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High Density Bands of GN Dislocations Formed by Multi Body Interaction in Compatible Type Multi Crystal Models

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Abstract. Slip deformation phenomena in compatible type multi crystal models subjected to tensile load are analyzed by a finite element crystal plasticity analysis code, and accumulation of geometrically-necessary and statistically-stored dislocations (GNDs and SSDs) are evaluated in detail. Crystal orientations for the grains are chosen so that mutual constraint of deformation through grain boundary planes does not take place. We call these models as compatible type multi crystals, because “compatibility requirements” at grain boundaries are automatically maintained by slip deformation only on the primary systems and uniform deformation is expected to occur in each grain. Results of the analysis, however, show non-uniform deformation with high density of GNDs accumulated in a form of band. Growth of such kind of structure of GNDs caused localized accumulation of SSDs at grain boundary triple junctions. Mechanism for the band-shaped accumulation of GNDs in the compatible type multi crystals are discussed from the viewpoint of multi body interactions which arise from shape change of crystal grains after slip deformation.

Introduction

When plastic deformation occurs in polycrystalline material, crystal grains mechanically interact with each other and mutual constraint of deformation takes place between adjacent grains [1-3]. As a result of this mutual constraint between crystal grains, non-uniform deformation and accumulation of dislocations occurs near grain boundaries and also in the interior of grains. Since these dislocations are necessary where the gradient of plastic shear strain exists, they are called geometrically-necessary-dislocations (GNDs) [4].

Accumulation of dislocations causes strain hardening of crystal grains, and as a result of this, mechanical characteristics of polycrystalline materials changes with the progress of deformation. Conventionally, mechanical interaction between crystal grains in polycrystalline material is understood to take place through grain boundary planes. Recently, we made a detailed analysis of slip deformation in compatible type multi crystals where crystal orientations for the crystal grains are chosen so that mutual constraint of deformation through grain boundary planes does not take place [1]. Results of the analysis, however, shows high density of GNDs and statistically-stored-dislocations (SSDs) accumulated at grain boundary triple junction. This fact indicates that mechanical interaction between crystal grains in polycrystalline material takes place not only by mutual constraint of deformation through neighboring crystal grain boundary planes, but also by effects of multi-body-interaction around grain boundary triple junction. The latter interaction causes developments of dislocation structure and non-uniform deformation field [5]. In this paper, effects of displacement field around grain boundary triple junction in compatible type

6-crystals model are studied from the viewpoint of multi-body-interactions which arise from shape change of crystal grains after slip deformation.

Basic Equation

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

$$P_{ij}^{(n)}\sigma_{ij}=\theta^{(n)},\quad P_{ij}^{(n)}\dot{\sigma}_{ij}=\dot{\theta}^{(n)},\qquad (n=1,2,\quad,12), \tag{1}$$

and

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

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 vector $v_i^{(n)}$ and slip direction vector $b_i^{(n)}$ define the Schmid tensor $P_{ij}^{(n)}$. Increment of the critical resolved shear stress is written as follows:

$$\dot{\theta}^{(n)}=\sum_m h^{(nm)}\dot{\gamma}^{(m)}, \tag{3}$$

here, $\dot{\gamma}^{(m)}$ denotes the increment of plastic shear strain on slip systems *m*. $h^{(nm)}$ denote the strain hardening coefficient. If the slip deformation is small and rotation of the crystal orientation is neglected, the constitutive equation is written as follows [6]:

$$\dot{\sigma}_{ij}=\left[S_{ijkl}^{e}+\sum_n\sum_m\{h^{(nm)}\}^{-1}P_{ij}^{(n)}P_{kl}^{(m)}\right]^{-1}\dot{\varepsilon}_{kl}, \tag{4}$$

where, S_{ijkl}^{e} denote elastic compliance. Summation is made over the active slip systems.

