Molecular Dynamics / Discrete Dislocation Dynamics Simulations on the Dislocation Behavior in Ni-Based Superalloys

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Summary

Dislocation behaviors in the matrix-precipitate microstructure of Ni-based superalloys are investigated by means of molecular dynamics (MD) and discrete dislocation (DD) dynamics simulations. MD results suggest that a dislocation is not blocked by the matrix-precipitate interface but decelerated by the stress field around the precipitate. A DDD–FEM analysis is then implemented to evaluate the stress field and treat the image force on dislocations from precipitates, showing good agreement with the MD results.

Introduction

Ni-based superalloys possess the characteristic microstructure where cuboidal γ' phases are precipitated in the γ matrix. The precipitates are decreased in the size down to about 0.5μm, and arranged with the distance of less than 0.1μm in the matrix. The main composition of γ' precipitate is Ni_3Al, $L1_2$ ordered alloy, while that of γ matrix is Ni of fcc. The small lattice mismatch between the γ and γ' makes the γ/γ' interfaces coherent; however, dislocations are affected by the interface and show complicated behavior depending on the morphology of the γ/γ' microstructure. The dislocation behavior in the array of γ' precipitates has attracted intense interest with respect to the understanding of the deformation mechanism of superalloys.

Numerous studies have been devoted to dislocations in the γ/γ' microstructure from the viewpoint of their role in the *rafting* process, or the directional coarsening of the precipitates under creep deformation [1]. It is still difficult, however, to explore further details of the interaction between the dislocation and the γ/γ' interface by experimental observations, since the scale of the phenomena is less than one micrometer and of a nanoscale. We have conducted several molecular dynamics (MD) simulations to reveal the fundamental aspect of dislocations at the γ/γ' interface in the atomistic scale [2,3]. The MD simulation, however, can not treat the collective behaviors of many dislocations nor thermally activated motions such as dislocation climb. Thus we have now been trying to scale-up our study with the discrete dislocation dynamics (DDD) simulation. In the present paper, an MD simulation is firstly presented to insist on the fact that the stress field around the precipitate dominates the dislocation behavior at the γ/γ' interface. Then we outline the DDD modelling and treatment of image force from the precipitate by

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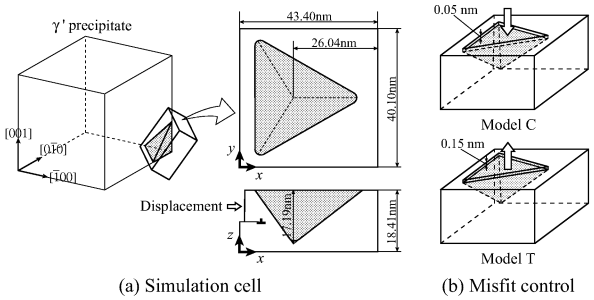

Figure 1: MD simulation model.

using the superposition with FEM analysis, and finally show an example by using the DDD-FEM code proposed by Zbib and Diaz de la Rubia [4].

MD Simulation of Dislocation at γ/γ' Interface

Simulation procedure The interatomic potential adopted is the embedded-atom method [5], in which parameters are fitted to the properties of the Ni, Al, and Ni-Al binary systems by Voter and Chen [6]. The details of the functions and parameters are described in the original papers [6] and our previous reports [2].

