deformation. It can be seen from Figure 3a that at this time the strain $\varepsilon \leq 4.8\%$ (point A), the model reaches the maximum elastic deformation, and the tensile strain does not exceed the critical value of dislocation emission, so there is no initiation of dislocation slip. Figure 3b–d show that the crystal has begun to undergo plastic deformation. As the strain increases, the model enters the plastic deformation stage, and more point defects appear on the surface of the hole. When the strain continues to increase, as shown in Figure 3b at $\varepsilon = 6.12\%$ (point B), the hole is slightly elongated in the tensile orientation and the dislocation nucleates on the surface of the hole. When strained $\varepsilon = 6.66\%$, the dislocation line grows, and a small hole appears on the right side of the hole. As the strain $\varepsilon = 6.84\%$ increases, the large pores and small pores aggregate during the strain, leading to further failure of the material.

Figures 3. Stretched atomic configuration diagram of [1210] crystal orientation

(a) $\varepsilon = 4.8\%$; (b) $\varepsilon = 6.12\%$; (c) $\varepsilon = 6.66\%$; (d) $\varepsilon = 6.84\%$.

It can be seen from Figure 4a that the strain at this time strain $\varepsilon \leq 5.52\%$ (point A’), except for the structural change of the atoms on the surface of the hole, the atoms inside the crystal still belong to the perfect hexagonal close-packed structure, and there are no defects such as dislocations and slippage. The model can still be restored to its original shape. Figure 4b–d show that the crystal has begun to undergo plastic deformation. In Figure 4b strain $\varepsilon = 6.18\%$ (point B’), the dislocations inside the crystal begin to nucleate near the holes. As the strain increases, it is observed that the dislocations are sliding to the model surface. At the same time, FCC crystal structure atoms and $\frac{1}{3}<1100>$ incomplete dislocations are generated in the process, resulting in stacking faults inside the crystal; in

![Figure 3](image-url)
the strained $\varepsilon = 8.28\%$ figure c, the crystal begins to appear twins, and then the twins continue to grow; when strained $\varepsilon = 10.74\%$, the lower half of the entire model is occupied by twins.

5. conclusions

1) The elastic modulus and yield strength of the $[0001]$ crystal orientation are larger than that of the $[1\bar{2}10]$ crystal orientation, and the dislocation nucleation stress in the $[0001]$ crystal orientation is greater than the $[1\bar{2}10]$ crystal orientation. The reason is that the critical decomposition shear stress (CRSS) of cylindrical or conical slip is much higher than the base slip and is not easy to be activated.

2) The microscopic plastic deformation mechanism of the $[1\bar{2}10]$ crystal orientation is mainly that small holes appear inside the crystal, and then as the loading progresses, the large and small holes aggregate to make the holes grow and cause the material to fail. 3) The microplastic deformation of the $[0001]$ crystal orientation is caused by the movement of dislocations and the growth of stacking faults and twins.

Acknowledgments

This work was supported by the National Natural Science Foundation of China (51164027, 51661024) and the Key Science and Technology Project of Jiangxi Provincial Department of Education (GJJ14502).

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