Discrete dislocation plasticity analysis of dispersion strengthening in oxide dispersion strengthened (ODS) steels

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Abstract: A discrete dislocation plasticity analysis of dispersion strengthening in oxide dispersion strengthened (ODS) steels was described. Parametric dislocation dynamics (PDD) simulation of the interaction between an edge dislocation and randomly distributed spherical dispersoids (Y$_2$O$_3$) in bcc iron was performed for measuring the influence of the dispersoid distribution on the critical resolved shear stress (CRSS). The dispersoid distribution was made using a method mimicking the Ostwald growth mechanism. Then, an edge dislocation was introduced, and was moved under a constant shear stress condition. The CRSS was extracted from the result of dislocation velocity under constant shear stress using the mobility (linear) relationship between the shear stress and the dislocation velocity. The results suggest that the dispersoid distribution gives a significant influence to the CRSS, and the influence of dislocation dipole, which forms just before finishing up the Orowan looping mechanism, is substantial in determining the CRSS, especially for the interaction with small dispersoids. Therefore, the well-known Orowan equation for determining the CRSS cannot give an accurate estimation, because the influence of the dislocation dipole in the process of the Orowan looping mechanism is not accounted for in the equation.

Key words: parametric dislocation dynamics; oxide dispersion strengthened steel; Orowan mechanism; critical resolved shear stress; dislocation dipole

1 Introduction

Fusion and fission reactors are now promising candidates for the next generation energy sources. One of problems to be solved for realizing the reactors is to design materials, which can show their extreme strength even under ultra-high temperature and irradiation conditions. As a material of the core structure of such reactors, oxide dispersion strengthened (ODS) steel is, so far, the most promising candidate. The ODS steel is strengthened by dispersing oxide particles, such as yttrium-oxide (Y$_2$O$_3$), which strongly impede the dislocation motion, and subsequently increase the onset stress of plastic deformation and creep resistance. Indeed, the extreme strength of the ODS steel has already been proven by a lot of experiments [1−9]. These experimental studies gave us the information on the macroscopic mechanical behavior of ODS steels, however, did not provide us with the microscopic deformation mechanism of the interaction between dislocations and Y$_2$O$_3$ dispersoids. In order to realize the practical use of the ODS steels, not only the macroscopic mechanical behavior under certain environmental conditions but also the detailed information on the microscopic mechanism of the deformation must be clarified, which determines the macroscopic mechanical behavior. Thus, understanding the information on the interaction between dislocations and Y$_2$O$_3$ dispersoids is crucial.

Recently, computers and computer simulation techniques are successfully developed, and provide us with an opportunity to investigate the detailed microscopic material strengthening mechanism. Dislocation dynamics (DD) method, which is originally developed for studying the meso-scopic plastic deformation based on the collective behavior of individual dislocations in bulk single crystals, has been extended for the simulation of plastic deformation in finite volumes [10], precipitation strengthened alloys [11] using the superposition principle. The interaction between a screw dislocation and Y$_2$O$_3$ dispersoids in PM2000 is studied using the DD method [12]. These studies extend the application of DD method to the interaction between dislocations and particles, and open a door to investigate numerically the interaction between...
dislocations and Y\textsubscript{2}O\textsubscript{3} dispersoids in ODS steels.

In this work, three-dimensional DD simulations of the interaction between an edge dislocation and multiple Y\textsubscript{2}O\textsubscript{3} dispersoids are performed for investigating the dependence of the critical resolved shear stress (CRSS) on the volume fraction and average size of Y\textsubscript{2}O\textsubscript{3} dispersoids. It has already been revealed that the dislocation interacts with Y\textsubscript{2}O\textsubscript{3} dispersoids, and passes the Y\textsubscript{2}O\textsubscript{3} dispersoids with the Orowan mechanism [13]. Therefore, in this work, the interaction between an edge dislocation and Y\textsubscript{2}O\textsubscript{3} dispersoids is assumed to be the Orowan mechanism. Applying a constant shear stress to the simulation volume containing an edge dislocation and multiple Y\textsubscript{2}O\textsubscript{3} dispersoids, the velocity of dislocation interacting with Y\textsubscript{2}O\textsubscript{3} dispersoids is measured. By considering the linear relationship between the applied constant shear stress and the dislocation velocity, the CRSS is statistically extracted from the numerical results of the DD simulations. The numerical results are then compared to the CRSS predicted by the corresponding theoretical equations in order to discuss the dominant microscopic mechanism that controls the CRSS and macroscopic mechanical behavior.