The simulation is implemented with a slab cell that mimics a local part of an apex of cuboidal Ni_3Al precipitate in a Ni matrix, as schematically illustrated in Fig. 1(a). The cell has the size of $43.4\,\mathrm{nm} \times 40.1\,\mathrm{nm} \times 18.4\,\mathrm{nm}$ and the total number of atoms is 2,880,000. The precipitate is made by substituting Al for Ni in the matrix, thus there is no lattice mismatch between γ and γ' and the interfaces are coherent in the initial arrangement. The edges of the cubic are rounded off to have the radius of 3.5 nm. This initial configuration is relaxed by molecular dynamics calculation of 5000 fs in order to redistribute the internal strain around the precipitate. Here, the motion of atoms is restricted in the yz or xy planes at the x or z boundaries, respectively, while the periodic boundary condition is adopted along the y axis. The temperature is kept at 300 K during the simulation by the velocity scaling. After the initial relaxation, the γ' precipitate is slightly pushed-in or pulled-out as shown in Fig.1(b) and relaxed again. Here the former cell is referred as "Model C" while the later as "Model T". This process aims to increase/decrease the compressive internal stress of γ' precipitate due to the lattice misfit. Mode II type displacement is then applied on each cell at the side of $x = 0$, to nucleate edge dislocations and proceed them toward the precipitate. Details of the displacement controll adopted is shown in our previous report [3].

Simulation results Figures 2(a) and (b) show the dislocation motion in Model C and Model T, respectively, on the slip plane where dislocations nucleated. Ni

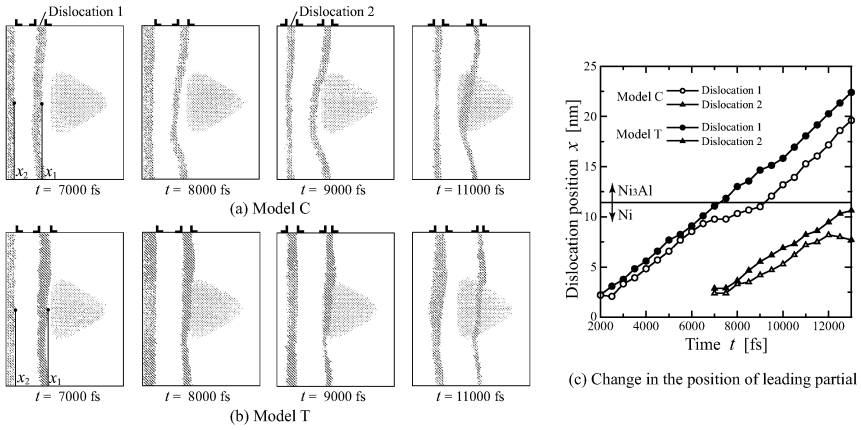

Figure 2: Motion of extended edge dislocations.

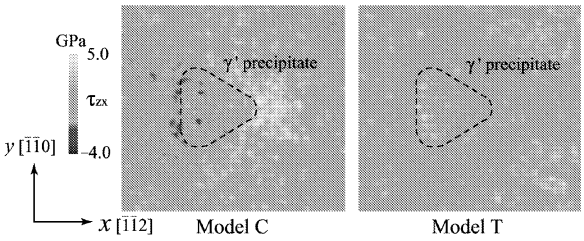

Figure 3: Distribution of shear stress, τ_{zx}, on the slip plane.

atoms in the stacking faults between leading and trailing partials are drawn with dark shade while Al atoms of the γ' are indicated with light shade in the figure. Figure 2(c) is the change in the position of leading partial evaluated at the center as indicated at $t = 7000$ fs of Figs 2(a) and (b). In the Model C, the first dislocation is decelerated at the front of the precipitate while it continues to glide at the other part, resulting in the dislocation bending. It is noteworthy that the slow-down takes place at far point about 3 nm from the interface as shown in Fig. 2(c). Then the bent dislocation begins to cut into the precipitate. On the other hand, the dislocation in Model T reaches the interface with constant speed and penetrates into the precipitate without any obstruction. This different behavior is explained in terms of the Peach-Koehlor (PK) force by the stress field around the precipitate. Figure 3 shows the distribution of shear stress, τ_{zx}, which generates the PK force in the x-direction on the edge dislocation. Negative stress can be found at the front of γ' precipitate in Model C, so that we can deduce this negative stress causes repulsive force on the approaching dislocation and decelerate it. This MD result suggests that the γ/γ' interface is rather continuum and the stress field around the precipitate would dominate the dislocation behavior in the γ/γ' microstructure.