The critical resolved shear stress is assumed to be given by the following modified Bailey-Hirsch type relation [7]:

$$\theta^{(n)}=\theta_0(T)+\sum_{m=1}^{12}a\mu\tilde{b}\Omega^{(nm)}\sqrt{\rho_s^{(m)}}, \tag{5}$$

where, θ_0 denotes the lattice friction term, a is a numerical factor, which is close to 0.1, μ and $\tilde{b}$ denote the elastic shear modulus and magnitude of Burgers' vector, $\Omega^{(nm)}$ denotes the interaction matrix which define the reaction between dislocations on slip systems *n* and *m*. $\rho_s^{(m)}$ denotes the density of SS dislocations that accumulate on the slip system *m*, respectively.

Increment of the SS dislocations is given as follows [7]:

$$\dot{\rho}_S^{(n)}=\frac{c\dot{\gamma}^{(n)}}{\tilde{b}L^{(n)}}, \tag{6}$$

where, c is a numerical coefficient of the order of 1. $L^{(n)}$ denotes the mean free path of dislocations on slip system *n* and we use the following dislocation density dependent model for it [8-9]:

$$L^{(n)}=\frac{c^{*}}{\sqrt{\sum_m\omega^{(nm)}\left(\rho_S^{(m)}+\left\|\rho_G^{(m)}\right\|\right)}}, \tag{7}$$

where, c^* is a material constant. In this paper, we assume $c^* = 15$. $\omega^{(nm)}$ is dislocation interaction matrix.

Norm of the edge and screw components of GN dislocations defines the scalar density for the GN dislocations [10]:

$$\left\| \rho_G^{(m)} \right\| = \sqrt{\left(\rho_{G,edge}^{(m)} \right)^2 + \left(\rho_{G,screw}^{(m)} \right)^2} , \tag{8}$$

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

here, $\xi^{(m)}$ and $\zeta^{(m)}$ denote directions parallel and perpendicular to the slip direction on the slip plane, respectively. The strain hardening coefficient in equation (3) is given by the following equation:

$$h^{(nm)} = \frac{1}{2} \frac{a c \mu \Omega^{(nm)}}{L^{(m)} \sqrt{\rho_S^{(m)}}} . \tag{10}$$

Model

Figure 1 shows multi crystals model employed in this study. The size of height (*h*), width (*w*) and thickness (*t*) of specimen are 600, 200 and 10 μm, respectively. Grain boundary planes are perpendicular to the *x-y* planes of the model. We uniformly divide the model into 9600 finite elements. The continuity requirements of strain components across the grain boundary plane between grain 1 and 2 is given by the following relationship [1]:

$$\varepsilon_{yy}^{(1)} = \varepsilon_{yy}^{(2)} , \quad \varepsilon_{zz}^{(1)} = \varepsilon_{zz}^{(2)} , \quad \varepsilon_{yz}^{(1)} = \varepsilon_{yz}^{(2)} , \tag{11}$$

here, $\varepsilon_{yy}^{(1)}$ for example, denotes the sum of elastic and plastic strain components and the number in superscript denotes the grain.

The continuity requirements of strain components across the other grain boundary planes, which are lying parallel to *z-x* plane, are represented by the following relationship:

$$\varepsilon_{xx}^{(n)} = \varepsilon_{xx}^{(m)} , \quad \varepsilon_{zz}^{(n)} = \varepsilon_{zz}^{(m)} , \quad \varepsilon_{zx}^{(n)} = \varepsilon_{zx}^{(m)} , \tag{12}$$

here, *n* and *m* denote number of neighboring crystal grains.

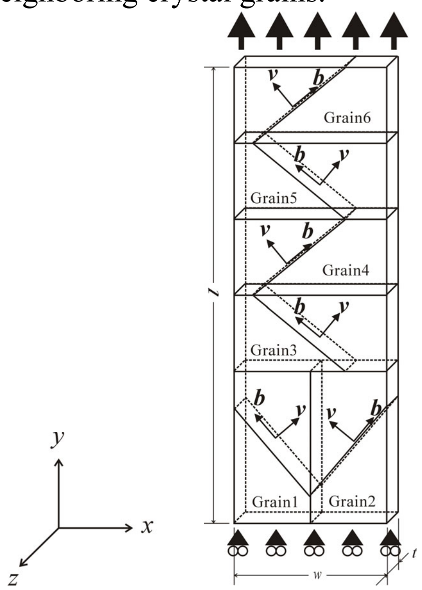

Fig. 1 Geometry and boundary condition for the models employed in this study

The elastic compliance data for standard crystal oriantation are S_{11} = 1.0, S_{12} = -0.25, S_{44} = 2.5 [$\times 10^{-11}$ m^2/N], and interaction of crystal grains due to the effect of the elastic incompatibility stress [11] does not occur through grain boundary planes.