2 Computational method

2.1 Dislocation dynamics

In this work, the interaction between an edge dislocation and multiple Y\textsubscript{2}O\textsubscript{3} dispersoids is simulated using DD method. Although there are a lot of versions of DD simulation technique, we choose to use the parametric dislocation dynamics (PDD) method [14], because of the high numerical accuracy and thermodynamical background of the basic equation. In the PDD method, dislocations are discretized with a number of segments. To avoid a numerical singularity at sharp corners of dislocation line, where two neighboring segments are connected, the segments are smoothly connected using a cubic spline function. In order to use the cubic spline function, the nodes at two ends of segments have generalized coordinate vector composed of the position vector, which is for describing the location of segments, and the tangent vector, which gives the information on the shape of segments. The dislocation velocity is assumed to have a linear relationship with the local shear stress. A variational form of the governing equation of motion of dislocation is given by

\[
\int f(F_k - B_{\alpha k}V_\alpha)\delta_k ds = 0
\]

(1)

where \(f\) is the dislocation line, \(F_k\) is the Peach-Koehler force acting at the infinitesimal integral element of the dislocation line \(ds\), \(B_{\alpha k}\) is the resistivity matrix and \(V_\alpha\) is the velocity of the generalized coordinate vector. By solving the equation, the velocity of generalized coordinate vector can be obtained, and is used for computing the temporal evolution of the position and shape of dislocation segments. Further details of the PDD method can be found elsewhere [14].

The influence of Y\textsubscript{2}O\textsubscript{3} dispersoids on the dislocation motion is incorporated into the PDD simulation. Under the influence of coherency strain, which is arisen from the lattice size difference between the matrix and dispersoid, the elastic stress generated by the Y\textsubscript{2}O\textsubscript{3} dispersoid is calculated. In this work, the shape of Y\textsubscript{2}O\textsubscript{3} dispersoid is assumed to be spherical so that the elastic stress can be calculated using the following elastic solution [15]:

\[
e_r = \frac{21 + \nu a^3}{31 - 4\nu r^3} \epsilon_{coh}
\]

(2)

\[
e_l = \frac{11 + \nu a^3}{31 - 4\nu r^3} \epsilon_{coh}
\]

(3)

where \(\nu\) is the Poisson ratio, \(a\) is the radius of the spherical dispersoid, \(r\) is the distance from the center of the spherical dispersoid, and \(\epsilon_{coh}\) is the coherency strain. In addition to the influence of coherency strain, we assume that the dislocation cannot penetrate the Y\textsubscript{2}O\textsubscript{3} dispersoid. In order to implement the assumption, the position of segments is checked at every time step. When a part of segment comes into inside a Y\textsubscript{2}O\textsubscript{3} dispersoid, the part is returned to the interface between the Y\textsubscript{2}O\textsubscript{3} dispersoid and the matrix. The artificial treatment of the position of segments can naturally introduce the Orowan mechanism into the PDD simulation. As the result of the Orowan mechanism, the dislocation goes around the Y\textsubscript{2}O\textsubscript{3} dispersoid, when the dislocation is likely to pass over the Y\textsubscript{2}O\textsubscript{3} dispersoid.

2.2 Distribution of Y\textsubscript{2}O\textsubscript{3} dispersoids (Ostwald growth)

In this work, we simulate the interaction between an edge dislocation and multiple Y\textsubscript{2}O\textsubscript{3} dispersoids so that, since the distribution should have a significant influence on the dislocation motion, and must be realistic, the distribution of Y\textsubscript{2}O\textsubscript{3} dispersoids is of great interest. Experimental studies have revealed that, in ODS steels, the Y\textsubscript{2}O\textsubscript{3} dispersoids are formed by the Ostwald growth process [16]. MOHLES and FRUHSTORFER [17] developed a method that can make a distribution of particles resulting from the Ostwald growth process. In this work, we use the method developed by MOHLES and FRUHSTORFER, and briefly review the procedure below.

1) The particle radius distribution function is given by

\[
\delta(R) = \frac{R}{9 R^3} \left(\frac{3}{3 + R / R^*}\right)^\frac{7}{3} \left(\frac{1.5 - R / R^*}{1.5 - R / R^*}\right)^\frac{11}{3}
\]

where \(R\) is the radius of the spherical dispersoid, and \(R^*\) is a reference radius.