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Influence of pore size on the plastic deformation of c-axis-compressed magnesium single crystals

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Abstract

The molecular dynamics method is used to establish a single crystal model of magnesium with different void sizes. Uniaxial compression along the c-axis is carried out at 300 K. Combined with the stress–strain curve, potential energy curve and dislocation density curve of the four models, the compression mechanical energy and structural evolution process of a single crystal of magnesium with different hole sizes are analysed. Results show that when the radius of the single spherical void is large, the elastic modulus is small, the yield stress is low, the potential energy value is large, and the absolute value is small, such conditions facilitate deformation. When the hole radius is small, complete closure under c-axis compression requires minimal time and deformation.

1. Introduction

Magnesium alloy exhibits good lightness, cutting, corrosion resistance, shock absorption, dimensional stability and impact resistance and is thus far superior to other materials [1–7]. These characteristics make magnesium alloys widely applicable to many fields. For example, magnesium alloys are commonly used in computers, consumer electronic products, high-speed rail, medical rehabilitation equipment and other fields [8–16]. The crystal structure of a magnesium alloy is a typical dense six-sided crystal that features minimal sliding. Its grains do not easily produce macro yields, and it easily generates large stress concentration.

Therefore, from a microscopic perspective, studying the hole defects of magnesium alloys will have positive effects. It will enrich the understanding of the evolution law of magnesium alloy microdefects, guide magnesium alloy processing and improve the performance of magnesium alloys. Numerous scholars at home and abroad have actively explored the theory and law of hole evolution. Xu Qian et al [17] established a dense six-sided titanium single crystal model according to molecular dynamics research methods to simulate the plastic deformation mechanism of a prefabricated hole closure. Kim et al [18] studied the structural evolution of magnesium nanocrystals in the stretching process on the basis of molecular dynamics; their results indicated that only extruded twins are produced in the crystal boundary under low stress and that compression twins are produced in the crystal boundary and inside the grain under high stress. Babak Kondori et al [19] studied the accumulation of damage in a rolled, partially annealed magnesium alloy by using synchronous radiation tomography, they observed and recorded a large number of pores in the nucleation, growth and aggregation stages, which are reminiscent of the most malleable and resilient metal materials. Tian Tang and Sungho Kim [20] studied pore growth and coalescence mechanism by using one-pore and two-pore samples with the same initial pore volume fraction. GROH [21] used a molecular dynamics method to simulate the stretching of magnesium single crystals and revealed the dependence of the strain rate, temperature and orientation of crystals on the damage evolution defined by pore growth. Huang Kaixin [22] studied the plastic deformation pattern of the twin crystal interface of magnesium with prefabricated holes at different strain rates. Liu Zhao [23] simulated the uniaxial compression of single crystal magnesium in the directions of c-axis and vertical c-axis and

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comparatively analysed the slip and dislocation properties in the stress–strain curve and microscopic deformation.

In view of the large number of holes in the inner hole of magnesium alloy, the current work proposes to study the micromodel of the evolution of the inner hole of magnesium alloy to reveal the variation law of the hole in the forming process. This work also aims to explore the microstructure of magnesium alloy under different hole sizes and determine its deformation mechanism. The results are expected to provide guidance in the processing of magnesium alloy.

2. Model building and simulation methods

The molecular dynamics method is used to study the influence law of hole size on the plastic deformation of magnesium monocrystalline. This study establishes four models through Atomsk software (figure 1).

Figure 1(a) shows a perfect single crystal model without holes, and figures 1(b)–(d) present a magnesium monocrystalline model with single holes with diameters of 1, 2 and 3 nm. The prefabricated holes are located in the hexagonal bodies inside the model. Hence, the model was cut along (100), as shown in figure 1. In this figure, the red colour represents the perfect tight-knit six-sided structure, and the grey colour represents the defect structure. The dense cubic system usually uses a four-axis coordinate system. Therefore, in the Cartesian coordinate system used in the modelling, the x, y and z coordinates correspond to the model’s [1210], [1010] and [0001] crystal directions. The z-axis corresponds to the c-axis of the magnesium monocrystalline model, and the three-way are periodic boundary conditions to effectively reduce the impact of the boundary effect (figure 2). The model size is 9.63 nm × 16.68 nm × 15.64 nm, and the numbers of atoms are 108 000, 107 817, 106 535 and 103 087. The potential function among the Mg atoms is the EAM (Embedded Atom Method) [24] potential function established by Wilson and Mendelev in 2016; this function is a variation of the simulated potential function of Sun et al [25]. The total potential energy of the system is:

