Crystal Plasticity Analysis of Mechanical Response and Size Effect in Two Phase Alloys with Dispersion of Fine Particles

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Abstract. Plastic deformation and dislocations accumulation in a steel alloy dispersed with vanadium carbide particles is numerically analyzed by a crystal plasticity finite element technique and work hardening characteristics are discussed. Increment of dislocation density that contributes to work hardening is calculated from the mean free path of dislocations. The mean free path is defined by the spacing of forest dislocations and the average spacing of dispersed particles. Obtained yield stress and work hardening characteristics was close to that of experimental result, except that the value of work hardening rate was higher than that of experimental one.

Introduction

Dispersion hardening where fine particles are dispersed in metal matrix is a typical strengthening method of metals. When hard particles are dispersed in the matrix, dislocations need to pass through them when metals deform by slip. Yield stress and plastic flow stress level as well as the work hardening rate are increased, which is known as the Orowan mechanism. So far, a number of studies have been made on the Orowan mechanism and yield stress is successfully estimated from the spacing of dispersed particles. After the movement of dislocations through particles, loops shaped dislocations [1] should theoretically be left around particles and the back stress that accompanies to the dislocation loops is considered to be the origin of work hardening. In experiments, Orowan loops are often observed at an initial stage of plastic deformation. However, dislocations accumulation after some amount of plastic slip deformation consists of tangled structures between particles. Therefore, a further examination of dislocation accumulation and work hardening characteristics are needed.

In this study, plastic deformation and dislocations accumulation in a steel alloy dispersed with vanadium carbide particles [2][3] is analyzed by a crystal plasticity finite element technique and work hardening characteristics are discussed.

Crystal Plasticity Analysis

We use a continuum mechanics-based crystal plasticity analysis code CLP and analyze plastic slip deformation. Densities of the geometrically necessary (abbreviated as GN, hereafter) and statistically stored (abbreviate as SS, hereafter) dislocations are evaluated.

Edge and screw components of the GN dislocation are defined from spatial gradient of plastic shear strain.

$$\rho_{G,edge}{}^{(n)} = -\frac{1}{\tilde{b}}\frac{\partial \gamma^{(n)}}{\partial \xi^{(n)}}, \quad \rho_{G,screw}{}^{(n)} = \frac{1}{\tilde{b}}\frac{\partial \gamma^{(n)}}{\partial \varsigma^{(n)}}. \tag{1}$$

Here, $\tilde{b}$ and $\gamma^{(n)}$ denote the magnitude of Burgers vector and the plastic shear strain on slip system n, respectively. ξ and ζ denote directions parallel and perpendicular to the slip direction on the slip plane, respectively. The density norm of the GN dislocation is defined by the following equation.

$$\left\|\rho_G^{(n)}\right\| = \sqrt{\left(\rho_{G,edge}^{(n)}\right)^2 + \left(\rho_{G,screw}^{(n)}\right)^2}. \tag{2}$$

Increment of the SS dislocation density is calculated from the increment of shear strain and the mean free path of moving dislocations.

$$d\rho_S = \left(\frac{c}{\tilde{b}L^{(n)}} - \frac{D}{\tilde{b}} \rho_S^{(n)} \right) d\gamma^{(n)}. \tag{3}$$

Here, L and D denote the mean free path of moving dislocation and a distance of dislocation annihilation.

The mean free path is an average distance where the dislocations stop moving. In this study, the distance is defined by the spacing of forest dislocations and the average spacing of dispersed particles, as follows.

$$L^{(n)} = Min\left[\frac{c^*}{\sqrt{\sum_{m=1}^{24} w^{(nm)} \left(\rho_S^{(m)} + \left\| \rho_G^{(m)} \right\| \right)}},\ \lambda \right]. \tag{4}$$

Here, c^* is a numerical factor of obstruction weight of moving dislocations. w is the weight matrix which controls the contribution of SS and GN dislocations accumulated on the slip system m to the mean free path of moving dislocations on slip system n. The value of w is 1 when the dislocations on the slip system m act as forest dislocations against the ones on slip system n, while w=0 when the dislocations on the m slip system are co-planar. λ is the average spacing of dispersed particles and given by the distance of randomly dispersed particles on the slip plane subtracted by the diameter of particles [7].

