Effect of secondary orientation on micromechanical properties of nickel base single crystal superalloy

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Abstract. In this paper, the mechanical properties and microstructure evolution of Ni based single crystal superalloy with different secondary orientations under stress loading were studied by molecular dynamics (MD) simulation. The MD model is a supercell structure established with three-dimensional cubic mosaic units, and the volume fraction of the γ′ precipitated phase is 65%, which is similar to the structure of the actual material. The effect of secondary orientation on the tensile properties of superalloy was analyzed on the atomic scale, and the mechanism of the secondary orientation on tensile deformation and fracture was discussed systematically. The work in this paper will be helpful to understand the tensile deformation behavior of superalloy from an atomic point of view.

1. Introduction
Nickel base single crystal superalloy has become the main material for turbine blade of advanced aviation gas turbine engine due to its excellent comprehensive properties [1-2]. Anisotropy is an intrinsic property of single crystal metal materials. Therefore, the mechanical properties of single crystal superalloy such as tensile, durability, creep, and fatigue all show obvious anisotropy. In aero-engines, the principal stress axis under working conditions is usually parallel to the [001] orientation of single crystal turbine blades, which is also the preferred direction for its fastest growth. However, in the process of single crystal growth, it will be affected by many factors, and it often does not grow in strict accordance with the [001] direction. We call the angle deviating from [001] as primary orientation, while the deviation in the horizontal plane perpendicular to [001] as secondary orientation. At present, many scholars have studied the orientation of superalloy. Zhao et al. [3] prepared AM3 single crystal superalloy with orientations [001] and [011], and found that the primary crystal orientation also affects the primary dendrite arm spacing. The study of the orientation and temperature dependence of the stress fracture properties of nickel-based superalloy single crystals shows that at 760-871°C, the stress fracture life of crystals oriented near [001] and [111] is significantly improved. In contrast, single crystals
oriented near [011] exhibit extremely short lifetimes. As the temperature increases, the influence of orientation on the superalloy decreases [4-5].

With the development of computer, the research efficiency can be greatly improved by using the method of simulation [6]. Many researchers have studied the mechanical properties and damage mechanisms of superalloy through atomic-scale MD simulations. Zhou et al. [7] used the mega parallel three-dimensional MD method to simulate the system of 35 million atoms and studied the mechanical behavior of plastic fracture on the atomic scale. Terentyev et al. [8] studied the propagation and passivation behavior of metal cracks in BCC and FCC under different strain rates, temperatures and crack shapes. The results show that molecular dynamics is an effective method to study the initiation and propagation of micro cracks.

Most of the previous researches focused on primary orientation, while the secondary orientation was less researched, and the tensile strength and influence mechanism of nickel-based single crystal superalloy are still not clear. In view of the above background, this paper takes the simplified model of nickel based single crystal superalloy as the main research object, and uses MD as the research method to simulate the influence of different secondary orientation on the tensile strength of nickel based single crystal superalloy, and explains the deformation and fracture mechanism of nickel based single crystal superalloy under tensile load.

2. Models and methods

Ni based cast superalloy are usually composed of two basic phases, the matrix phase and the strengthening phase. The main component of the γ phase is Ni, which has a FCC structure, and the lattice constant of γ is 0.352nm. At the same time, the same sample with Ni3Al as strengthening phase also has a FCC structure, and the lattice constant of γ’ is 0.3567nm. The structure of γ’ phase is similar to γ phase, and the lattice constants are almost the same.

In this study, in order to simulate the characteristics of superalloy, as shown in Figure 1, we set up two components of γ and γ’ according to actual situation, and embedded the 6 * 6 * 6 γ’ phase into the 7 * 7 * 7 γ’ phase to establish the mosaic model. The cell contains 1689 atoms and the volume fraction of γ’ phase in the model is in the range of 60 ~ 70%, which is in line with the actual situation.

![Figure 1 Cell model of nickel base single crystal superalloy](image)

The experimental model of molecular dynamics was obtained by extending the obtained γ / γ’ supercell according to the proportion of the actual stretching workpiece. As shown in Figure 2, the whole model consists of 90 unit cells (γ phase and γ’ phase) and it contains 152010 atoms.
In this paper, MD simulations are carried out with the LAMMPS software and the potential function is EAM. Periodic boundary conditions are applied in XY direction and aperiodic boundary conditions are applied in Z direction.

