Molecular dynamics simulation of temperature effect on void propagation in Magnesium single crystal

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Absrtact: The propagation and fracture process of void in magnesium single crystal at the nanoscale have been investigated using molecular dynamics simulation and embedded atom method at different temperature. The results show that the temperature has a significant effect on the potential energy and yield strength of the system, the system potential energy and yield strain increase with the increase of temperature. When the temperature is 100K, the plastic deformation mode of the specimen belong to mainly dislocation movement. And the plastic deformation belong to mainly dislocation movement and a small amount of base plane slip at 300K. Furthermore, the plastic deformation is mainly non basal surface slip at 500K.

Introduction

Magnesium alloys have the characteristics of small density and excellent cutting processing, etc. There are expected to become the third largest metal material to replace steel and aluminum alloy. Microscopic hole is one of the important defects of the material, which affects its mechanical properties to a certain extent. The evolution of defects will lead to material fracture failure. Therefore, it is necessary to study the fracture mechanism of microscopic holes. In recent years, Luo et al [1]. simulated the effect of hole defects on the nucleation of shear bands of metallic glass by means of molecular dynamics methods. Studies have shown that hole defects can indeed lead to nucleation of non-uniform shear bands of metallic glass. Zhang et al [2]. simulated the effect of hole density of nickel single crystals on the shrinkage mechanism of holes based on molecular dynamics. The results show that the density of holes can affect the yield strain of nickel single crystals. The higher the hole density, the higher the shrinkage rate of nickel single crystals. Tang et al [3]. used molecular dynamics methods to simulate the expansion and fracture mechanism of single-crystal γ-TiAl nanopores. The results show that the generation of dislocation nucleus and the propagation of shear rings expand the pores.

In summary, most scholars have used molecular dynamics methods to conduct various researches on nano-scale pores under different materials and achieved many high-level results. However, the mechanism of pore expansion of Mg single crystals has not been reported from the nanoscale. In this paper, the molecular dynamics simulation software LAMMPS (Large-scale Atomic Molecular Massively Parallel Simulator) [4] was used to perform visual processing using OVITO to study the fracture process of magnesium single crystals with central pores at the nanometer scale.

Atomistic model and stress calculation

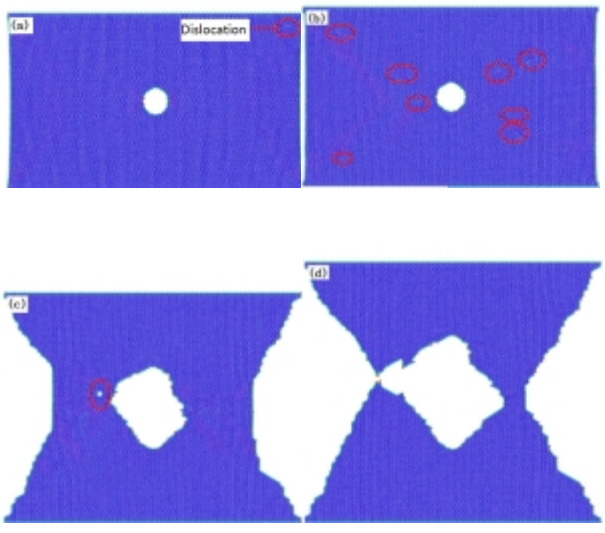
Magnesium has a close-packed hexagonal structure (*hcp*), the lattice constants at room temperature are: $a=b$=3.21Å, c=5.21 Å, and the axial ratio c/a=1.62. The model ruler (X×Y×Z) is $80a\times80b\times3c$. Remove some atoms in the center of the model and get a hole with a diameter of 3 Å. The total number of atoms is 76,932, and the crystal orientations of the three coordinate axes are respectively X—[1 $\bar{2}$ 1 0], Y—[1 0 $\bar{1}$ 0], Z—[0 0 0 1].

A 2a-thick surface layer atom is fixed at the top and bottom boundary for applying the load. In order to eliminate the boundary effect, the displacement of the left and right boundary in the X direction is set to zero. Periodic boundary condition was used in the Z direction, and the X and Y directions are nonperiodic boundary conditions.

In all simulations, energy minimization and relaxation with 10,000 time steps were performed to bring the total energy of the system into equilibrium before the uniaxial tensile load was applied. Subsequently, a uniaxial tensile load was applied in the Y direction. The tensile strain rate was $4\times10^{9}s^{-1}$, and the tensile simulation was performed until the specimen broke. The time step for the entire simulation was set to 1*fs*, and the NVT ensemble was used to control the temperature during stretching.

Simulation results and discussion

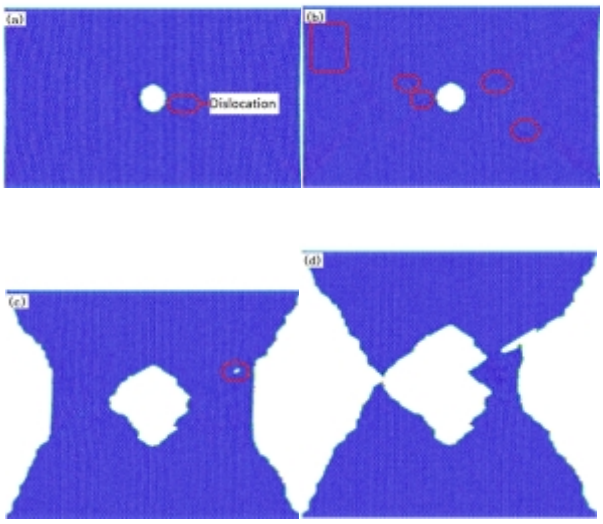
Analysis of Atom Configuration During Stretching. Fig. 1, Fig. 2 and Fig. 3 are the corresponding atomic configurations of three different temperature. When the temperature is 100K.At 3.4% of strain, dislocation nucleation occurred on both the boundary angle and the left and right sides of the hole, and the first dislocation was emitted in the upper right corner of the boundary, as shown in Figure 1(a). At 4.6% of strain, the sample contains 8 dislocations (red circled part), and the dislocations emitted from both sides of the hole and the boundary angle move relative to each other, as shown in the fig 1(b). At 33.8% of strain, the holes continued to expand, and the atoms on the upper and lower boundaries contracted inward. The dislocations of the relative motions met at the left end of the hole to form a vacancy defect (red defect), as shown in Fig. 1 (c). At 58% of strain, the specimen finally shows a neck-type fracture, as shown in Fig. 1 (d).



