Modelling and Crystal Plasticity Analysis for the Mechanical Response of Alloys with Non-uniformly Distributed Secondary Particles

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The relationship between yield stress and the distribution of microscopic plastic deformation was numerically investigated by using a crystal plasticity finite element method (CP-FEM) in the model where particles were randomly distributed. It was in order to reveal which particle spacing, i.e., the maximum, minimum or average particle spacing, can be taken as the representative length which controls yielding. The critical resolved shear stress for the onset of the slip deformation in any element was defined under the extended equation in the Bailey-Hirsch type model. The model includes the term of the Orowan stress obtained from the local values of the representative length. Each particle spacing was distributed with a standard deviation of approximately 2 to 3 times larger than the average particle spacing. The macroscopic mechanical properties obtained with CP-FEM were in good agreement with those experimentally obtained. The onset of microscopic slip deformation depended on the particle distribution. Plastic deformations started first in the area where the particle size is larger, then the plastic region grows in the areas where the particle spacing is smaller. Slip deformation had occurred in 90% of the matrix phase by the macroscopic yield point. The length factor in the Orowan equation was the average spacing of the particles in the model, which is in good agreement with Foreman and Makin. The CP-FEM indicated that in dispersed hardened alloys, microscopic load transfer occurred between the areas where the large particles spacing and the small one at the yielding.

KEY WORDS: crystal plasticity finite element analysis; dispersion hardening; mechanical response.

1. Introduction

Dispersion hardened alloys have superior mechanical strength due to the precipitation of hard secondary phase particles throughout the matrix. These particles enable the alloy to have high yield strength and work hardening rates. Plastic deformation of crystalline metallic materials occurs due to the movement of dislocations. If second phase hard particles are finely dispersed in the matrix, dislocations must pass through these fine particles and are blocked from advancing, increasing yield strength compared to the single phase alloys. The mechanism of dislocations passing between particles1,2) is understood as follows. When the movement of a dislocation line is blocked by particles, the dislocation protrudes between particles, and protruding parts of the dislocation line annihilate each other,3) which allows them to avoid particles. The shear stress necessary for dislocations to move around particles is obtained by the following equation:

\[
\tau_{\text{Orowan}} = \frac{\mu \bar{b}}{l} \tag{1}
\]

where \(l\), \(\mu\), and \(\bar{b}\) are intervals between the surface of each particle, elastic shear modulus of the matrix, and the magnitude of Burgers vector of the matrix, respectively. The dislocation mechanism described above is called the Orowan mechanism and the shear stress given by Eq. (1) is called the Orowan stress. For dispersion hardened alloys to achieve macroscopic yielding, short and localized movement of dislocations is not enough but they must move a long distance through a number of particles. Consequently, the average particle interval is used for Eq. (1) to calculate the yield stress of materials. The average interval \(\bar{t}\) between particles can be obtained with the following equation using the square approximation of the average diameter of particles \(d\) and volume fraction \(V_f\):

\[
\bar{t} = \frac{\pi}{6V_f} \sqrt{d} \tag{2}
\]
where the average interval $T$ is the distance between the center of particles. When multiple particles are irregularly dispersed throughout the alloy matrix, the square approximation given by Eq. (2) must be modified and Foreman and Makin calculated the shear stress necessary for dislocations to pass through the particles. Their result showed that when the critical angle of the passing dislocation between particles was about $10^\circ$ (hard particle), the stress was about 0.8 times the Orowan stress calculated from the average interval of particles $\tilde{T}$ using the square array approximation. As such, the average interval of particles $T$ is multiplied with a correction factor of 1.25, and the average diameter of particles is subtracted to obtain effective spacing of dispersed particles $\lambda$. In our previous papers, we examined a model that expresses the macroscopic mechanical responses (yield strength and work hardening rate) using this effective spacing of dispersed particles, and applied it to the crystal plasticity finite element method (CP-FEM). The results showed that the macroscopic mechanical responses of dispersion hardened alloys were expressed fairly well with the effective spacing of dispersed particles. CP-FEM allowed for analysis of the onset and propagation of microscopic plastic deformation. In these analyses, the critical resolved shear stress (CRSS) obtained from the effective spacing of dispersed particles, $\lambda$, was assumed to be a constant in the matrix; however, if we consider in more detail, particles are dispersed unevenly in dispersion hardened alloys and thus, the Orowan stress should vary from place to place. Therefore, the start of microscopic plastic deformation should be non-uniform in the microstructures.