\[
U = \sum_i F_i(\rho_i) + \frac{1}{2} \sum_{j=1}^{\infty} \phi_{ij}(r_{ij})
\]

where \(F_i\) is the embedded energy function; \(\rho_i\) is the sum of the density of the electron cloud produced at i by all atoms, except the i atom; \(\phi_{ij}\) is the function of the potential action between the i atom and the j atom; \(r_{ij}\) is the distance between the i atom and the j atom.

Simulation process: The simulation temperature of the model was controlled at 300 K, and the magnesium single crystal model atoms were fully relaxed (30 ps) using NPT ensemble to ensure that the simulation system reached the equilibrium of specified temperature before loading and had sufficient time to reach the minimum state of energy. Then, the strain rate of 1010 s\(^{-1}\) is compressed uniformly along the z-axis with a time step of 0.001 ps until the total strain reaches 20%. In the simulation process, the stress, total energy, potential energy, kinetic energy and atomic coordinate position of the atom in all directions are recorded every 100 steps. The calculation process is carried out using the Lammps program, and visualisation is performed in Ovito software.

3. Effect of nanohole size on the c-axis compression of magnesium monocrystalline

3.1. Effect of hole size on compression stress-strain curve of magnesium monocrystalline

Figure 3 shows the influence of the hole size of a nanohole on the plastic behaviour of a single crystal of magnesium. The yield strength of the effect is obvious, and the impact on elastic mode is small. The analysis of the stress–strain relationship indicates that in the early stage of compression for elastic deformation, stress linearly increases, and the grid arrangement of a single crystal of magnesium remains unchanged. With increasing strain, the single crystal of magnesium enters the plastic deformation stage. The hole not only changes the local stress state but also reduces the critical stress required for dislocation nucleation and emission. The
single crystal of magnesium without holes can withstand great deformation, and the maximum stress of a yield point is 8.69 GPa. With the increase of hole diameter, the corresponding degree of deformation and the stress value of the single crystal of magnesium at the yield point decrease. When the pore diameter is 3 nm and the strain is 7%, the maximum yield stress is 4.89 GPa. The larger the hole diameter is, the higher the stress value is in the stable stage; however, the difference is small. After the yield point, the stress strain–curve of the magnesium single crystal with c-axis-compressed holes is flatter than that for the defect-free condition. The existence of the hole enhances the plasticity of the magnesium single crystal to a certain extent. As the bond breaks between the atoms on the surface of the preformed hole and the adjacent atoms, the coordination number of the atoms is different from that of the other atoms in the model. Thus, the surface of the hole is equivalent to the free boundary condition, which contains certain surface residual energy. In this case, the model contains a certain amount of prestress when the strain is 0.

As the actual metal material contains numerous gaps, impurities and other defects, the molecular dynamics model makes a defect-free idealisation hypothesis on the metal material crystals. The only error is caused by the atomic scale modelling and the simulation of the atomic scale of a small number of atoms. Hence, the
metamorphic stress obtained by the numerical molecular dynamics simulation is 1–2 orders of magnitude larger than the stress measured by the macro-image experiment.