The critical resolved shear stress for slip system n is given by the extended expression of the Bailey-Hirsch type model [6].

$$\theta^{(n)} = \theta_0 + \sum_{m=1}^{24} a\mu\tilde{b}\Omega^{(nm)}\sqrt{\rho_S^{(m)}} + c_T \beta \frac{\mu\tilde{b}}{d}. \tag{5}$$

Here, the first term in the right hand side of eq.(5) stands for lattice friction stress for moving dislocations, the second term defines slip resistance of SS dislocations and the third term defines size effect of microstructure. Here, $\Omega^{(nm)}$ is the interaction matrix between slip systems. a is a numerical factor of the order of 0.1, μ denotes the elastic shear modulus and $\rho_S^{(m)}$ denotes the density of SS dislocations accumulated on the slip system m. c_T and β are numerical factor for the moving dislocations and d is the representative length scale of microstructure. The third term of dispersion strengthened alloy is the Orowan stress. Therefore, c_T and β are given 1 and d is equal to λ: the average spacing of dispersed particles.

Analysis Model

Fig.1 shows the geometry of the model employed. Sphere shaped second phase is placed at the center of the cube shaped matrix. Lateral dimension of the cube of 135.8 nm and the diameter of the particle of d_p=39 nm are used in accordance with experimental data by Nakada et al [2][3]. With this dimensions, the volume fraction of the particles is V_f=1.24%. For the purpose of comparison, another model with the lateral dimension of 101.2 nm and same diameter of particle of d_p=39 nm was also made where the volume fraction was V_f=3%. The average distance of randomly dispersed particles are 286.2 nm for the model with V_f=1.24% and 173.0 nm in the model with V_f=3%. Crystal structure is body-centered cubic. Crystal orientation is chosen so as that the normal to the primary slip plane and the slip direction make an angle of $\pi/4$ to the y-axis. Uniform tensile displacements are given on the surfaces perpendicular to the y-axis, while side surfaces are traction free. Under this condition, the Schmid factor for the slip system is 0.5. For the purpose of simplicity, we assume slip deformation only on the primary systems.

Matrix and second phase of material are iron and vanadium carbide, respectively. Table 1 shows material constants. Lattice friction of iron matrix and vanadium carbide precipitate are decided as 50MPa and 4GPa, respectively.

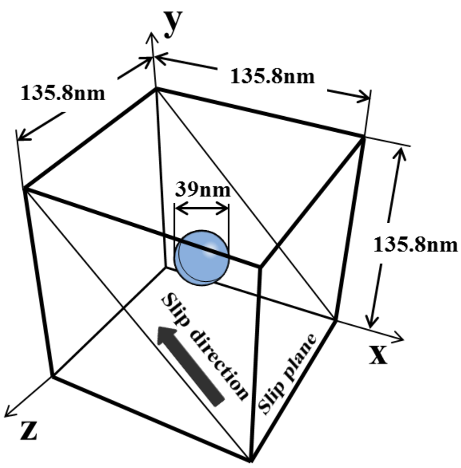
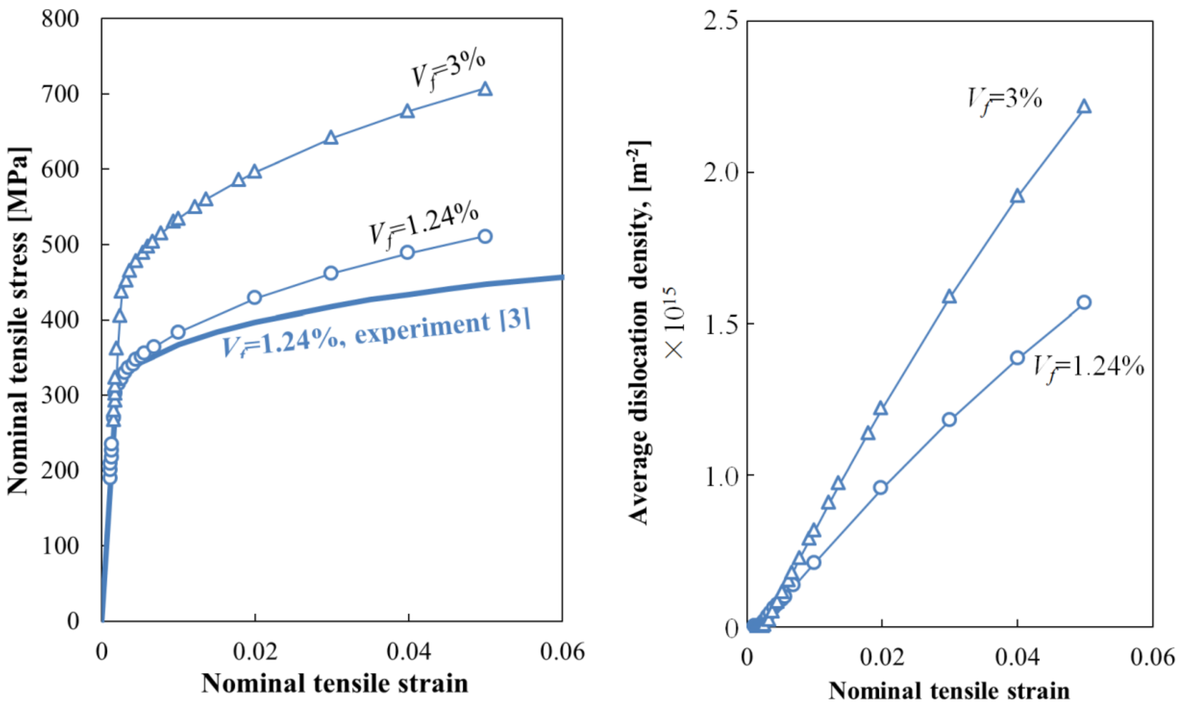