In this MD simulation, we conduct a z-direction uniaxial tensile test on the model. Before the external loading we need to let the system be relaxed, the time step is 1 fs, and the ensemble is NVT, then run 50000 steps until the system reaches equilibrium. The temperature is kept at 300K, the initial pressure is zero-stress state, and then the pulling force is gradually applied to stretch until it breaks. The Verlet algorithm is used to solve Newton's equation of motion, and the uniaxial stretching process is carried out in NPT ensemble.

3. Results and discussion

3.1 Effect of secondary orientation on tensile properties

As shown in Figure 3, the simulation results of different secondary orientations against tensile strength (a) and low cycle fatigue test results (b) [9] are compared. Since there is no completely relevant literature data, fatigue life can also be used as a measure of mechanical properties, so preliminary comparison is made between them for a while.

It can be seen that the secondary orientation has a great influence on the mechanical properties of nickel base single crystal superalloy: in the range of 0°-20°, the tensile strength of the nickel-based single crystal superalloy first decreases and then increases, and reaches the lowest point when the secondary orientation is 5°. In the range of 20°—60°, the tensile strength of the nickel-based single
crystal superalloy fluctuates with the change of the secondary orientation angle. In the range of 60°-90°, the tensile strength of the nickel-based single crystal superalloy reaches the lowest point when the secondary orientation is about 70°. When the secondary orientation is 90°, the tensile strength is basically the same as when the secondary orientation is 0°. We speculated that due to the symmetry of the unit cell model of the nickel-based single crystal superalloy in the XOY plane, the secondary orientation is the same when the secondary orientation is 0° and 90°.

Regarding the change law of tensile strength with secondary orientation, the analysis reasons are as follows. No matter at room temperature or high temperature, there is the activation of the octahedral slip system during the stretching process. The included angle of the slip direction is 60°, which causes the material to be more likely to break at about 30° and 60°, so it will show a tendency to fluctuate around this angle.

3.2 Evolution of microstructure during stretching

Figure 4 shows the microstructure evolution of Ni based single crystal superalloy with secondary orientation of 0° at room temperature under primary orientation (001), in which the green part is the FCC structure, the red part is HCP structure and the white part is amorphous structure. It can be seen that with the tensile process, the strain of the single crystal superalloy model increases gradually, and the material phase structure undergoes a certain transformation, from the orderly FCC structure to the HCP structure and the amorphous structure, and also the degree of amorphous in the fracture zone is higher. However, for 760°C, due to the more intense atomic vibration at high temperature, the structure is transformed into amorphous earlier, and the effect is not as good as that at room temperature. There is still a problem of simulation distortion, which needs to be solved in the field of computational science.

When the elongation is 1%, the deformation of the material occurs, and a certain proportion of HCP structure begins to appear in the microstructure. When the elongation increased to 5%, the proportion of HCP phase increased by 3%. When elongation increased to 15%, it reaches its maximum value of 7.9%. Then, with the increase of elongation, voids appear in the simulated structure and grow rapidly, resulting in rapid failure of the material. Therefore, in this simulation, we think that the tensile strength at 15% elongation can be defined as the tensile strength of the material.
In addition, according to the latest research report by Koglin [10], based on in-situ observation, the damage and failure of the material are attributed to the formation of a large number of cavities, which is also consistent with the MD simulation results.

4. Conclusions
In summary, the secondary orientation of nickel-based single crystal superalloy will have a certain impact on its mechanical properties. In terms of tensile strength, it is affected by the octahedral slip system. The tensile strength of the secondary orientation of 30° and 60° is lower than the other secondary orientations and easier to fracture.

In the aspect of micro morphology, the ordered FCC structure in Ni based single crystal superalloy will be transformed into HCP structure or disordered amorphous structure during the tensile process. The degree of amorphization increases with the increase of strain. The deformation mechanism is dislocation twinning and large-scale amorphization, which is an important reason for the formation of voids and the expansion of voids to the surrounding area, resulting in the fracture of the material.

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