Euler angles (κ, θ, ϕ), components of slip direction and normal direction of slip plane on the primary slip systems are summarized in Table 1. Values of Schmid tensor for the primary slip systems are summarized in Table 2. In this case, Since $v_z^{(9th)}$ and $b_z^{(9th)}$ are equal to 0, components of Schmid tensor $P_{33}^{(9th)}$, $P_{23}^{(9th)}$ and $P_{31}^{(9th)}$ are also equal to 0. Then, increments of plastic strain $\dot{\varepsilon}_{zz}^{p}$, $\dot{\varepsilon}_{yz}^{p}$ and $\dot{\varepsilon}_{zx}^{p}$ are equal to 0, also. Since the values of $P_{22}^{(9th)}$ for grain 1 and 2 are the same, the strain $\dot{\varepsilon}_{yy}^{p}$ for both grains are the same and Eq.(11) is satisfied.

The combination of crystal orientations for grains 1, 2 and 3 are chosen so that the angle(α) between loading direction and slip direction of the primally slip system are $\alpha^{(1)}=\alpha^{(2)}$=44° and $\alpha^{(3)}$=46°, here, the number in superscript denotes the crystal grain number. In this case, since the values of $P_{11}^{(9th)}$ for grain 1, 2 and 3 are the same, the strain ε_{xx}^{p} for each grain are also the same and Eq.(12) is satisfied. Crystal orientation for the grain 5 is the same as the one given for the grain 3. Cristal orientation for the grains 4 and 6 is given by rotation of that for the grain 3 by 180 degree around *y*-axis. The strain ε_{xx}^{p} for grain 3 and 4 are the same and Eq.(12) is satisfied. Therefore, strain incompatibility do not occure in this model. Iinitial dislocation densities ρ_0 for twelve slip systems are supposed to be 1.0×10^9 [m^{-2}]. This model is deformed under tensile load in *y*-axis.

Dislocations formed by multi body interaction

Figure 3(a)-(d) show distribution of plastic shear strain, SS dislocations, edge and screw components of GN dislocations on the primary slip system $(11\bar{1})[101]$, respectively. Figure 3(e) show density distribution of norm of GN dislocation on a secondary slip system $(111)[10\bar{1}]$ when average tensile strain $\bar{\varepsilon}_{yy}$ is equal to 1%. Non-uniform deformation occurs (Fig. 3(a)) and pattern of GN dislocations develops in accordance with the non-uniform deformation (Fig. 3(c)-(d)).

Mechanism of these non-uniform deformation and development of some patterns in the density distribution of GN dislocation are understood in two stages shown in Fig. 4(a)-(b) and Fig. 4(b)-(c).

Table 1 Grain number, Euler angles (κ,θ,ϕ), Value of components of slip direction vector $\boldsymbol{b}^{(9th)}$ and slip plane normal vector $\boldsymbol{v}^{(9th)}$ of primary slip systems

Grain Num.	(κ, θ, ϕ) [deg]	$b_x^{(9th)}$	$b_y^{(9th)}$	$b_z^{(9th)}$	$v_x^{(9th)}$	$v_y^{(9th)}$	$v_z^{(9th)}$
1	(74.983, 24.535, 79.469)	-0.6947	0.7193	0	0.7193	0.6947	0
2	(74.983, 24.535,259.469)	0.6947	0.7193	0	-0.7193	0.6947	0
3, 5	(79.645, 24.973, 75.236)	-0.7193	0.6947	0	0.6947	0.7193	0
4, 6	(79.645, 24.973,255.236)	0.7193	0.6947	0	-0.6947	0.7193	0