The start of microscopic plastic deformation occurring in dispersion hardened alloys could be described as follows. Regions with dense and sparse distributions of particles coexist and local value of $T$ should be different from the value in Eq. (2). In the region of dense particle distribution, where the particle interval is narrow, high shear stress is necessary to start slip deformation. On the other hand, in the region with sparse particle distribution, wide particle interval allows for slip deformation to start at lower shear stress. If there is a mixture of regions with different shear stress requirements for slip deformation, microscopic yield will start in the region of low CRSS and expand to the regions with higher CRSS. Close examination of such process will enable us to understand in more detail the macroscopic yielding phenomena of alloys with unevenly dispersed hard particles.

In the present paper, we first analyze the microstructure of dispersion hardened alloys; i.e., three-dimensional particle distribution, and obtain localized particle intervals. From these obtained particle intervals, we introduce the condition that the CRSS is not uniform in the matrix but given as a function of distances between neighboring particles. We then elucidate the relationship between the start of microscopic slip deformation and the macroscopic mechanical responses and examine a numerical model that is able to express the macroscopic mechanical responses from crystal plasticity analysis of the microstructure.

2. Representative Length Involved with Spatial Arrangement and Deformation of Dispersed Particles

We prepared a model as shown below to perform crystal plasticity analysis that considers non-uniform distribution of many particles in three-dimensional space. First, we dispersed particles in three-dimensional space using pseudo-random numbers. At that time, we set the particle diameter and volume fraction. In the present paper, we prepared a three-dimensional region by assuming a material in which vanadium carbide (VC) particles with average diameter of 39 nm are dispersed in the ferrite matrix at a volume fraction of 1.24%. Figure 1(a) shows this three-dimensional model. Within a cube with a side of 1.36 µm, 1 000 particles with a diameter of 39 nm were irregularly dispersed. Based on this three-dimensional model, we analyzed a finite element model where a particle interval was determined for each element.

The domain treated by the finite element model was a part of the three-dimensional space in Fig. 1(a). The reason for this decision was when the dimensions of the analytical model shown in Fig. 1(a) and particle dispersion space are the same, there would be regions without particles near the edges. It is possible to create a model with larger thickness (e.g., cube). However, in order to use an element size with sufficient spatial resolution with this model, a massive number of elements become necessary, and such a calculation using the finite element method (FEM) is presently too difficult. Therefore, the present finite element model was a thin and flat model (Fig. 1(b)). The analytical model has the center of the three-dimensional region extracted. If we assume the origin of the three-dimensional region and the analytical model, a coordinate point in the three-dimensional region, $x = 150$ nm, $y = 150$ nm, $z = 650$ nm, and the origin of the analytical model become the same. On the other hand, analysis of the localized particle intervals used this three-dimensional region that is the basis of the finite element model to obtain particle intervals (representative length of microstructure) based on the three-dimensional particle distribution.

The particle interval for each element; in other words, the representative length involved with slip deformation, was analyzed as follows. Analysis of the particle interval was performed independently for each element and each slip system. Here, we present an example for one element and one slip system. Crystal orientation of this slip system is $\kappa = 77.33^\circ$, $\theta = 24.73^\circ$, and $\varphi = 257.33^\circ$ when using the definition of Euler angle in Fig. 1(c). Next, we discuss the slip plane and slip direction shown in Fig. 1(b). As shown in Fig. 2(a), we identify a plane parallel to the slip plane of the slip system to be analyzed that passes through the center of the element of interest in the analytical three-dimensional model. Among particles in the plane identified in Fig. 2(b), particles surrounding the element of interest are further identified. These particles surrounding the element of interest is defined as follows. We performed Voronoi tessellation using the center point of the element of interest and the center point of the particles, and as in the two-dot chain line shown in Fig. 2(b), we determine and define particles that form the core of the Voronoi region adjacent to the Voronoi...
region of the element of interest as particles surrounding the element of interest. The interval between particles surrounding the element of interest (Fig. 2(c)), $l_i$, is defined as the

Fig. 1. (a) Distribution of particles in 3 dimensional space. The number of particles is 1,000. Diameter and volume fraction of distributed particles are 39 nm and 1.24%, respectively. (b) The model used for the finite element analysis. The model is a part of the 3 dimensional region shown in (a). (c) Definition of the Euler angles between the crystal and specimen coordinate systems.

