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Molecular dynamics study of mosaic structure in the Ni-based single-crystal superalloy*

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The mosaic structure in a Ni-based single-crystal superalloy is simulated by molecular dynamics using a potential employed in a modified analytic embedded atom method. From the calculated results we find that a closed three-dimensional misfit dislocation network, with index of $\langle 011\rangle\{100\}$ and the side length of the mesh 89.6 Å, is formed around a cuboidal γ' precipitate. Comparing the simulation results of the different mosaic models, we find that the side length of the mesh only depends on the lattice parameters of the γ and γ' phases as well as the γ/γ' interface direction, but is independent of the size and number of the cuboidal γ' precipitate. The density of dislocations is inversely proportional to the size of the cuboidal γ' precipitate, i.e. the amount of the dislocation is proportional to the total area of the γ/γ' interface, which may be used to explain the relation between the amount of the fine γ' particles and the creep rupture life of the superalloy. In addition, the closed three-dimensional networks assembled with the misfit dislocations can play a significant role in improving the mechanical properties of superalloys.

Keywords: Ni-based single-crystal superalloy, mosaic structure, molecular dynamics simulation
PACC: 6185, 6170N, 6155H

1. Introduction

Since their introduction in the early 1980's,[1,2] Ni-based single-crystal superalloys have been widely used as turbine aerofoil materials in jet engines and industrial gas turbines to increase the turbine inlet gas temperatures so as to improve the thermal efficiencies. It is well known that these alloys can be optimized by a series of thermal heat treatments which produce the precipitation of $L1_2$ ordered coherent γ' particles embedded in a face-centred-cubic (fcc) γ matrix. The shape of the precipitates is cuboidal with roughly $\{100\}$ faces and they are approximately aligned along the common $\langle 100\rangle$ directions. The crystal structures of the fcc γ matrix (Ni) and the $L1_2$ γ' precipitate (Ni_3Al) are shown in Fig.1.

In order to increase the strength of the initial simple Ni–Cr–Al–Ti alloys, adding other elements that can be brought into substitutional solid solution has been used to strengthen the matrix phase and to increase the volume fraction of γ'. It is found that in modern single-crystal superalloys, the γ' volume fraction can reach 70% or even higher, and the γ' precipitate-particle size of about 0.45μm appears to be optimum for the yield strength and creep strength, and also for hot hardness.[3,4]

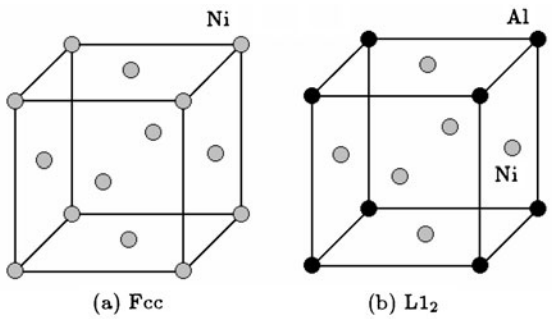

Fig.1. Crystal structures of (a) γ and (b) γ'.

For the similar fcc structure of both γ and γ', the microstructures containing the γ' precipitates coherent with the γ matrix will form in the course of heat treatment, which means the formation of 'mosaic structure'.[3,4] Since the mechanical properties are strongly dependent on the morphology of the γ' precipitates, it is important to investigate the configuration of the mosaic structure, which can be a great

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help for further understanding of the physical mechanisms responsible for the better creep resistance of the Ni-based single-crystal superalloy.

Molecular dynamics (MD) is a powerful tool in material researches and can provide an atomistic view of the deformation process.[5,6] This method has been developed to enable studies of the properties of material volumes containing millions to billions of atoms with effective interatomic potentials. Many physical properties such as the lattice parameter, cohesive energy, elastic constants, phonon-dispersion relations, point defect behaviour, phase diagrams, stacking fault energies, surface structure, reconstruction and energy, etc., are well reproduced in this method.[7,8] In the present paper, the MD method is used to simulate the mosaic structure of cuboidal γ' precipitate in a pure γ matrix, or the idealized γ/γ' structure in a Ni-based single-crystal superalloy.

2. Modelling and simulation

In superalloys, the precipitated phase γ' has a different lattice parameter from that of the γ matrix phase. It is possible to measure this difference in lattice parameters in terms of the mismatch δ, which is defined as $\delta = 2 \times \dfrac{a'_\gamma - a_\gamma}{a'_\gamma + a_\gamma}$, where a_γ and a'_γ are the lattice parameters for the γ and γ' phase and chosen as 3.52 Å and 3.567 Å (expt) or 3.62 Å (calc), respectively. For the γ/γ' phase system in the present work, δ is 2.8% (calc), which indicates that the stress field resulting from the lattice misfit will be created at the interface between γ and γ'. Therefore, the γ/γ' interface with the stress field is unstable, and the atoms on the phase interface will rearrange to release the elastic stress and to decrease their energy towards the stable state, i.e. a relaxation process occurs. Then the network of the phase interface dislocations will be created and the interphase coherence will be affected. This process shows that the formation of dislocation networks is an important way to reduce the distorted energy, and it can be supposed that the phase interfaces with dislocation networks exist widely in the single-crystal superalloy, and will have great influence on the mechanical properties of the superalloy.