Table 2 Grain number and values of Schmid tensor $P_{ij}^{(9th)}$

Grain Num.	$P_{11}^{(9th)}$	$P_{22}^{(9th)}$	$P_{33}^{(9th)}$	$P_{12}^{(9th)}$	$P_{23}^{(9th)}$	$P_{31}^{(9th)}$
1	-0.4997	0.4997	0	0.0174	0	0
2	-0.4997	0.4997	0	-0.0174	0	0
3, 5	-0.4997	0.4997	0	-0.0174	0	0
4, 6	-0.4997	0.4997	0	0.0174	0	0

Figure 4(a)-(b) show free deformation of individual crystal grains that are supposed to deform by slip on the primary slip system. Figure 4(b)-(c) schematically show interaction of crystal grains via grain boundary planes and non-uniform deformations. Mutual interaction of crystal grains and non-uniform deformation take place in order to satisfy boundary conditions and continuity of the displacement at grain boundaries. Displacement field around grain boundary triple junction formed by grain 1, 2 and 3 is similar to the one for wedge type disclination as shown in Fig. 4(d)-(e).

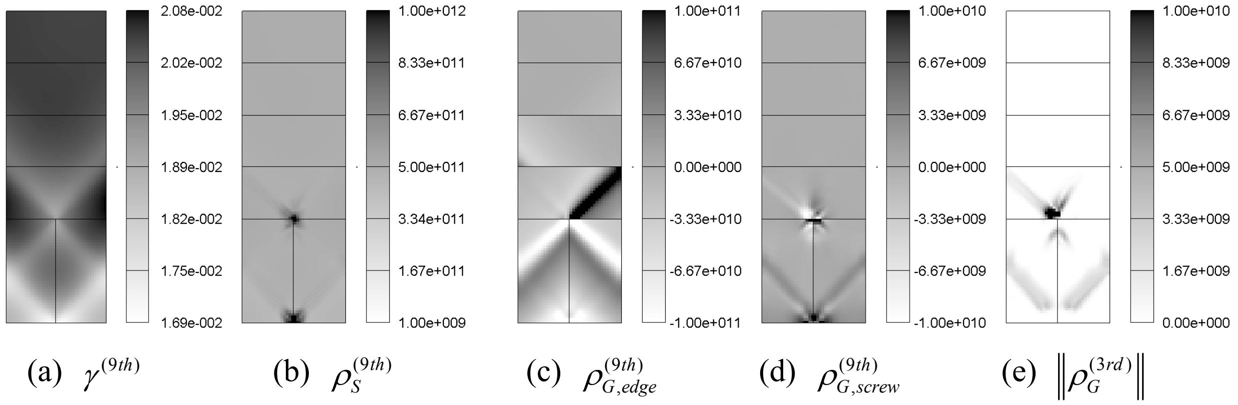

Fig. 3 (a) Distribution of plastic shear strain, (b) density distribution of SS dislocations, (c) edge and (d) screw components of GN dislocations on the primary slip systems $(11\bar{1})[101]$ and (e) density distribution of norm of GN dislocation on the 3rd slip systems $(111)[10\bar{1}]$ when the average tensile strain $\bar{\varepsilon}_{yy}$ is 1%. Unit of dislocation density is m^{-2}.