3.2. Effect of hole size on the potential energy–strain property of magnesium monocrystalline under compression

Figure 4 shows the potential energy and strain diagram of holes with different diameters. According to figure 3, in the elastic deformation stage, the average spacing of atoms decreases with the increase of strain. Thus, the system’s potential energy increases. When the yield critical point is reached, the dislocation or twin is produced by the plastic deformation of the magnesium single crystal, and the potential energy of the system gradually decreases and then becomes stable. Figure 4 shows the single hole of the magnesium single crystal with a hexahedral centre; the larger the diameter of the hole is, the greater the potential energy is. The potential energy curve of the defect-free magnesium single crystal changes rapidly and presents a sharp peak when it enters the plastic stage. The energy curve lift process of the single-hole magnesium single crystal with a prefabricated single-hole centre is relatively smooth and moderate. This result is consistent with the trend of the stress–strain curve changes. As shown in the single-hole magnesium single crystal with a hexahedral centre (figure 4), the larger the radius of the spherical hole is, the greater the value of the potential energy, the smaller the absolute value, and the smaller the change of potential energy.

3.3. Common neighbour analysis (CNA)

Near-neighbour analysis based on local crystalline structure is used to visualise atoms (figure 5). The red colour represents the complete dense arrangement of six-sided structural atoms, the grey colour represents the surface and unrecognised structural atoms, the blue colour represents the body-centred cubic atomic structure, and the green colour represents the surface-centred cubic atomic structure. The smaller the radius of the prefabricated spherical single hole is, the shorter the time required for complete closure under c-axis compression, and the smaller the deformation. When the degree of deformation reaches 5%, the model with a hole radius of 1 nm collapses severely while the other two models collapse to a lower degree; all three models show changes in atomic structure and a body-centred cubic atomic structure. The model with a 1 nm hole radius has the minimum number of atoms with atomic structural change, whereas those with a 3 nm hole radius has the largest number of such atoms. When the deformation degree reaches 8.75%, the model with a 1 nm hole radius completely collapses. When the deformation reaches 10%, the model with a 2 nm hole radius completely collapses. Figure 5 shows that when the strain is less than 5% in an area far from the prefabricated spherical hole, the atomic structure is enough to maintain a perfect and tight six-sided structure. Overall, the crystal structure does not change greatly, and the prefabricated hole remains spherical. With the increase of strain, the single crystal model of magnesium with preformed holes gradually reaches the yield point, and the preformed spherical single hole gradually collapses or even completely closes under the action of c-axis compression. This result is due to the atoms in the inner edge of the hole being rearranged constantly to release strain energy and emit dislocation, thereby forming a disordered region. The propagation speeds of spherical holes in different directions vary, thus leading to the uneven change of the inner edges of the holes.

The co-neighbour analysis can visually observe the distribution of various atomic structures under different deformation levels and generate data on the number of atomic structures in the system structure for quantitative

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Figure 4. Potential energy strain curve.
analysis. Figure 6 shows the number of atomic structures with different hole radii. The numbers of BCC, FCC, HCP, ICO and unknown structures with different hole radii are calculated. Figure 6 shows that the HCP structure in the four compression models of magnesium single crystal first changes into an unknown structure. When the stress variable reaches the yield strength, the BCC and FCC structures begin to appear, and the number tends to be stable after the stress is stable. The magnesium single crystal model without preformed holes rises slowly after the HCP structure suddenly decreases and finally reaches equilibrium. The magnesium single crystal model with different radius sizes has a relatively smooth process of HCP structure decreasing to equilibrium. The comparison shows that the larger the hole radius is, the smoother the change trend of the HCP.

Figure 5. Structure characterization of deformed nanocrystals by CNA.

Figure 6. Number diagram of atomic structures with different hole radius.
structure quantity is. The other structure increases sharply after the yield point, and the corresponding number tends to be stable after the stress is stable; however, the number of holes is inversely proportional.

