Crystal Plasticity Analysis of Non-uniform Deformation in Symmetric Type Bicrystals under Tensile Load and Formation of Geometrically Necessary Dislocation Bands*

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Abstract
Slip deformation in symmetric type bicrystal models subjected to tensile load is analyzed by a finite element crystal plasticity analysis code and accumulation of geometrically necessary dislocations (GNDs) is studied in detail. Uniform deformation was expected to take place because mutual constraint of crystal grains through the grain boundary plane does not occur in symmetric type bicrystals, but, some results of the analysis show non-uniform deformation and the high density of GNDs accumulated in the form of band. Such kind of non-uniform deformation is observed regardless of the model size and the strain-hardening characteristics. Mechanism of non-uniform deformation and accumulation of GNDs in the form of band in the symmetric type bicrystals is discussed from the viewpoint of the boundary condition and shape change of grains after slip deformation

Key words: Crystal Plasticity Analysis, Geometrically Necessary Dislocation, Grain Boundary, Grain Size Effect, Symmetric Type Bi-Crystal, Compatibility

1. Introduction

Slip deformation of metal crystal grains largely depends on the dislocation density and the crystal orientation because the deformation takes place due to the change in the relative position of an atomic plane defined crystallographically with respect to another atomic plane by the motion of dislocations. Plastic deformation of a metal polycrystal largely depends on the dislocation density and the crystal orientation in a combination of slip deformation that takes place in the crystal grains. However, these are not independent of each other and the deformation takes place while mechanical deformation constraint is imposed on each other between neighboring crystal grains. Because of this, when plastic deformation takes place in a polycrystal, normally, in order to satisfy the continuity of displacement at the grain boundary, non-uniform deformation takes place in the vicinity of the grain boundary and at the same time, “geometrically necessary (GN) dislocations” (1) accumulate.

The main cause of the accumulation of GN dislocations in a polycrystal is thought to be the non-uniform deformation that takes place in the vicinity of the grain boundary in order to satisfy the continuity of displacement at the grain boundary. However, there is a phenomenon which is thought to be caused not only by this. For example, the GN dislocations do not necessarily accumulate only in the vicinity of the grain boundary but in some cases accumulate in high density in a band-like area that has developed in the inward direction of the crystal grain (2) (3). Although the structure of this GN dislocation is
regarded as the “GN dislocation band” from its aspect or a newly formed pseudo crystal grain boundary, details are not known. However, the motion or the accumulation of a dislocation group is not only the cause but also the result of an extremely complex mechanical phenomenon, so it is difficult to discuss the cause of formation of the “GN dislocation band” based on experiments.

On the other hand, theoretical, analytical methods \(^{(4)(5)}\) that utilize continuum mechanics have recently been put to practical use. And the methods \(^{(3)(6)}\) of evaluating the dimension effect that resides in a material, such as the average crystal grain radius that could not be evaluated by conventional continuum mechanics, are beginning to be discussed. With these, it is possible to analyze the non-uniform deformation, the accumulation of dislocations, and the motion of the dislocation group inside the material by imposing arbitrary mechanical boundary conditions on the material having an arbitrary shape, dimensions, crystal orientation, dislocation density, and material constant.

In this study, in order to clarify the cause of formation of the “GN dislocation band”, crystal plasticity analysis of tensile deformation in symmetric type bicrystals, the most fundamental model of polycrystal, is performed, and the results of discussing the non-uniform deformation and GN dislocation are described.

2. Model

As an analysis model, Model A and Model B, which are two kinds of bicrystals shown in Fig. 1, are used. In order to discuss the effect of the dimensions of the model on the deformation state and the accumulation of dislocations, three kinds of combinations are used, that is, the length \(l\) of a side and the thickness \(t\) are 2,000 \(\mu\)m and 100 \(\mu\)m, 200 \(\mu\)m and 10 \(\mu\)m, and 20 \(\mu\)m and 1 \(\mu\)m. The grain boundary plane is perpendicular to the model surface. Finite element division of the model is carried out uniformly using eight-node hexahedron elements and the total number of elements is 3,200 in each case.

