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THREE-DIMENSIONAL STRUCTURES OF THE GEOMETRICALLY NECESSARY DISLOCATIONS GENERATED FROM NON-UNIFORMITIES IN METAL MICROSTRUCTURES

Tetsuya Ohashi

Kitami Institute of Technology,
Koencho 165, Kitami, 090-8507, Japan
E-mail: ohashi@newton.mech.kitami-it.ac.jp

Abstract: Slip deformation in microstructures of f.c.c. type metals are analyzed by a finite element technique and the density distribution of the geometrically necessary dislocations is evaluated. Results show development of wall like structure of dislocations in some of single crystals and also dislocation half loops within grains and their pile up at grain boundaries in multiple crystal models.

Key words: single and multiple crystals, microstructure, crystal plasticity analysis.

1. INTRODUCTION

Development of dislocation structures during deformation has long been studied. Two types of dislocation densities can be evaluated; the statistically stored (SS) and the geometrically necessary (GN) dislocations (Ashby, 1970). Density increment of the SS dislocations is related to the increment of plastic shear strain and the mean free path of moving dislocations, while the density of the GN ones is related to the spatial gradient of the plastic shear strain on slip systems. Scale dependent characteristics of the GN dislocations have been attracting much attention in the research field of solid mechanics and some models for scale dependent crystal plasticity constitutive laws were proposed (for example, Fleck, *et al.*, 1994). On the other hand, the structure of the aggregate of the GN dislocations is less studied, although some typical structures such as the Orowan loops formed around precipitates or piled up dislocations at grain boundaries result from non-uniform deformation and thus, be understood as the ones made up of the GN dislocations.

In the present paper, we analyze slip deformation in single and multiple crystals of the face centered cubic type metals and evaluate edge and screw components of the GN dislocations. Their density norm and direction vector of the dislocation line segments are also deduced from the edge and screw components. After this process, we can reconstruct images for three-dimensional structures of the GN dislocations in deformed microstructures.

2. BASIC EQUATIONS

Slip deformation is supposed to take place on {111} crystal plane and in <110> crystal direction. The activation condition of the slip system *n* is supposed to be given by the Schmid law;

$$P_{ij}^{(n)}\sigma_{ij} = \theta^{(n)}, \ P_{ij}^{(n)}\dot{\sigma}_{ij} = \dot{\theta}^{(n)}, \quad (n = 1,\cdots,12), \tag{1}$$

and,

$$P_{ij}^{(n)} = \frac{1}{2}\left(\nu_i^{(n)}b_j^{(n)} + \nu_j^{(n)}b_i^{(n)}\right), \tag{2}$$

where, σ_{ij} and $\theta^{(n)}$ denote the stress and the critical resolved shear stress on the slip system *n*, respectively. The slip plane normal $\nu_i^{(n)}$ and the slip direction $b_i^{(n)}$ define the Schmid tensor $P_{ij}^{(n)}$. Quantities with dot indicate increments of them. Increment of the critical resolved shear stress is written as follows;

$$\dot{\theta}^{(n)} = -q\dot{T} + \sum_m h^{(nm)}\dot{\gamma}^{(m)}. \tag{3}$$

Here, $\dot{T}$ and $\dot{\gamma}^{(m)}$ denote the increments of temperature and the plastic shear strain on slip system *m*, respectively. If the deformation is small and rotation of the crystal orientation is neglected, the constitutive equation is written as follows (Hill, 1966, Ohashi, 1987, 1994),

$$\dot{\sigma}_{ij} = D_{ijkl}(\dot{\varepsilon}_{kl} - \alpha_{kl}^{*}\dot{T}), \tag{4a}$$

where,

$$D_{ijkl} = [S^{e}_{ijkl} + \sum_{n}\sum_{m}\{h^{(nm)}\}^{-1}P^{(n)}_{ij}P^{(m)}_{kl}]^{-1}, \qquad (4b)$$

and,

$$\alpha^{*}_{kl} = \delta_{kl}\alpha + q\sum_{n}\sum_{m}\{h^{(nm)}\}^{-1}P^{(m)}_{kl}. \qquad (4c)$$

S^{e}_{ijkl}, α, and δ_{kl} denote elastic compliance, thermal expansion coefficient and the Kronecker's delta, respectively. Summation is made over the active slip systems.

