Molecular dynamics simulation of the effects of temperature on the microscopic deformation of single crystal magnesium containing a void and a crack

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Abstract: Mechanical properties of a material are intensively influenced by the presence of flaws. While temperature is the significant factor of the deformation. An embedded atomic potential function is used to simulate the micro-defect deformation behavior under different temperatures loading in HCP Mg with various defects. Defects consisting of a fixed distribution of void and an edge crack. The results of the simulation were analyzed by the stress-strain curve and atomic trajectory diagram. The results show that the tensile deformation behavior of single crystal magnesium with defects changes obviously with temperature. Increases in temperature lead to decreased peak stress and ascending crack propagation speeds, and toughening the material to fracture ultimately. But the increase of crack-propagating speed is not obvious when the temperature is above 600K. The time that the crack extends to the void and in combination with it at low temperature is delayed as compared to that at high temperature.

1. Introduction

One consequence of the crack-void interaction is the changes of the stress field around the crack tip. The voids can change the effective stress intensity factor in the close proximity of the crack tip due to the different location and the separate distance [1] S. Chandra et al. [2] investigated the crack shear behavior of face-centered cubic aluminum in no defects or defects with random vacancy distribution under I type loading. The interaction between the crack tip and the cavity changes the stress concentration at the crack tip, and the increase of the content of the cavity leads to the increase of the passivation at the crack tip, the decrease of the crack growth rate, which will make the material fracture limberly. Liu et al. [3] studied the crack-cavity interaction in α-iron at the nanoscale, and considered three different crack-cavity samples. It is found that the increase of temperature leads to the reduction of the dislocation nucleation stress, and the crack propagation becomes blunt after deflection. Yashiro [4] et al. carried out various molecular dynamics simulations of cracks, including prismatic cracks and pyramidal cracks in HCP-Mg, and found that different crack types are adapted to different deformation modes while loading. Tang et al. [5] investigated the fatigue crack propagation behavior of magnesium single crystal, showing the crystal orientations have a big influence on fatigue crack growth. Crack-propagating also affected by other crystalline defects like vacancies, interstitials and clusters, which changed the stress field around the crack tip by reducing or amplifying the crack tip stress intensity factor [6]. Musazadeh et al. [7] studied the effects of the material types and shapes of the inclusions on the crack-propagating in Ni nanocrystals. Their studies indicated that the shape of the inclusion has an intensive influence on crack-propagating, while the material types of the inclusion
show no significant effect on the crack growth.

The defects performance of the microscopic particle has a significant effect on the single crystal material especially at different temperatures. However, there is no report on the deeper level of the defecting performance of the microscopic particle with different temperatures. The molecular dynamics simulation based on embedded atomic method have advantages for the research of the defects analysis characteristics. In terms of studying the mechanism of action and defects analysis characteristics, it can satisfy the study of the microscopic deformed mechanism of single crystal Mg. In this paper, 4 different temperatures are studied through molecular dynamics, and the stress-strain curve and atomic stress fields are obtained by analyzing the crack growth rates and defect evolution.

2. Calculation method and model

The crystal structure of Mg single crystal is HCP, its atomic structure is shown in figure 1. The three crystal directions [1 2 1 0], [1 0 1 0], [0 0 1] are corresponded as the x, y, z axis direction. According to the characteristics of crystal structure, the lattice constant is set as a = 3.2094 Å, c = 5.2105Å. The Figure 2 is the initial atomic model of molecular dynamics simulation and its corresponding geometric model. The model’s size is 54a * 21a * 32c, and there're a total of 86153 atoms in the system. The (0 0 1) [1 2 1 0] crack is established on the edge of the model by eliminating the inter-atomic forces. The length of the crack is 9a. The x direction is set as the extended direction of the crack. In addition, a spherical void with a radius of 4.5a was added in the model, and its location is 2a offset the center of the model by the opposite direction of x axis. The model would be loaded along the z-direction. In the simulation process, the speed loading mode with one end fixed and the other end stretched was adopted. In order to study the influence of temperature on the micromolecular deformation of single crystal magnesium containing void and crack, the model was simulated under the conditions of different temperatures as 150K, 300K, 450K and 600K respectively. The simulation process is divided into relaxation and loading stages. The model will be relaxed for 400ps under the NVT ensemble to make the system balance before loading firstly. The three directions of the model will be set as free boundary condition. After the relaxation process, the loading stage starts. The loading stage will run 60000 steps under the NVE ensemble, and use the Velocity Scaling Method to control the temperature. Besides, the simulation system’s time step will be set as 1 fs, the stretching speed as 0.2 Å/ps. The embedded atomic method (EAM) can express the inter-relationship of metal atoms. It can be divided into two portions; one is the interacting pair potential energy and the other is the embedded energy. The total potential energy of the crystal can be formulated as:

$$U = \sum_i F_i (\rho_i) + \frac{1}{2} \sum_{i \neq j} \Theta_{ij} (r_{ij})$$

(1)

In the formula, the first item $F_i$ is embedded energy; the second item $\frac{1}{2} \sum_{i \neq j} \Theta_{ij}$ is pair potential; $\rho_i$ is the sum of the electron cloud density formed on the location of $i$th atom by all the extranuclear electrons except the $i$th atom. $\Theta_{ij}$ is the interaction potential function between the $i$th atom and the $j$th atom; $r_{ij}$ is the distance between the $i$th atom and the $j$th atom. In this experiment, EAM potential function is used to describe the interaction between atoms, and Velocity-Verlet algorithm is used to solve the trajectories of atoms. In this paper, open source LAMMPS is used for simulation, and visualization software OVITO is used to process and analyze the simulation results.