When Grains 1 and 2 in Models A and B deform independently of each other, if their combination produces a difference between the strain components in the direction of the grain boundary plane, deformation constraint occurs between the crystal grains when Grains 1 and 2 couple with each other and deform. The condition under which interaction of such deformation constraint is not produced is called the “compatible condition” \(^{(7)(8)}\). The “compatible condition” of Models A and B is given by the following expressions

\[
\begin{align*}
\varepsilon_{xx}^{(1)} &= \varepsilon_{xx}^{(2)}, & \varepsilon_{zz}^{(1)} &= \varepsilon_{zz}^{(2)}, & \varepsilon_{xz}^{(1)} &= \varepsilon_{xz}^{(2)}, & \text{(Model A)}, \\
\varepsilon_{yy}^{(1)} &= \varepsilon_{yy}^{(2)}, & \varepsilon_{zz}^{(1)} &= \varepsilon_{zz}^{(2)}, & \varepsilon_{yz}^{(1)} &= \varepsilon_{yz}^{(2)}, & \text{(Model B)},
\end{align*}
\]

where, \(\varepsilon_{ii}^{(1)}, \varepsilon_{ii}^{(2)}\), etc., are strain components (the sum of the elastic component and the plastic component) produced when Grains 1 and 2 deform independently of each other, and the superscripts indicate the crystal grain numbers. Those which satisfy the “compatible condition” are called the “compatible type” and those which do not are called the “incompatible type”. It should be noted that the “compatible condition” here is different in
meaning from the compatible condition in solid mechanics.

Hook and Hirth\(^{(9)}\) state that the incompatibility of bicrystals is induced also by elastic anisotropy and non-uniform deformation and multiple slips occur in the vicinity of the grain boundary. Here, a virtual face-centered cubic crystal metal that does not produce the effect of elastic anisotropy\(^{(9)}\) is supposed and it is assumed that the combined elastic compliances of the crystal reference axis orientation are

\[
S_{11} = 1.0, \quad S_{12} = -0.25, \quad S_{44} = 2.5 \times 10^{-11} \text{m}^2/\text{N}
\]

so that the elastic anisotropy ratio

\[
\frac{S_{11}}{S_{12}} = 1.
\]

If it is assumed that the rotation of orientation accompanying slip can be ignored under minute deformation, the plastic strain increment produced in the crystal grain due to the plastic shear strain increment \(\dot{\gamma}^{(n)}\) on the slip plane in the \(n\)-th slip system is represented by the following equation

\[
\dot{\varepsilon}_p^{(n)} = \sum_{\gamma} \dot{\gamma}^{(n)} P^{(n)}_p = \frac{1}{2} \left( \psi_\phi^{(n)} b^{(n)} + \psi_\psi^{(n)} b^{(n)} \right), \quad (3)
\]

where, \(P^{(n)}_p\) is the Schmid tensile, and \(\psi_\phi^{(n)}\) and \(b^{(n)}\) are unit vectors in the plane normal direction and the slip direction.

As shown in Fig. 2, the relationship between the crystal coordinate system constituted by the unit vectors \([100]\), \([010]\), and \([001]\) and the material coordinate system \((x, y, z)\) is represented by Euler angles \((\kappa, \theta, \phi)\). Coordinate transformation is represented by the following expression

\[
\begin{bmatrix}
100 \\
010 \\
001
\end{bmatrix} =
\begin{bmatrix}
\cos \theta \sin \kappa & \cos \phi & \sin \theta \sin \kappa \\
\sin \theta \cos \kappa & \cos \theta \sin \phi & \sin \theta \cos \kappa \\
-\sin \phi & \cos \phi & 0
\end{bmatrix} \begin{bmatrix}
x \\
y \\
z
\end{bmatrix}
\]

(4)

Fig. 2  Definition of Euler angles \(\kappa, \theta, \phi\)