Let us suppose that the critical resolved shear stress is a function of the Bailey-Hirsch type and given by the following equation (Ohashi, 1987, 1994);

$$\theta^{(n)} = \theta_0(T) + \sum_{m}\Omega^{(nm)}a\mu\tilde{b}\sqrt{\rho^{(m)}_{a}}, \qquad (5)$$

where, $\theta_0(T)$ denotes the lattice friction term, which is, in general, dependent on temperature, and $\rho^{(m)}_{a}$ denotes the dislocation density that accumulate on the slip system *m*. Reaction between dislocations on slip systems *n* and *m* defines the magnitude of the interaction matrix $\Omega^{(nm)}$. In the present study, we choose parameters to express pseud-isotropic hardening character for every slip system.

The dislocation density on the slip system *n* is given by the following equation;

$$\rho^{(n)}_{a} = s\rho^{(n)}_{S} + g\left\|\rho^{(n)}_{G}\right\|, \qquad (6)$$

where, $\rho^{(n)}_{S}$ and $\left\|\rho^{(n)}_{G}\right\|$ denote the densities of the SS and GN dislocations, respectively.

Increment of the SS dislocations is given as follows;

$$\dot{\rho}^{(n)}_{S} = c\dot{\gamma}^{(n)} \Big/ \tilde{b}L^{(n)}, \qquad (7)$$

where, $L^{(n)}$ is the mean free path of dislocations on slip system *n* and, in this paper, we use the modified Seeger's model for it;

$$L^{(n)} = \begin{cases} L_0^{(n)} \\ \dfrac{\Lambda}{\sum_k \gamma^{(k)} - (\gamma^{**} - \Lambda / L_0^{(n)})} \end{cases}, \quad \text{for} \begin{cases} \text{single slip} \\ \text{multiple slip} \end{cases}, \tag{8}$$

where, Λ is a material constant and γ^{**} denotes the plastic shear strain when multiple slip start.

The edge and screw components of the geometrically necessary dislocations are obtained from the strain gradients (Ohashi, 1997);

$$\rho_{G,edge}^{(n)} = -\frac{1}{\tilde{b}}\frac{\partial \gamma^{(n)}}{\partial \xi}, \qquad \rho_{G,screw}^{(n)} = \frac{1}{\tilde{b}}\frac{\partial \gamma^{(n)}}{\partial \zeta}. \tag{9}$$

Here, ξ and ζ denote directions parallel and perpendicular to the slip direction on the slip plane, respectively. Norm of two components defines the scalar density for the GN dislocations,

$$\left\| \rho_G^{(n)} \right\| = \sqrt{\left(\rho_{G,edge}^{(n)}\right)^2 + \left(\rho_{G,screw}^{(n)}\right)^2}. \tag{10}$$

Evaluation of the edge and screw components for the GN dislocations enables one to calculate the tangent vector $\mathbf{l}^{(n)}$ of the dislocation line segments (Ohashi, 1999);

$$\mathbf{l}^{(n)} = \frac{1}{\left\| \rho_G^{(n)} \right\|}\left(\rho_{G,screw}^{(n)} \cdot \mathbf{b}^{(n)} + \rho_{G,edge}^{(n)} \cdot \mathbf{b}^{(n)} \times \mathbf{v}^{(n)}\right). \tag{11}$$

Data for GN dislocations are obtained for each finite element and then, we can draw line segments of dislocations in three-dimensional space. We will draw one line segment at the center of each element. Direction of the line segment is given by eq. (11) and its length and thickness is determined by the density norm $\left\| \rho_G^{(n)} \right\|$.

Numerical parameters s and g in the equation (6) are introduced to control the complexity of the simulation. In the present paper, we suppose s=1 and g=0 for simplicity and the strain hardening coefficients in equation (3) are given by the following equation;

$$q = \frac{\partial}{\partial T}\theta_0(T), \tag{12a}$$

$$h^{(nm)} = \frac{1}{2} ac\Omega^{(nm)} / \left[L^{(m)} \sqrt{\rho_a^{(m)}} \right]. \tag{12b}$$

3. RESULTS AND DISCUSSION

3.1 Single crystals with non-uniform initial dislocation densities

Let us examine tensile deformation of single crystal bars where distribution of the initial dislocation densities is not uniform. Figure 1 shows the geometry of the specimen employed for the analysis. The specimen is divided into 8x30x8 finite elements of composite type with eight nodes and the top surface is subjected to a uniform displacement in y direction, while the bottom surface is fixed. Initial dislocation densities on twelve slip systems in each elements are decided by a normally distributed deviates with the mean value $\rho_0 = 10^9$ m^{-2}. Crystal orientation of specimens #1 - #3 is the same and positioned so as that the Schmid factor of the primary slip system is at the maximum value of 0.5. Slip plane and slip direction for the primary system in the specimens #1 - #3 are schematically shown in Figure 1. While, the orientation of the specimen #4 is very close to double slip orientation. The standard deviations of the initial dislocation densities in the specimens #1 - #3 are 0, $0.1\rho_0$, and $0.25\rho_0$, respectively. The standard deviation for the specimen #4 is $0.1\rho_0$.