Fig. 2. Determination of the local particle spacing around a point in the specimen. (a) Extraction of particles on the slip plane passing through the point of interest from 3 dimensional region of Fig. 1(a). (b) Selection of particles surrounding the point of interest on the slip plane. (c) Distance between surrounding particles.
localized representative length of the microstructure.

In most cases, the evaluation method of the yield stress of dispersion hardened alloys is based on the study of, “dislocation movement of the region in which particles are irregularly dispersed” calculated by Foreman and Makin. The calculation by Foreman and Makin shows that after the moving dislocation becomes caught by a group of particles, it passes through wide areas in between particles that are irregularly dispersed. Plastic deformation in this model is assumed to be occurring preferentially in this region, where slip deformation occurs with ease. In other words, in this model, macroscopic yielding occurs when moving dislocations pass through a large number of localized particle intervals $l_{\text{ave}}$. Since localized CRSS is determined by $l_{\text{ave}}$, the macroscopic yield stress is likely dominated by $l_{\text{ave}}$. If the dislocation source is present in the region of the element of interest, for the dislocation loop released from this dislocation source to continuously move, the existence of a large number of moving dislocations that pass through the narrowest interval ($l_{\text{min}}$) among particles surrounding this region is necessary. Therefore, since localized CRSS is determined by $l_{\text{min}},$ localized yield stress is dominated by $l_{\text{min}}.$ As such, it is unclear which interval of particles is the appropriate expression of the microstructure characteristics. Therefore, in this paper, in addition to $l_{\text{max}}$ and $l_{\text{min}}$ without limiting to a specific mechanism, we considered the average interval $l_{\text{ave}}$ of particles surrounding the element of interest as the representative length of microstructure. Under these three conditions, we performed the analysis to examine the representative length of the localized microstructure of dispersion hardened alloys. Here, $l_{\text{ave}}$ is defined with the following equation, and $n$ is 8 in Fig. 2(c).

$$l_{\text{ave}} = \frac{1}{n} \sum_{i=1}^{n} l_{i} \text{..................................(4)}$$

### 3. The Crystal Plasticity Analysis Model

For the analysis in the present paper, we used the three-dimensional crystal plasticity analysis software code based on FEM.\textsuperscript{10,11} In past studies,\textsuperscript{7,8} the conventional crystal plasticity model has been expanded to include dispersion hardened alloys. However, in the past models, it was limited to the introduction of the representative length of the microstructure for each phase and grain of the crystal plasticity model. In the present paper, we expanded the model even further, so that the representative length of the localized microstructure could be introduced to the model for each element. Here, let us discuss the CRSS model dependent on the representative length of microstructure and the model associated with dislocation density.

The CRSS of a slip system, $n$, for each element is provided by the following equation with the extended expression of the Bailey-Hirsch type model:\textsuperscript{12}

$$\dot{\rho}^{(m)} = \dot{\rho}^{(m)}(T) + \sum_{n=1}^{N} \Omega^{(m,n)} a \mu b \sqrt{\dot{\rho}^{(m)} + \frac{\mu b}{f^{(m)}}} \text{............(5)}$$

where $T$ is temperature, the first term on the right side of Eq. (5) is the lattice friction stress $\dot{\rho}^{(m)}(T)$ of the slip system $n$, the second term is the deformation resistance due to dislocation accumulated in the crystal, and $\rho^{(m)}$ is the density of statistically stored (SS) dislocations accumulated in the slip system $m$. $\Omega^{(m,n)}$ is the moving dislocation of the slip system $n$ and interaction matrix of dislocation accumulated in the slip system $m$. The fact that the interaction of moving dislocations and accumulated dislocations is different based on the combination of the slip system is expressed by the values of the matrix elements. In the present paper, we assumed isotropic hardening where $\Omega^{(m,n)}$ was 1. $N$ is the number of slip systems. $a$, $\mu$, and $b$ are a numerical coefficient, elastic shear modulus and the magnitude of Burgers vector, respectively. The third term on the right side is the Orowan stress value dependent on the representative length $f^{(m)}$ of microstructure. For example, it has been proposed to use grain diameter\textsuperscript{12} and lamellar thickness\textsuperscript{3} as the representative length of the microstructure for polycrystals and lamellar structures, respectively. In the present paper, we used the method discussed in Chapter 2 to calculate the interval of particles surrounding the element and used this value as the representative length of microstructure for each element.