It is assumed that Euler angles \((\kappa, \theta, \phi)\) in Grains 1 and 2 are \((77.0, 24.705, 77.636)\) and \((77.0, 24.705, 257.636)\) [deg], respectively. At this time, the crystal orientation of Grain 1 is as follows: \(v^{(0)}\) of the primary slip system \((11\bar{1})[101]\) is \(v_x^{(0)} = 0.7089, v_y^{(0)} = 0.7053, v_z^{(0)} = 0\), and \(b^{(0)}\) is \(b_x^{(0)} = -0.7053, b_y^{(0)} = 0.7089, b_z^{(0)} = 0\). The crystal orientation of Grain 2 will be one when Grain 1 is rotated about the y-axis through 180 degrees. In this case, because of \(v_x^{(0)} = b_x^{(0)} = 0\), the plastic strain components produced in Grains 1 and 2 are only \(\varepsilon_{pp}', \varepsilon_{pp}',\) and \(\varepsilon_{pp}'\). Further, for both Grains 1 and 2, \(\psi_\phi^{(0)}b^{(0)} = -0.4999\) and \(\psi_\psi^{(0)}b^{(0)} = 0.4999\), and therefore, from equation (3), the values of the Schmid tensile \(P_{11}^{(0)}\) and \(P_{22}^{(0)}\) are equal, \(\varepsilon_{pp}'\) and \(\varepsilon_{pp}'\) produced in Grains 1 and 2 are equal, and both Models A and B satisfy the “compatible condition” of expressions (1) and (2).

Further, \(v^{(0)}\) and \(b^{(0)}\) of the slip system of Grains 1 and 2 are symmetrical with respect to the grain boundary, so Models A and B will be bicrystals having the same dimensions and shape. It is assumed that the initial dislocation density \(\rho_0\) is uniform, \(1.0 \times 10^9 \text{ m}^{-2}\). The displacement in the y-axis direction at all the nodes on the bottom plane of the model is constrained, a uniform forced displacement in the y-axis direction is imposed on all the nodes on the top plane, and pulling is performed until the average tensile strain \(\varepsilon_{yy}\) becomes 1%.

3. Analysis method

3.1  Analysis of deformation by finite element method
If it is assumed that the activation condition of the slip system is given by the Schmid law, the following equation will hold true between the stress tensor \( \sigma \) under the activation condition and the critical resolved shear stress \( \tau \) in the \( n \)-th slip system.

\[
\theta^{(n)} = P_{ij}^{(n)} \sigma_{ij} \\
\dot{\theta}^{(n)} = P_{ij}^{(n)} \dot{\sigma}_{ij}
\]

(5)

The strain increment \( \dot{\varepsilon}_{ij} \) is acquired from the sum of the elastic component \( \dot{\varepsilon}_{ij}^{e} \) and the plastic component \( \dot{\varepsilon}_{ij}^{p} \) using the following equation

\[
\dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^{e} + \dot{\varepsilon}_{ij}^{p} \\
\dot{\varepsilon}_{ij}^{e} = S_{ijkl}^{*} \sigma_{kl}
\]

(6)

where, \( S_{ijkl}^{*} \) is an elastic compliance.

If it is assumed that the strain hardening coefficient is \( h^{(nm)} \) and the strain hardening law is represented by the following equation

\[
\gamma = \sum h^{(nm)}
\]

(7)

then, the elastic/plastic constitutive equation (10) is represented by the following equation.

\[
\sigma_{ij} = \left[ S_{ijkl}^{*} + \sum h^{(nm)} \right]^{-1} \dot{\varepsilon}_{ij}^{p}
\]

(8)

However, \( n \) and \( m \) are added to obtain their sum only in the active slip systems. Based on the elastic/plastic constitutive equation, deformation is analyzed using the finite element method.

3.2 Analysis of dislocation density

Dislocations present inside the material having been subjected to deformation hysteresis are roughly classified into two kinds, that is, the “statistically stored dislocations” (SS dislocations) and the GN dislocations. Their density is calculated from the increment of the strain, which is the result of analyzing deformation.

The relationship between the increment \( \dot{\rho}_{S}^{(n)} \) of the SS dislocation density and the plastic shear strain increment \( \dot{\gamma}_{ij} \) is represented by the following equation (4)

\[
\dot{\rho}_{S}^{(n)} = \frac{c \rho_{S}^{(n)}}{b L^{(n)}}
\]

(9)

where, \( c \) is a coefficient of the order of one, \( b \) is the magnitude of Burgers vector, and \( L^{(n)} \) is the mean free path of dislocation.