Because there is no external stress applied to the system, only the internal elastic stress has effect on the lattice redistribution in the two-phase alloy systems containing coherent precipitates. When the precipitated phase is thin or the lattice parameter difference between the precipitate and the matrix is small, the strains induced by the misfit will be accommodated by elastic deformation, which retains the coherence between them. If the mismatch exceeds the limit of elasticity, the misfit dislocation will form on the phase interface to reduce the distorted energy of the system.[9]

Based on the idea of constructing the γ/γ' interface in our previous work,[10,11] it can be understood easily that a γ' structural unit of 35×35×35 (defining the side length of the cuboidal γ' precipitate as α) has almost the same volume and shape as a γ structural unit of 36×36×36. Then by substituting the 35×35×35 γ' structural unit for the 36×36×36 γ structural unit in the centre of a 40×40×40 γ block with the [100], [010] and [001] lattice directions, we can obtain the initial unit cell of the mosaic structure. In this mosaic structure, the cuboidal γ' precipitate will not be squeezed by the γ matrix, and the γ' volume fraction of the model is $\left(\dfrac{36}{40}\right)^3 \approx 73\%$, which is in agreement with the experimental value. The initial unit cell in the mosaic structure, named model (a), is shown in Fig.2(a).

For further investigation of the possible difference caused by the size and number of the cuboidal γ' precipitates, we construct another two mosaic models: model (b) contains eight unit cells forming a cube, and model (c) is a large mosaic model with the same volume of γ' precipitates as in model (b). From the model construction process, we can find that the orientations of crystal lattices in the models are all arranged along the [100], [010], and [001] directions as indicated in Fig.2(a), and then the γ/γ' interfaces will be the {100} plane, which is consistent with the experimental results.

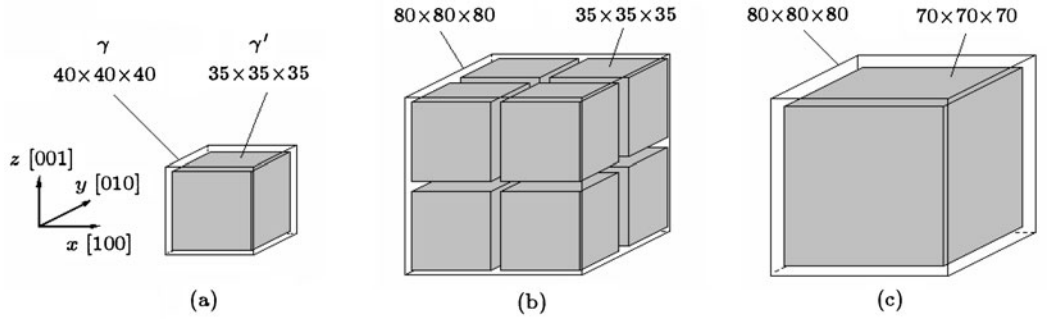

Fig.2. Initial models of the mosaic structure. (a) Initial unit cell of the mosaic structure. (b) Initial model with eight cuboidal precipitates. (c) Initial model with a large cuboidal precipitate.

In order to eliminate the surface effect, all the three initial models are relaxed by MD calculation under the periodic boundary conditions. Here, the simulation is based on the potential employed in modified analytic embedded atom method (MAEAM), which is developed by Zhang *et al*[12−14] in the framework of Johnson's theory.[15−17] The potential in MAEAM has been successfully applied to the study of monatomic metals, alloys, as well as intermetallic compounds, and the calculated results are in good agreement with the experimental values and other calculated results.[18,19]

3. Results and discussion

As discussed in Section 2, when γ' precipitates coherently from the γ matrix with interfaces parallel to the common {100} shared by them, the γ/γ' interface with the stress field distributed on it will be in a metastable state. After MD relaxation, the atoms on the phase interface will rearrange to minimize the elastic stress so as to decrease their energy towards the stable state. It is found that the misfit will be concentrated in some defect region and form the misfit dislocations. These misfit dislocations are separated by a relatively larger perfect region and then form the dislocation networks. The formation of misfit dislocation networks is regarded as an important way to reduce the distorted energy induced by misfit. It is reasonable to consider that the phase interfaces with dislocation networks widely exist in the Ni-based single-crystal superalloys.