(a)ε=0.034 (b) ε=0.046 (c) ε=0.338 (d) ε=0.52

Fig. 1 Atomic configuration of different strain corresponding to 100K

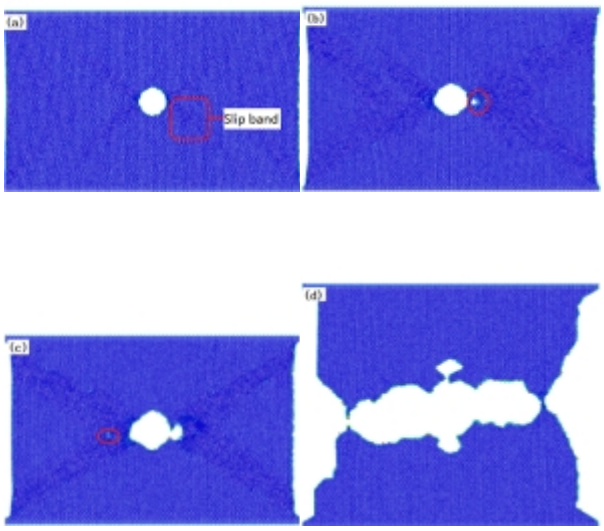
When the temperature is 300K.At 4.2% of strain, the first dislocation is emitted first on the right side of the hole, as shown in Fig. 2(a). At 5% of strain, the sample contains 4 dislocations, and the number of dislocations is significantly reduced compared to the temperature of 100K, but a small number of basal slip bands are generated (the red rectangle is a slip zone, and the red circle is a dislocation. Because the critical shear stress of the base slip system is smaller than the critical shear stress of the non-basal surface, the base slip is easier to start and there is no obvious deformation of the hole, as shown in Fig. 2(b). At 34.4% of strain, the dislocations on the right side of the hole meet to form a vacancy defect (red circled portion), as shown in Fig. 2(c). At 56.8% of strain, because of the atomic anisotropy, the left side of the specimen is necking-type fracture. The strain at break and the strain at 100K fracture are about the same, because the effect of low temperature and room temperature on the fracture toughness of the material is relatively small, such as Fig 2(d) shows.



(a)ε=0.042 (b) ε=0.05 (c) ε=0.344 (d) ε=0.568

Fig. 2 Atomic configuration of different strain corresponding to 300K

When the temperature is 500K. At 5.8% of strain, only the non-basal slip zone appeared in the whole specimen, because the critical shear stress of the non-basal slip system decreases greatly with increasing temperature, resulting in the critical point of the non-basal slip system, as shown in Fig. 3(a). At 7.6% of strain, a vacancy defect appears on the right side of the hole, and the strain when the vacancy defect occurs is significantly smaller than that when the vacancy defect occurs at 100K and 300K, as shown in Fig. 3(b). At 10% of strain, the vacancy defect on the right side of the hole is connected with the hole, and the vacancy defect on the left side of the hole is formed. As shown in Figure 3(c). At 41.6% of strain, the specimen finally showed a double-cup fracture, and the strain at break was the smallest among the three. The reason for this was that the temperature increased and the vacancy defects increased. Under the effect of external forces, vacancy defects would be easier to follow along, as shown in Fig. 3(d).



(a) ε=0.058 (b) ε=0.076 (c) ε=0.1 (d) ε=0.416

Fig. 3 Atomic configuration of different strain corresponding to 500K

Conclusions

1) Temperature has a significant effect on the potential energy and yield strength of the system. As the temperature increases, the potential energy and the yield strain increase, but the yield strength decreases.

2) The plastic deformation mechanism of the specimen changes with temperature. The plastic deformation is mainly dislocation movement at a temperature of 100K, dislocation movement at 300K and a small amount of basal slip, and non-basal slip at 500K. The higher the temperature is, the more slip is easier to start and the dislocation movement is inhibited.

Acknowledgements

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References

[1] Luo Yun，Yang Guan-nan，Shao Yang，Yao Ke-fu. The effect of void defects on the shear band nucleation of metallic glasses[J].Intermetallics.94 (2018) 114-118.

[2] Zhang Yan-yiu, Jiang Shu-yong, Zhu Xiao-ming, Zhao Ya-nan. Influence of void density on dislocation mechanisms of void shringkage in nickel single crystal based on molecular dynamics simulation[J]. Physica E.90 (2017) 90-97.

[3] Tang Fu-ling, Cai Hou-min, Bao Hong-wei, Xue Hong-tao, Lu Wen-jiang, Zhu Liang, Rui Zhi-yuan. Comput[J]. Mater.Sci.84(2014)232-237.

[4] Plimpton S J. Comput[J]. Phys.117(1995)1-19.http://lammps.sandia.gov/.