Figure 2 shows numerical results for the load-elongation curve. In specimens #2 - #4, slip on a secondary (conjugate) slip system superimpose after some amount of slip on the primary one and this causes decrease in the mean free path of the dislocations as shown in eq. (8) and result in the onset of the deformation stage II. Duration of the stage I depends on the crystal orientation and the magnitude of the non-uniformity of the initial dislocation density. Figure 3 compares density distributions of the GN and SS dislocations on the primary slip system in the specimen #3 when the average tensile strain is 4.625%. Walls of GN dislocations, which consist mainly of edge type dislocations, develop in the direction perpendicular to the slip plane and extend as wide as the width of the whole specimen. On the other hand, the distribution of the SS dislocations remains to be random, although the density is one order higher than that of GNDs. Tri-axial stress field, which accompanies to non-uniform slip is supposed to be responsible to the generation of the long-range structure of GNDs.

3.2 A multi-crystal plate of copper

Figure 4(a) shows the multi-crystal model we employed in this study.

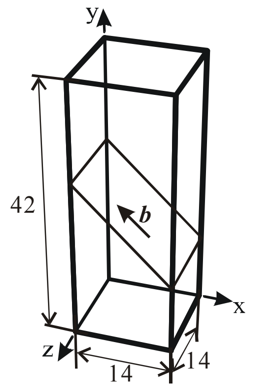

Figure 1 Geometry of the single crystal specimen employed in this study. Dimensions are given in unit of μm.

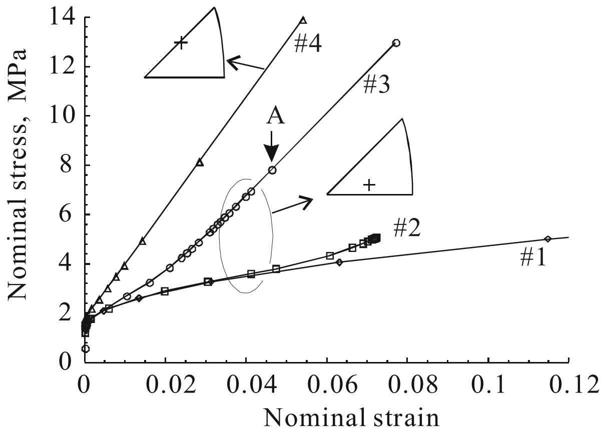

Figure 2 Load-elongation curves calculated for single crystal specimens #1 - #4. The initial dislocation density for the specimens #2 - #4 is not uniform and given by normally distributed deviates. See text for details.

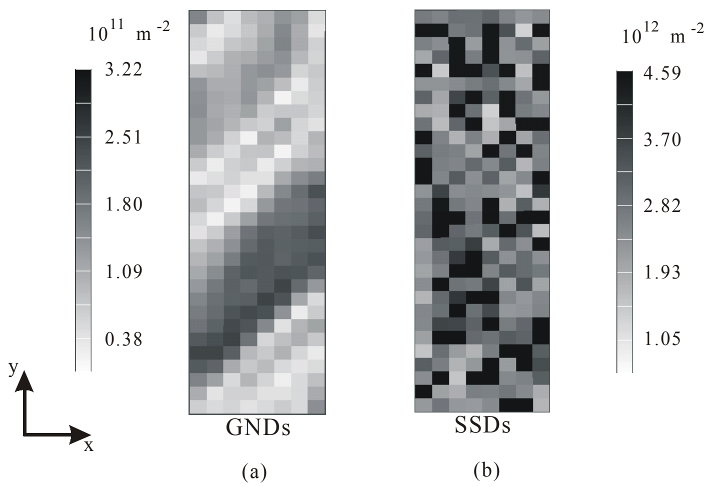

Figure 3 Cross sectional views for the distribution of the geometrically necessary dislocations (a), and statistically stored ones (b) in the single crystal specimen #3, when the mean tensile strain is 4.625 %.