Based on the MD calculation results, we have selected the atoms with the higher potential energies in the dislocation core area and drawn them in Fig.3. From Fig.3 we find that the square dislocation networks appear on the phase interfaces, and the side length of the mesh is 89.6 Å. The side length of the mesh can be obtained by using the equation[10] $d = \frac{\sqrt{2}}{2}\left(\frac{1}{\delta}+\frac{1}{2}\right)a_\gamma \approx \frac{\sqrt{2}a_\gamma}{2\delta}$, which is consistent with the experimental results.[20] Figure 3 displays that six square misfit dislocation networks on a cube are connected with each other and assembled into a closed three-dimensional network system. Further investigation shows that all the dislocations are the ⟨011⟩{100} edge dislocations.

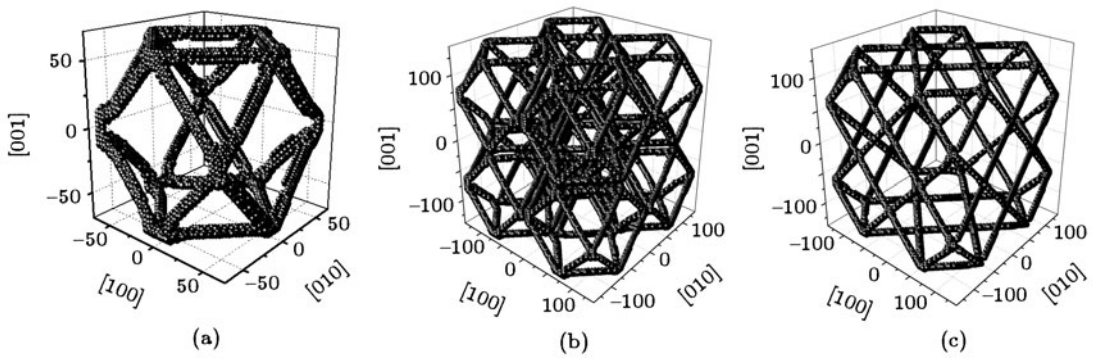

Fig.3. Patterns of the misfit dislocation networks obtained by MD simulation.

Figure 3 shows that each of the eight network systems in model (b) possesses the same shape and size as that in model (a), and the network system in model (c) possesses the same shape but is double the size of that in model (a). The simulation results indicate that the side lengths of the mesh in models (a), (b) and (c) are equal, i.e. 89.6 Å, which means that the side length of the mesh only depends on the lattice parameters of γ phase and γ' phase as well as the γ/γ' phase interface direction, but is independent of the size and number of the cuboidal γ' precipitates. Through the calculated results we can consider that the misfit dislocation will be formed only on the γ/γ' phase interface, and the similar patterns have been observed in experiments by transmission electron micrograph (TEM) and high resolution electron microscopy (HREM).[20−23]

Careful observation will show that the total dislocation length l in model (b) is twice as long as that in model (c). In other words, the amount of dislocations is proportional to the total area of the γ/γ' interface, indicating that the smaller the size of the cuboidal γ' precipitate, the larger the dislocation density $\left(\lambda = \dfrac{l}{\alpha^3}\right)$. The relation between λ and α can be given simply as $\lambda \propto \frac{1}{\alpha}$, which may be used to explain the relation between the amount of the fine γ' phase and the creep rupture life of the superalloys. In addition, the closed three-dimensional networks consisting of the misfit dislocations can play a significant role in improving the mechanical properties of superalloys.

4. Summary

In the present paper, several molecular dynamics simulations are conducted for the dislocation mechanism in the idealized Ni-based superalloy composed of Ni_3Al cuboidal precipitates γ', and the pure Ni matrix γ. The simulation for the formation of mosaic structure reveals the properties of dislocation networks as follows. (1) In the mosaic models, six square dislocation networks, with index of $\langle 011\rangle\{100\}$ and the side length of the mesh 89.6 Å, are formed on the corresponding phase interface, and these six square misfit dislocation networks are connected with one another and assemble into a closed three-dimensional network system. (2) In the mosaic models with eight piled-up small cuboidal γ' precipitates and with a whole large cuboidal γ' precipitate, it is found that the side length of the mesh depends only on the lattice parameters of γ phase and γ' phase as well as the γ/γ' interface direction, but is independent of the size and number of the cuboidal γ' precipitates. (3) It can be regarded that the misfit dislocation is formed on the γ/γ' interface, and the density of dislocations is inversely proportional to the size of the γ' cube: i.e., the amount of dislocations is proportional to the total area of the γ/γ' interface. This result may be used to explain the relation between the amount of the fine γ' phase and the large creep rupture life of the superalloys. In addition, the closed three-dimensional networks formed by the misfit dislocations can play a significant role in improving the mechanical properties of superalloys.

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