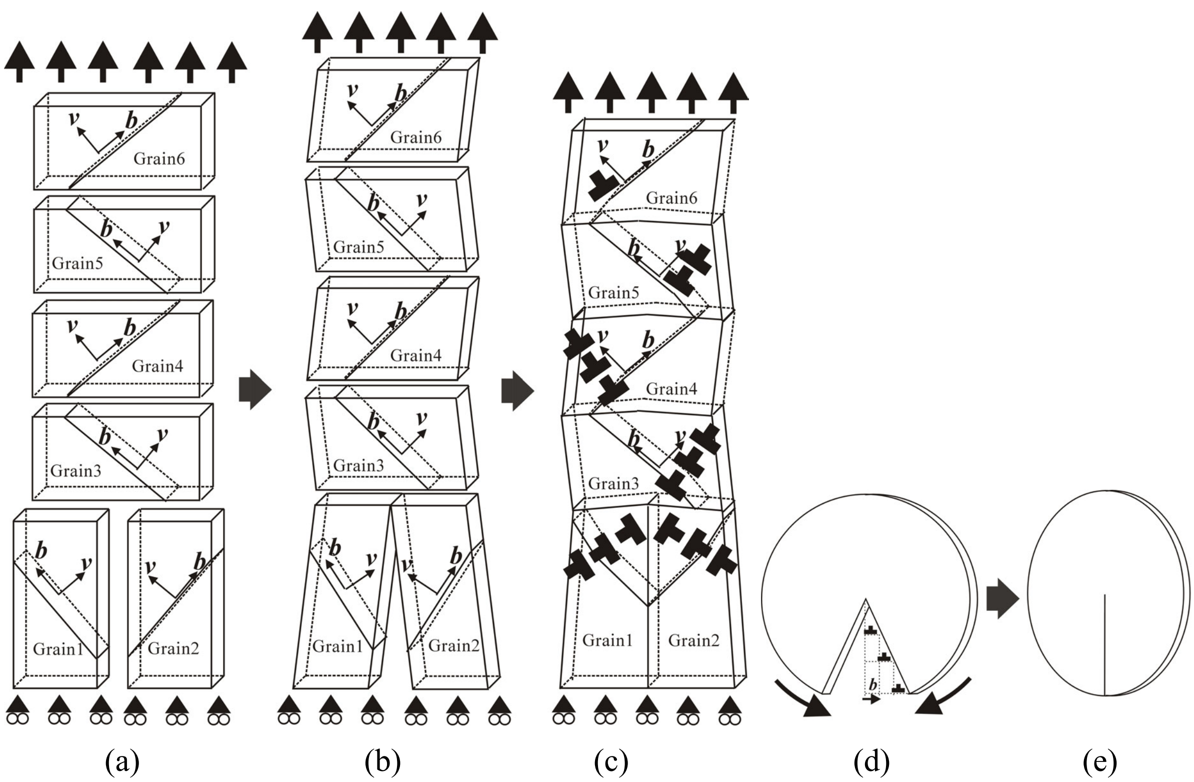

Fig. 4 Schematic illustration of (a) initial condition of each grain of compatible type multi-crystal, (b) imaginary slip deformation without multi-body-interaction, (c) when crystal grains have to deform in compatible manner, the displacement field corresponds to that for (d)-(e) wedge type disclination with its core placed at the grain boundary triple junction.

Defect of wedge type disclination spread depend on distance from its core and similar to line of edge dislocation when direction of disclination core is perpendicular to direction of Burgers' vector (Fig. 4(d)). Since line of edge dislocation is geometrically necessary existence on the primary slip plane, pattern of GN edge dislocations band which corresponds to kink band develop from grain boundary triple junction to inside of grain 1, 2 and 3. Since accumulation of GN dislocation change value of critical resolve shear stress of primary and secondary slip systems, secondary slip system $(111)[10\bar{1}]$ active near grain boundary triple junction (Fig.3 (e)). Dislocation interaction between primary and secondary slip systems causes accumulation of SS dislocation (Fig.3 (b)) and formation of GN screw dislocation bands which corresponds to secondary slip band (Fig.3 (f)). In this way, wedge type displacement field around grain boundary triple junction causes developments of non-uniform deformation and pattern formation of dislocation in grain 1, 2 and 3 and remote grain 4 in order to satisfy continuity of the displacement at grain boundaries. Then, non-uniform deformation field and pattern of dislocation formed with long-range in multi crystal models.

Summary

Slip deformation and acumulation of dislocation in the compatible type multi crystal models subjected to tensile load are studied by crystal plasticity anaylsys. The results of analysis are sammarized as follows;

1. Non-uniform deformation with high density of GN dislocation accumulated in compatible type multi cyrstal models are disclibable by imaginary disclination type displacement field at grain boundary triple junction.
2. Effects of displacement field at grain boundary triple junction causes developments of pattern of GN dislocation with non-uniform deformation in remote crystal grains.

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