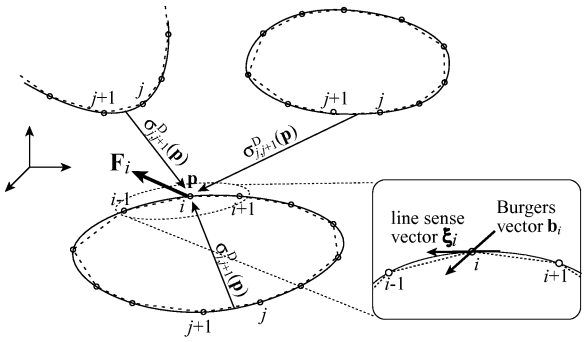

Figure 4: Nodes and segments on dislocation loops.

DDD Simulation of Dislocation at Matrix-Precipitate Interface

Outline In the framework of 3D discrete dislocation dynamics proposed by Zbib et al. [4], all dislocation lines and loops of arbitrary shape are discretized into short line segments, and the time evolution of each dislocation is pursued by calculating the force acting on each segment on the basis of the dislocation theory. The PK force on the node i at the position vector $\mathbf{p}$ is calculated by the following equation,

$$\mathbf{F}_i = \sum_{j=1}^{N-1} \left(\boldsymbol{\sigma}^{\mathrm{D}}_{j,j+1}(\mathbf{p}) + \boldsymbol{\sigma}^{\mathrm{a}}(\mathbf{p})\right) \cdot \mathbf{b}_i \times \boldsymbol{\xi}_i + \mathbf{F}_{i-\mathrm{self}} \tag{1}$$

where $\sigma^{\mathrm{D}}_{j,j+1}(\mathbf{p})$ is the stress at $\mathbf{p}$ generated by a remote segment [4], $\sigma^{\mathrm{a}}(\mathbf{p})$ the applied stress, N the number of all nodes, $\mathbf{b}_i$ and $\boldsymbol{\xi}_i$ are the Burgers vector and line sense vector at node i, respectively, as shown in Fig. 4. $\mathbf{F}_{i-\mathrm{self}}$ represents the line tension evaluated by the curvature at the node i. Evolution of dislocations are traced by solving the following equation of motion numerically.

$$m\dot{\boldsymbol{v}}_i + \frac{1}{M(T,p)}\dot{\boldsymbol{v}}_i = [\boldsymbol{F}_i]_{\mathrm{glide-component}} \tag{2}$$

Here $\boldsymbol{v}_i$ is the glide velocity, m the effective mass per unit dislocation, T and p are the temperature and pressure, respectively. M is the mobility accounting for the different character of screw and edge dislocations in fcc and bcc crystals.

DDD-FEM coupling The formulation of $\sigma^{\mathrm{D}}_{j,j+1}(\mathbf{p})$ is defined in the infinite body of homogeneous material, so that it could not be directly applied to the problem containing surface or heterogeneous interface. The superposition principle is used to treat the problem. The displacement u, strain ε, and stress σ in a finite body containing a precipitate is given by the sum of two solutions:

$$u = u^{\infty} + u^{*},\ \varepsilon = \varepsilon^{\infty} + \varepsilon^{*},\ \sigma = \sigma^{\infty} + \sigma^{*} \tag{3}$$

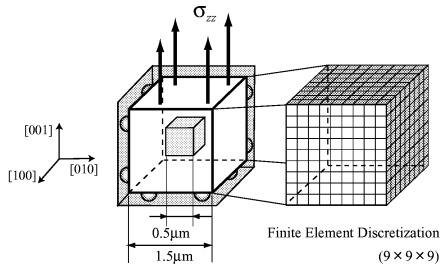

Figure 5: DDD–FEM simulation model.