In crystal plasticity analysis based on continuum mechanics, dislocation is separated into SS dislocations and geometrically necessary (GN) dislocations.\textsuperscript{14}

The increase in the SS dislocation density in the slip system $n$ is provided with the following equation with the Kocks-Mecking model:\textsuperscript{15,16}

$$d\rho^{(n)} = \frac{1}{D/b} \frac{dL^0}{b} \text{.....................(6)}$$

where $L^0$ is the mean free path of the dislocation in a slip system $n$. $D$ is the coefficient associated with the annihilation of the accumulated dislocations. The value of $D/b$ was proposed to be between 4.1–4.5;\textsuperscript{17} thus, we chose $D = 5b$ for the present paper. Equation (6) is based on the fact that the dislocation that increased with plastic deformation accumulates in the material after moving the distance of $L$, and if the density of accumulated dislocations, $\rho^{(n)}$, becomes high, this dislocation, and the dislocation of the opposite sign at a distance of about $D$ annihilate each other.

The mean free path $L^0$ of the dislocation is the distance from where the dislocation starts moving on the slip plane and is captured by an obstacle. A possible obstacle can be forest dislocations in the slip system $n$; in other words, dislocations accumulating in other slip systems from the viewpoint of the dislocation of interest. In dispersion hardened alloys, dispersed particles capture moving dislocations. Therefore, the mean free path of dislocation depends on the average interval of dislocation accumulated in the crystal or the distance between dispersed particles, whichever is smaller, and is determined by the following equation:

$$L = \text{Min} \left[ \sum_{n=1}^{N} w^{(m)} \left( \rho^{(m,n)} + \left\| \rho_{G}^{(n)} \right\| \right) , \frac{c^*}{\left\| \rho_{G}^{(n)} \right\|} \right] \text{............(7)}$$

where $\left\| \rho_{G}^{(m,n)} \right\|$ is the density norm of the GN dislocations that accumulated in the slip system $m$ as it will be discussed later. In Eq. (7), SS dislocations and GN dislocations are involved with the mean free path of the slip system $n$ through the weight $w^{(m)}$ at the same time as the mean free
Path being involved with accumulation of SS dislocation by means of Eq. (6). Here, \( w^{nm} = 0 \) for slip systems with the same slip plane, and \( w^{nm} = 1 \) for slip systems with a different slip plane. \( c^* \) is a numerical coefficient associated with the resistance of accumulated dislocation against moving dislocations, and empirically, the values between 10 to 100 is usually used.\(^{10}\) In the present paper, we used 15. \( n^* \) is a numerical coefficient that is dependent on the movement state of the dislocation in the crystal where micro particles are dispersed, and its value becomes 1 if the moving dislocation is captured in each average interval of dispersed particles. Previous studies have shown that in the crystal where hard particles are irregularly dispersed, \( n^* = 2 \) is a good approximation.\(^{7}\) However, in the present paper, we first performed the calculation with \( n^* = 1 \). We will refer to the first and second elements on the right side of Eq. (7) as effective forest dislocation spacing and effective particle spacing (associated with the mean free path of dislocation), respectively in the present paper. With Eq. (7), if the dislocations are accumulated densely in the crystal, the effective forest dislocation spacing becomes the mean free path of dislocation, but if its effective particle spacing is less than the effective forest dislocation spacing, the effective particle spacing becomes the mean free path of dislocation.

Density of the edge component and the screw component of GN dislocations are obtained in the partial derivative of plastic shear strain \( \gamma \) with respect to the \( \zeta^{(n)} \) and \( \zeta^{(n)} \) directions as follows:\(^{1}\)

\[
\rho_{\text{edge}}^{(n)} = -\frac{1}{b} \frac{\partial \gamma^{(n)}}{\partial \zeta^{(n)}} \tag{8}
\]

\[
\rho_{\text{crew}}^{(n)} = \frac{1}{b} \frac{\partial \gamma^{(n)}}{\partial \zeta^{(n)}} \tag{9}
\]

where \( \zeta^{(n)} \) and \( \zeta^{(n)} \) are parallel and normal to the slip direction on the slip plane. \( \mid \rho_c^{(n)} \mid \) is the density (density norm) of the GN dislocation in the slip system \( n \) consisting of two components, and is given by:

\[
\mid \rho_c^{(n)} \mid = \sqrt{\left(\rho_{\text{edge}}^{(n)}\right)^2 + \left(\rho_{\text{crew}}^{(n)}\right)^2} \tag{10}
\]