Fig.1. The geometry of the model for numerical analysis. The diameter of particles is 39nm. The slip direction and the slip plane of the primary slip system are shown.

Table 1 Material constans

		iron	VC
Elastic compliance [$\times 10^{-11}$m^2/N]	s_{11}	0.7720	0.2325
	s_{12}	-0.2850	-0.0512
	s_{44}	0.9020	0.6369
Magnitude of Burgers vector [nm]		0.248	0.294
Lattice friction [MPa]		50	4000
Initial dislocations density [m^{-2}]		24.0×10^9	



(a) (b)

Fig.2. (a) Nominal tensile stress-strain curves of models with V_f=1.24%, V_f=3% specimens and experimental result [3] and (b) change in average density of SS dislocations in the models with V_f=1.24% and V_f=3%.

Results and Discussion

Fig.2 shows the numerical results of the stress-strain relations with experimental result [3]. In the model with V_f=1.24%, deformation at an initial stage of deformation agrees very well with experimental one, but work hardening is higher than that of experimental one. Yield stress of V_f=3% model is about 81MPa higher than that of V_f=1.24% model and plastic flow stress of V_f=3% model at nominal strain of 5% is about 191MPa higher than that of V_f=1.24% model. That is, both yield stress and work hardening are higher in the model with higher volume fraction of secondary particle and this fact is consistent with existing theoretical and experimental results. Fig.2(b) shows the evolution of the average density of SS dislocations plotted as against nominal strain. Density of SS dislocations grows faster in the model of V_f=3% and this brings about the higher value of strain hardening.

In the present model, the mean free path of moving dislocations is limited to the average spacing of dispersed particles and obtained work hardening characteristics was close to that of experimental one. The average spacing of particles becomes smaller by increase of volume fraction and yield stress and work hardening are increased by the Orowan mechanism and dislocations accumulated.

There were some discrepancies between the numerical and experimental results in the work hardening rate. The reason for this is considered as follows. In this study, we used the averaged values for diameter of particles and their spacing. But in reality, the diameter and the spacing have distributions. In that case, the increase of dislocation density is quicker in narrower space and this brings about a local work hardening there and requires an increase of stress, but plastic deformation will continue in another space where particle spacing is larger and the increase of dislocation density is lower. In this way, plastic deformation is considered to expand from place to place without much increase in applied stress, and this will bring about a lower strain-hardening rate. Details of this mechanism should be discussed further.

Summary

Slip deformations and macroscopic mechanical response of two-phase alloys with dispersion of fine particles were analyzed by a crystal plasticity finite element method. The results obtained are summarized as follows.

I. Scale dependent characteristics of the yield stress and strain hardening were successfully reproduced by an introduction of the extended Bailey-Hirsch type model for the critical resolved shear stress as well as the model for the dislocation mean free path where mean spacing of dispersed particles contribute.

II. Numerical results for the yield phenomenon agreed very well with experimental results, while the strain hardening ratio was higher than that of experimental one. This discrepancy was considered to come from the fact that present model consists of only one particle.

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