where ∞ implies the solution of DDD analysis for a domain V in the inifinite homogeneous body, while $*$ does that of FEM for the finite body of which volume is V. The constitutive equation in domain V is defined as follows;

$$\sigma^{\infty} = [C^{\mathrm{m}}]\varepsilon^{\infty} \quad \text{in} \quad V \tag{4}$$

where C^{m} is the elastic stiffness tensor of matrix. In the FEM analysis, the following constitutive equations are defined for matrix and precipitate, respectively.

$$\begin{array}{ll} \sigma^{*} = [C^{\mathrm{m}}]\varepsilon^{*} & \text{in } V_{\mathrm{m}} \\ \sigma^{*} = [C^{\mathrm{p}}]\varepsilon^{*} + [C^{\mathrm{p}} - C^{\mathrm{m}}]\varepsilon^{\infty} & \text{in } V_{\mathrm{p}} \end{array} \tag{5}$$

Here C_{p} is the elastic stiffness of precipitate, V_{m} and V_{p} are the volume of matrix and precipitate in the finite body V, respectively. The dislocation stress σ^{∞} of Eq. (4) in whole domain V and the "eigenstress" of $[C^{\mathrm{p}} - C^{\mathrm{m}}]\varepsilon^{\infty}$ in the precipitate V_{p} is subtracted as body force in the FEM analysis. The boundary conditions are:

$$\begin{array}{lcll} t^{*} & = & t^{\mathrm{a}} - t^{\infty} & \text{on} \quad \partial V \\ u^{*} & = & u^{\mathrm{a}} & \text{on} \quad \text{part of } \partial V \end{array} \tag{6}$$

where t^{a} is the externally applied traction while t^{∞} is the traction by dislocations due to the infinite-homogeneous domain problem.

Simulation example The simulation is implemented with the cubic cell containing a cuboidal precipitate as shown in Fig. 5. The cell has the size of 1.5μm in the length while that of the precipitate is 0.5μm. $9 \times 9 \times 9$ mesh blocks are used in the FEM analysis. A Frank-Read source is set near the precipitate and a dislocation is propagated from the source and approaching the precipitate under the tensile stress of 150MPa. The shear moduli of matrix and precipitate are 80GPa and 160GPa, respectively. Poisson's ratio is set at 0.3 for both materials.

Figure 6 illustrates the motion of dislocation on the (111) slip plane simulated by the DDD-FEM analysis. For comparison, the results of the homogeneous matrix without precipitate are also shown. At the figure of $t = 600\,\mathrm{step}$, the dislocation loop near the precipitate grows slower than that in the homogeneous matrix. This suggests that the dislocation receives the repulsive force.

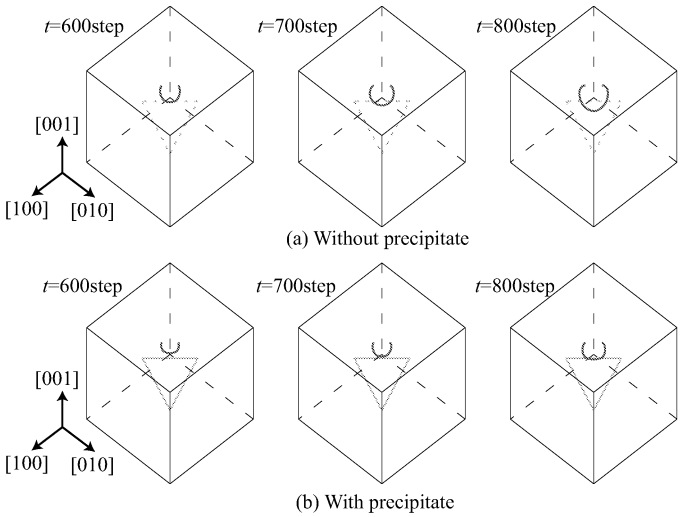

Figure 6: Motion of dislocation in DDD-FEM analysis

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