4. Analytical Conditions

The analytical target of the present paper is particle dispersion strengthened steel\(^9\) in which hard VC particles are dispersed and precipitated in the ferrite matrix. The analytical model extracted a portion from the region in which fine particles were irregularly dispersed in the matrix crystal (Fig. 1(b)). In the present paper, we used a flat model with about 10 particles dispersed. On the other hand, the representative length of the localized microstructure, which is an important parameter of analytical conditions, is determined based on the region where 1 000 particles were irregularly dispersed in a three-dimensional space as discussed in Chapter 2. The conditions were a particle diameter of 39 nm, and a volume fraction of 1.24\% based on the experiment.\(^9\) In this manner, yield stress in the three-dimensional particle distribution and work hardening properties due to dislocation accumulation are expressed. Dimensions of the model was \( 1 \mu m \times 1 \mu m \times 0.0066 \mu m \). The number of elements was \( 300 \times 300 \times 2 = 180,000 \) elements.

Figures 3(a), 3(b), and 3(c) show localized \( l_{\text{min}} \), \( l_{\text{ave}} \), and \( l_{\text{max}} \) distributions obtained by considering three-dimensional particle distribution in the same region. A grayscale contour is used to show the values from 40 nm to 700 nm, where the maximum value in Fig. 3(c) was 1 065 nm. The average interval of particle centers obtained from the particle diameter using Eq. (2) and volume fraction, was 253 nm; thus, particle intervals in the three-dimensional region with irregularly dispersed particles was four times wider than the average interval in some places.

The primary material constants used for analysis are shown in Table 1. The matrix was ferrite with a BCC structure, and we used the elastic compliance\(^19\) of a single iron crystal at room temperature as the elastic constant. At this time, the Young’s modulus of the main axial direction (100) was about 130 GPa. The lattice friction stress was 50 MPa, and numerical coefficient \( a \) of extended expression of the Bailey-Hirsch type model (Eq. (5)) was 0.1. The second phase particles to be dispersed were VC with FCC structure, and elastic compliance was determined so that Young’s modulus, Poisson’s ratio, and elastic shear modulus value\(^20\) would be 430 GPa, 0.25, and 157 GPa, respectively at room temperature. VC is very hard and does not easily occur.

Fig. 3. Distribution of the representative length on the primary slip system determined by (a) \( l_{\text{ave}} \), (b) \( l_{\text{ave}} \) and (c) \( l_{\text{max}} \), respectively.
plastic deformation; thus, the lattice friction stress of the VC was set sufficiently large to prevent slip deformation. For the crystal orientation, we used $\kappa=77.33^\circ$, $\theta=24.73^\circ$, and $\varphi=257.33^\circ$ using the definition of the Euler angle (Fig. 1(c)) for both the matrix and the second phase. The primary slip system in this direction was (101)[111], and the normal direction of the slip plane and the slip direction were $x'$ and $y'$, respectively (Fig. 1(b)). If we set the $y'$-axis direction as the tensile axis, the Schmid factor of the primary slip system becomes 0.5. The slip planes of the matrix with BCC structure were {110} and {112}; and thus, there would be 24 active slip systems. However, with dispersion hardened alloys, it is known that the activity of the secondary slip system has little impact on the macroscopic mechanical responses with up to a nominal strain of 0.05.9) Thus, in the present paper, we assumed only the primary slip system would be active for simplification.

5. Results and Discussions

5.1. Yield Behavior

Figure 4 shows the nominal stress-strain curves obtained from tensile deformation analysis using crystal plasticity analysis. The results of the referenced experiment are shown with a solid line,9) and the analytical results of the present study is shown with symbols and a dashed line. Symbols, ○, □, and △ represent results for localized particle intervals of $l_{\text{ave}}$, $l_{\text{max}}$, and $l_{\text{ave}}$, respectively. If we assume 0.2% offset stress as the yield stress, the yield stress of the $l_{\text{ave}}$ interval becomes about 600 MPa. The yield stress of the experiment we referred to was about 340 MPa, and the yield stress of the $l_{\text{ave}}$ interval was about 1.8 times higher than the present experiment. The yield stress of the $l_{\text{max}}$ interval was about 270 MPa, being about 0.8 times lower than the experimental result. On the other hand, the yield stress of the $l_{\text{ave}}$ interval was about 350 MPa, mostly consistent with the experimental result.