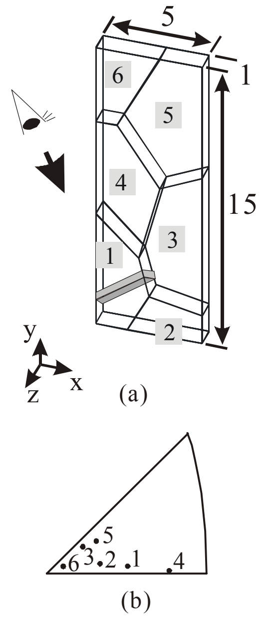

Figure 4(a) Geometry of the multi-crystal model. Dimensions are given in μm.
(b) Crystal orientation of grains 1-6.

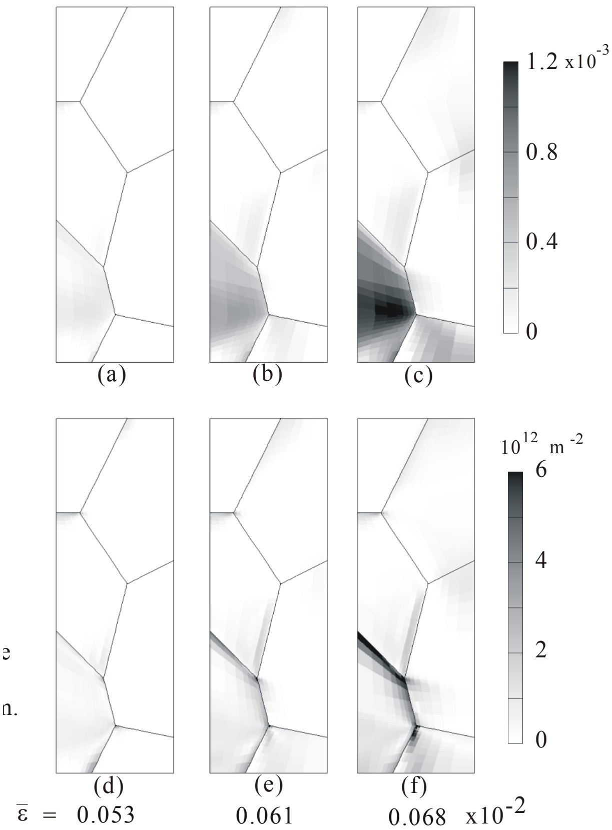

Figure 5(a)-(c): Distribution of plastic shear strain on the primary slip system when the average tensile strain is 5.3, 6.1, and 6.8 x10^{-4}, respectively.
(d)-(f) Density distribution of the geometrically necessary dislocations which correspond to the primary slip shown in (a)-(c).

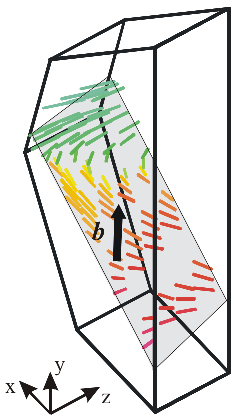

Figure 6 Dislocation segments in a thin foil in the grain 1. The foil is parallel to the primary slip plane and its thickness is 0.4 μm. View direction of this figure and position of the foil is illustrated in Figure 4(a).

The model is made from six copper crystal grains and their orientations are determined by random numbers and exhibited in Figure 4(b). All grain boundary planes are flat and positioned perpendicular to the x-y plane. The specimen is divided into 4864 finite elements and uniform tensile displacement is given to the top and bottom surfaces.

Figure 5(a)-(c) show evolution of the plastic shear strain on the primary slip systems at three stages of deformation. The first plastic slip takes place in the grain 1 near a grain boundary between the grains 1 and 2, although the slip at the interior of the grain 1 starts immediately after it and grows faster. Slip deformation in the grain 1 induces slip deformation in the grains 2, 3 and 4, which start from grain boundary triple junctions. Figure 5(d)-(f) show distribution of GN dislocations. Rather uniform accumulation of GN dislocations in the grain 1 is observed first, and then the density near grain boundaries gradually builds up. To examine the structure of GN dislocations in more detail, we cut out a foil from the grain 1 and observe the structure. The foil is schematically illustrated as a platelet in the grain 1 in Figure 4(a). The foil is parallel to the slip plane and its thickness is 0.4 μm. Figure 6 shows the line segments of GN dislocations, which are positioned within the volume of the foil. Half loop shaped structure of dislocations is observed to expand from specimen surface and the grain boundary pile up of dislocations is also observed.

4. SUMMARY

We analyzed plastic slip deformation in FCC type single- and multi-crystals and three-dimensional structure of the geometrically necessary dislocations were evaluated. Results for single crystals showed a development of wall shaped structure of GN dislocations and fairly random distribution of SS dislocations. GN dislocations in a multi-crystal model were depicted to emerge from specimen surface and grow in the shape of half-loops before they pile-up at grain boundaries.

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