![Fig.1 Atomic model of Magnesium single crystal](image-url)
3. Results and discussion

Figure 3 shows the stress-strain curves of magnesium single crystal atoms at different temperatures. The chart present that the stress increases sharply in the elastic deformation stage and then decreased when moving into the plastic deformation phase, and fluctuated stably finally. In this experiment, a constant temperature was used for stretching, and the model was relaxed to the corresponding temperature before each stretching, and two layers of atoms in the top and bottom are fixed, so the initial stress is different under different temperature. The higher the temperature is, the more severe the initial atomic motion is. When the atoms of an ideal infinite crystal without external loads were placed in equilibrium position, the atomic stress is zero. But for single crystal magnesium with free surfaces, which losing adjacent atoms in space and forming fractured bonds due to that the atoms on the surface have different ligancies than the inside. Then the atoms on surface are out of balanced because the symmetry is broken. The atoms departure the equilibrium position of the original ideal lattice and caused the tension on surfaces when the model relaxed. Therefore, the stress value of the crystal is not zero at the beginning of the stretching. Before ε=0.06, it corresponds to the elastic deformation stage of single crystal magnesium. In this stage, with the increase of temperature, the stress under the same strain condition decreases, so does the peak stress. It can be seen that the temperature affects the properties of the material on the elastic deformation stage mainly. with the strain continues to increase, the curve of the stress descends sharply due to the intensely decrease of interatomic forces, and the material move on to the stage of plastic deformation.

The statistic of energy, stress and strain of the system were calculated by LAMMPS software. The
calculation results are processed by Ovito software. The Ovito software is used to get the motion trajectory of the atom at the temperature of 150K, 300K, 450K and 600K respectively. The following figures show four characteristic moments on the process of stretching.

Fig.4 Microscopic defects evolution of Mg single crystal at T=150K: (a) t=29ps, (b) t=98 ps, (c) t=170ps, (d) t=509ps.

In the figure, the color from green to red represents that the stress increases in turn. According to Fig.4a, 4b, 4c and 4d, the stress is concentrated at the crack tip in the process of crack propagation, and there arise the phenomenon that the sub-crack spread from the parent-crack. The figure.4 (a) shows that at t=29ps the stress value is larger than the interaction force of the atoms, Stress concentration appears at the crack tip and the void, the crack started to fissure. At t=98ps, the crack tip appeared a large stress concentration, so did the center of void and the right side of the model. This moment the stress level of the whole model is approaching to the maximum. The crack started to extend in the direction of [ 1 2 1 ]. Shown in Fig.4c are the dislocations that nucleating from the model. This moment the integral stress value descended to a lower level rapidly during a short time. The crack tip became large and rounded due to the partial strong strain. From previous evolution diagram of atomic defects, the nucleation of dislocations can gather energy then lead to the reduction of stress, while the accumulation of dislocations can release energy and lead to the increment of stress. The centralization of stress result in producing sub-cracks. The stress reduced at the time that the sub-cracks combined with the main crack. Such process repeated a period of time until the material fractured. In the plastic deformation stage of the crystal, the stress is fluctuant, and the speed of descending slowed down gradually with the increases of temperature. Then some cracks began to arise around the void. Finally, at t=509ps, it is obvious that the model’s main crack did not combined with the sub-crack, which is due to the fact that the single crystal of magnesium has few slip systems start at a low temperature. We can also see sub-crack propagation phenomenon near the void.

Fig.5 Microscopic defects evolution of Mg single crystal at t=325ps: (a) T=150K, (b) t=300 K, (c) t=450K, (d) t=600K.

The Fig.5 shows the different changes of the model in different temperatures at t=325ps. From Fig.5(a) to Fig.5(c), the areas of the void get larger one by one. That means the crack and void growth rates are affected by temperature. And the crack and void growth rates get faster when the temperature
increases as we observed from the first three picture in Fig.5. but the propagation rate did not get faster when the temperature add up to 600K as compared to t=450K. so the excessive temperature also can restrain the propagation of crack.

4. Conclusions
(1) The elastic modulus and yield strength of the [1 2 1 0] crystal orientation at low temperature is larger than that at high temperature. And the peak stress of the material decreases when temperature increases.

(2) The stress configuration is changed by the join of void, the crack tip becomes blunted when the void added, so a higher strain is required for further crack extension. The appearance of blunted crack tip result in decreasing speeds of crack extension.

(3) The crack extension and void growth rates are intensely affected by the temperature due to the substantially different plastic deformation forms of the crack tip at different temperatures. This increase in crack-propagating speed is pronounced as the temperature goes up. But the excessive temperature can restrain the propagation of crack to some extent.

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