In the case of the $l_{\text{ave}}$ interval, the yield stress was twice as large as the experimental result, deviating notably from the stress-strain curve of the experiment. In contrast, in the case of the $l_{\text{max}}$ interval, the yield stress remained at about 0.8 times that of the experiment. The reason for this is because in Eq. (5), which determines the CRSS, the value for the Orowan stress is obtained with $\mu b / l$. In other words, as shown in Fig. 5, the contribution of the Orowan stress to the CRSS is in inverse proportion to the particle interval $l$. Figure 5 shows that as the particle interval decreases, the Orowan stress increases, and its rate of increase varies based on the particle interval. For example, the average value of $l_{\text{ave}}$, $l_{\text{min}}$, was 96 nm with an Orowan stress of 286 MPa, the average value of $l_{\text{ave}}$, $l_{\text{ave}}$, was about 263 nm with an Orowan stress of 105 MPa, and the average value of $l_{\text{ave}}$, $l_{\text{max}}$, was about 417 nm with Orowan stress of 66 MPa. If we add the lattice friction stress of 50 MPa, and consider the value of the CRSS, the CRSS for $l_{\text{ave}}$ is 336 MPa, which is 2.2 times higher than the CRSS for $l_{\text{ave}}$. But since the CRSS for $l_{\text{ave}}$ is 116 MPa, it remains at 0.75 times the CRSS for $l_{\text{ave}}$. Therefore, the calculation result for the $l_{\text{ave}}$ interval does not deviate much from calculation of the $l_{\text{ave}}$ interval and experimental result unlike the result of $l_{\text{ave}}$ interval.

In the present paper, the irregular distribution of particles

| Table 1. Material data used for the analysis. |
|---------------------------------------------|
| iron | VC |
|------|----|
| $s_{11}$ | 0.7720 | 0.2325 |
| $s_{12}$ | -0.2850 | -0.0512 |
| $s_{44}$ | 0.9020 | 0.6369 |
| Magnitude of Burgers vector [nm] | 0.248 |
| Lattice friction stress [MPa] | 50 |
| Initial dislocations density $[m^{-2}]$ | $24.0\times10^8$ |

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was generated with uniform random numbers, and there is no extreme bias in particles. Therefore, wherever the slip plane is assumed in the three-dimensional space, the dispersion of particles on the plane could be close to the slip plane, defined by Foreman and Makin in which particles are irregularly dispersed. We analyzed the particle interval on such a slip plane and performed CP-FEM with an average interval of particles surrounding each elemental point as the representative length of the microstructure. In this manner, we showed that the result of obtaining the shear stress for the yield by calculating the movement of the dislocation, and the result of mechanical calculation with FEM using a dislocation model presented almost the same yield behavior.

Let us now focus on the result for $l_{ave}$ interval. With the method of the present paper, the localized difference in representative length of the microstructure causes the initial CRSS to be determined by Eq. (5) to differ between each element. If we convert the average CRSS (164 MPa) for each element of the matrix to the yield stress with a Schmid factor of 0.5, it becomes 328 MPa, which is consistent with the value of the 0.2% offset yield stress obtained from the experiment (340 MPa). Here, the average value of representative length of each element was 263 nm. On the other hand, the average surface interval of the particles in the square array approximation obtained by subtracting average diameter of particles from Eq. (2) is 223 nm. The ratio of these values was 1.18. This value was slightly smaller but close to the coefficient (1.25) that corrects the difference between the shear stress necessary for dislocation to pass through the region with irregularly dispersed particles, proposed by Foreman and Makin and the Orowan stress obtained from the average interval in the square array approximation.

Next, let us look at the details of the beginning of the microscopic slip deformation and the slip deformation during macroscopic yielding in the analytical model with locally different CRSS distributions (Fig. 4). Figure 6 shows the representative length of each element in the $l_{ave}$ interval using frequency distribution. The maximum, minimum, and average values of the representative lengths were 627 nm, 46 nm, and 263 nm, respectively, with a standard deviation of 628 nm. In the initial stage of deformation when the nominal strain is 0.00152, and the nominal stress is 256 MPa; thus at 73% stress level of the 0.2% offset stress, 6.6% of the matrix element volume experienced plastic strain. Microscopic yielding occurred at the early stage of deformation, where plastic deformation began from the area of wide representative length. Here, the top 6% of the matrix element volume with high representative length had a value of about 350 nm or higher. In contrast, at 0.2% offset stress, at a nominal strain of 0.0038–0.0044 it becomes macroscopic yielding, 83%–87% of the matrix element volume experienced plastic strain. Meaning, about 10% of the matrix element volume was the region of non-plastic deformation. As such, during macroscopic yielding of dispersion hardened alloys, not only stress partitioning is observed by the hard particles and the soft matrix, but also stress partitioning occurs in the regions with wide and narrow particle intervals in the matrix. Such stress partitioning due to elastoplastic deformation is generally observed in dual phase steel, but it was discovered that it is also seen in the matrix of dispersion hardened alloys.