3.4. Radial distribution function analysis

The radial distribution function can represent the particle distribution probability in space with distance changes. In the molecular dynamics simulation process, the ordering degree of a crystal dot matrix structure can be characterised by analysing the radial distribution function. Figure 7 shows the radii of different holes. The c-axis-compressed magnesium single crystal model is not compressed after relaxation and should be variables 5%, 7.5%, 8.75% and 10% of the radial function distribution. The four c-axis-compressed magnesium monocrystalline models at the end of the process are not compressed, and they show a long-range order and obvious curve fluctuations at long distances. With the increase of deformation degree, the curve fluctuation slows down and presents obvious and regular peaks at a distance. The radial distribution function after reaching the strain corresponding to the maximum yield point gradually slows down and even disappears at a long distance. The magnesium single crystal model without prefabricated holes does not reach the maximum yield point under the deformation condition of the c-axis compression reaching 10%. Therefore, its radial distribution function is still shown as a strong long-range order. As the simulation progresses, the first peak of the four magnesium monocrystalline models shifts to the left and presents a certain degree of widening. As the hole radius size increases, the offset and the degree of width gradually decrease. This result is explained as follows. The first adjacent atom of the dense six-sided crystal structure is at 2.90 Å, containing 12 atoms; the second nearest atom is at 3.2 Å. As a result of the vibration shift, the two peaks partially overlap and widen. As the degree of deformation increases, the atoms move relatively, and the crystal structure gradually transforms into a body-centred cubic structure with 8 atoms, with the first nearest-neighbour atom at 2.84 Å. The height of the first peak decreases, and the width increases due to the decrease of the coordination number.

3.5. Dislocation density analysis

The dislocation density is the ratio of the total length of the crystal inline misalignment to the solid volume v, i.e.

\[ \rho_d = \frac{l}{V} \]  

Figure 8 shows the change of dislocation density under different hole radii. In the process of the molecular dynamics simulation of the magnesium single crystal model under the compression effect, the atomic spacing

Figure 7. Change of radial distribution function under different hole radius.
gradually decreases, and the potential energy increases. When the yield point is reached, non-stop atomic lattice fractures, recombination and misalignment are observed. This result is due to the presence of a stress concentration area in the edges of the prefabricated hole. Such feature greatly reduces the stress required for sliding, and the prefabricated hole provides the simulation material a large internal space. In this case, the simulation material becomes easy to use in the process of molecular dynamics simulation. Figure 8 shows four dislocation types in the molecular dynamics simulation of the four magnesium single crystal compression models: \( \frac{1}{3} \langle -110 \rangle \) dislocation, \( \frac{1}{3} \langle 1120 \rangle \) dislocation, \( \frac{1}{3} \langle 1123 \rangle \) dislocation and \( \langle -110 \rangle \) dislocation. Other dislocations are not easy to identify. The deformation degree of the magnesium single crystal model with prefabricated holes is significantly reduced relative to that of the magnesium single crystal model without defects. The maximum bit misalignment density of the magnesium monocrystalline model containing prefabricated holes is larger than that of the non-defective magnesium monocrystalline model. The total bit misalignment density of the magnesium single crystal model containing prefabricated holes increases sharply and decreases sharply, followed by a jagged rise. The larger the radius of the hole is, the smaller the first peak of the total dislocation density is, and the larger the width of the peak is.

4. Conclusions

The molecular dynamics simulation method is used to calculate the plastic deformation process of spherical single-hole magnesium single crystal models with different radii and obtain the relationship between stress and potential energy and strain changes. Ovito software is used to visualise the different atomic structures corresponding to different strains and to calculate the numbers of different atomic structures, radial distribution functions and densities of various dislocations under different strains. After the statistical analysis of the data, relevant discussions are carried out, and the following conclusions are derived:

1. The effect of nanometer hole radius on the plastic behavior, especially the yield strength, of magnesium single crystal is very obvious and the impact on elastic modulus is small. When the hole radius is large, the degree of deformation and the stress value corresponding to the magnesium single crystal at the yield point are small, the potential energy is high, the absolute value is low, and the potential energy changes only slightly, the results are expected to provide guidance in the processing of magnesium alloy.
(2) According to the nearest–neighbour analysis method according to the local crystalline analysis of atoms, the smaller the radius size of the prefabricated spherical single hole is, the less time required for complete closure under the c-axis compression action, and the smaller the amount of deformation will be.

(3) According to the analysis of the dislocation extraction algorithm, the deformation degree of the magnesium single crystal model with prefabricated holes is significantly reduced relative to that of the magnesium single crystal model without defects. The larger the hole radius is, the smaller the first peak of the total dislocation density is, and the larger the peak width will be.

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