Here, in the $l_{ave}$ interval, the average of the top 85% of the representative length for the matrix element is about 280 nm. The ratio of this value to the average particle surface interval in the square array approximation (223 nm) is about 1.26, which is quite consistent with the above-mentioned correction factor presented by Foreman and Makin (1.25). Let us discuss the factors below. The image of the dislocation passing over the slip plane with irregularly dispersed particles calculated by Foreman and Makin was expressed as follows. When the moving dislocation passes between particles, in the region of dense and narrow particle intervals, it does not pass through the group of particles by the Orowan mechanism but avoids such groups of particles. In other words, moving dislocations bypass by treating the group of particles as a mass, leaving a dislocation loop around such a mass. This shows that there is no slip deformation in the region with dense particles distribution. Calculation by Foreman and Makin defines the stress of when the dislocation has finished passing through the region with a large number of dispersed particles as yield stress. Therefore, though the non-slip region is included in yielding as discussed above, the deformation resistance of such non-slip deformation region would not appear in the calculation due to its calculation properties. Therefore, the correction factor shown by Foreman and Makin (1.25) is the value obtained when only considering the slip deformation region. This is why it is consistent with the correction factor of 1.26 obtained in the present study by only considering the slip deformation region.

The present result shows that during macroscopic yielding of dispersion hardened alloys, there are elastic deformation regions and elastoplastic deformation regions. However, it...
It is difficult to accurately determine the distribution of the elastoplastic deformation regions that should be reflected on the stress-strain curve in the experiment. Therefore, we could set the correction factor obtained from the average particle interval of the whole matrix as 1.18. In addition, the correction factor likely changes with the dispersion of particles. In the present paper, we dispersed particles using the uniform random number and analyzed particle intervals. As a result, we discovered that localized particle interval distribution was normal distribution. If the particle interval distribution is lognormal or bimodal, it is unlikely to see the plastic deformation distribution and volume fraction that are similar to the present results. Thus, we need to examine the correction factor for the particle interval that expresses the yield strength of dispersion hardened alloys with different particle distributions in the future.

5.2. Work Hardening Behavior
Next, in this Section, we examine properties of work hardening. As shown in Fig. 4, if we focus on the result of the $l_{\text{ave}}$ interval where the yield stress was consistent, the work hardening rate was higher than the experimental value. In this calculation, dimension factors associated with the start of slip deformation, and the dimension factors involved with the accumulation of dislocations in Eq. (7) are the same, and the same representative length of microstructure is used. However, the authors pointed out the necessity of making these dimension factors different.7) Thus, in the present paper, we set the numerical coefficient $n^*$ that is dependent on the style of movement of the dislocation in the crystal in Eq. (7) as 2. Figure 7 shows the stress-strain curve obtained from this calculation. The solid line shows the experimental result that we referred to, and dashed line and ▲ symbol show the result from the calculation. Both yield stress and work hardening rate are consistent with

![Nominal stress-strain curves obtained by experimental and numerical analysis.](image)

Fig. 7. Nominal stress-strain curves obtained by experimental and numerical analysis.

![Distribution of plastic shear strain on the primary slip system when the nominal tensile strain is (a) 0.00165, (b) 0.00314, (c) 0.02 and (d) 0.05, respectively.](image)

Fig. 8. Distribution of plastic shear strain on the primary slip system when the nominal tensile strain is (a) 0.00165, (b) 0.00314, (c) 0.02 and (d) 0.05, respectively.
experimental results, recreating the stress-strain curve from the experiment. In short, similar to the conclusion in the previous report, the mean free path of dislocation for this alloy should be double the average particle interval for good approximation.

Next, let us discuss development of the slip deformation in the microstructure. Figure 8 shows plastic shear strain distribution ($\gamma_{xy}$) of the primary slip system for each nominal strain value. During the initial stage of deformation shown in Fig. 8(a) (nominal strain of 0.00165), the region where plastic deformation has begun was the region with sufficiently large representative length as shown in Fig. 3; in other words, it is limited to the region of low CRSS. Therefore, there is plastic strain dependent on the representative length distribution, where plastic strain is spread along the slip direction. When deformation progresses, plastic strain occurs in the areas that are wider in the matrix and propagates. When nominal strain is 0.05, as shown in Fig. 8(d), the value of strain itself is not uniform, and plastic strain occurs in about 99.7% of the matrix. Unlike the initial stage of deformation, in addition to the plastic strain distributed along the slip direction, there is a region with notable plastic strain in the normal direction to the slip plane. Such development of strain distribution is closely related to the stress field that forms in the structure.

Figure 9 shows the stress distribution at nominal strain of 0.05. Figure 9(a) is $\sigma_y$ distribution, Fig. 9(b) is $\sigma_x$ distribution, and Fig. 9(c) is $\tau_{xy}$ distribution. The stress distribution around the particles is similar to the result of the three-dimensional stress analysis of the model that includes one particle, where high compressive and tensile stress concentrations around particles stretch in the slip direction and the normal direction of the slip plane. The stress fields around each particle become connected, forming a non-uniform stress field in the wide area of the matrix.

As it was shown in Figs. 8(a) and 8(b), plastic slip in the initial stage of deformation begins in the region with high representative length of the microstructure, and subsequently, plastic slip is driven to the high stress field created by the presence of particles and spreads. When the nominal strain was 0.05, as stress distribution (Fig. 9) and plastic strain distribution (Fig. 8(d)) show, the plastic strain distribution is highly dependent on the stress field created by particles.

Non-uniform plastic strain distribution contributes to the accumulation of GN dislocations. Figure 10 shows the distribution of the GN edge dislocation density when the nominal strain was 0.05. Positive and negative edge dislocations accumulate at high density, sandwiching the particles. High-density bands of GN dislocations stretched in the normal direction of the slip plane, spreading over a wide area of the matrix. Edge dislocation accumulating at high density like this and accumulation of edge dislocation stretching in the normal direction of the slip plane from particles, have been observed in experiments. High-density bands consisting of positive and negative edge dislocations had a dislocation structure equivalent to the kink band. Dislocations with a structure equivalent to the kink band forms at a high density of $1 \times 10^{15} \text{m}^{-2}$ in the initial stage of deformation with a nominal strain if about 0.01. If the high-density band of the GN dislocations shown in Fig. 10 was about $\pm 5 \times 10^{15} \text{m}^{-2}$ or higher, the high-density band consisting of a pair of positive and negative edge dislocations equivalent to the kink band is not only present around particles, but spreads widely at double the length of the average interval of the dispersed particles $\lambda (= 286 \text{ nm})$ in the matrix. Since the kink band is a factor for transition from stage II with a high work harden-
ing rate of single crystal material, the high-density band of edge dislocations created in the initial stage of deformation by dispersed particles contributes to the high work hardening rate of the dispersion hardened alloys.

6. Conclusions

We analyzed the localized representative length of microstructures based on a three-dimensional particle distribution, and using the representative length, we examined the relationship between microscopic deformation and macroscopic mechanical responses in dispersion hardened alloys with CP-FEM.

I. The stress-strain curve that recreates the experimental conditions well is obtained by assuming that the localized representative length (particle interval) of the microstructure, where particles are dispersed, as the average interval of particles surrounding the point.

II. Distribution of the representative length that determines the localized CRSS has twice as much dispersion as the average. Macroscopic yielding (0.2% offset stress) under such a large dispersion only experienced slip deformation in 80 to 90% of the matrix element. In other words, during macroscopic yielding of the dispersion hardened alloys, the region of elastic deformation and the region of elastoplastic deformation become mixed, leading to stress partitioning. Hence, the yield stress of dispersion hardened alloys is determined by the inhibition of moving dislocations (Orowan stress) by particles and stress partitioning in the elastic deformation region.

III. The beginning of plastic slip deformation is dependent on the distribution of particle intervals in the matrix, and if deformation of material continues after reaching macroscopic yielding, the plastic slip deformation of the matrix progresses, and is dependent on the high stress field created by the hard particles that are difficult to deform plastically. As such, plastic strain distribution unique to dispersion hardened alloys and GN dislocation accumulation structures are created.

IV. In accumulated GN dislocations, positive and negative edge dislocations accumulate densely to sandwich particles, creating a structure equivalent to a kink band. The formation of kink bands is known to contribute to the transition to stage II with a high work hardening rate in single crystals. In dispersion hardened alloys, dispersion of numerous numbers of particles form multiple kink bands; thus, it could be a factor for high work hardening rates expressed by dispersion hardened alloys.

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