The slip deformation of the crystal grain is produced by the moving dislocations, and therefore, as shown in Fig. 3(a), in the area in which dislocations have passed, a slip occurs and in the area in which dislocations have not passed yet, no slip occurs. Consequently, at a place where a spatial gradient of the plastic shear strain \( \gamma^{(n)} \) is produced, dislocations must exist. This is called the GN dislocation (1).

Because a dislocation whose direction of the dislocation line is perpendicular to the slip direction is called an edge dislocation and one parallel to the slip direction is called a screw dislocation, as to the spatial gradient of \( \gamma^{(n)} \), as shown in Fig. 3(b), the component in the slip direction is referred to as an edge dislocation density component \( \rho_{G, \text{edge}}^{(n)} \), and a component in the direction perpendicular to the slip direction is referred to as a screw dislocation density component \( \rho_{G, \text{screw}}^{(n)} \). The density of norm of GN dislocations \( \rho_{G}^{(n)} \) is represented by the following equation using \( \rho_{G, \text{edge}}^{(n)} \) and \( \rho_{G, \text{screw}}^{(n)} \)

\[
\left\| \rho_{G}^{(n)} \right\|^2 = \left( \rho_{G, \text{edge}}^{(n)} \right)^2 + \left( \rho_{G, \text{screw}}^{(n)} \right)^2
\]

(10)
where, $\xi$ and $\zeta$ are the direction parallel to the slip direction and the direction vertical to the slip direction on the slip plane, respectively. As described above, the density of GN dislocations $\gamma^{(m)}$ is acquired from the spatial gradient, and therefore, the amount to be evaluated has dimension dependence.

![Diagram](a)  

Fig. 3 Schematic illustration of relationship between geometrically necessary dislocations and gradient of plastic shear strain.

### 3.3 Deformation hysteresis and method of evaluating dimension effect

The critical resolved shear stress $\theta^{(a)}$ in the slip system having been subjected to deformation hysteresis is represented as follows by the modified Bailey-Hirsch equation

$$
\theta^{(a)} = \theta_0(T) + \sum_a \frac{a \mu_b \Omega^{(a)}}{\sqrt{\rho^{(m)}}},
$$

where, $\theta_0$ is a resistance value that does not depend on the deformation hysteresis against moving dislocation, $a$ is a numerical value of about 0.1, $\mu$ is an elastic shear coefficient, and $\Omega^{(a)}$ is an interaction matrix. The interaction matrix indicates the strength of damage of the dislocations accumulated on the slip system imposed on the moving dislocation on another slip system, and can be represented by five kinds of parameters $R_1, R_2, R_3, R_3', and R_4$, the strength of interaction between the dislocations on the same slip system being the reference unit. Here, isotropic hardening is supposed and so $R_1 = R_2 = R_3 = R_3' = R_4 = 1.01$.

The strain hardening coefficient $k^{(mn)}$ of the material having been subjected to deformation hysteresis is represented by the following equation

$$
k^{(mn)} = \frac{1}{2} L^{(mn)} \sqrt{\rho^{(m)}}.
$$

As a method of calculating the mean free path $L^{(a)}$ in equations (9) and (12), many models have been proposed, such as the Seeger model depending on the plastic shear strain, the modified Seeger model that takes into consideration multiple slips, the dislocation density dependent type model, etc. Here, the dislocation density dependent type model is based on the concept that the moving dislocation comes to a stop after having moved the distance $c^*$ times the average interval of the accumulated dislocations, and is represented in a form dependent on the dislocation density, that is the quantity of state. Here, the following model in which the SS dislocation and the GN dislocation contribute to $L^{(a)}$ is used

$$
L^{(a)} = \frac{c^*}{\sqrt{\sum_n \Omega^{(mn)} \left( \rho^{(m)} + \rho^{(m)} \right)}},
$$

where, $c^*$ is a material constant, a value of about 1 to 100, and in this study, it is assumed that $c^* = 1, 15, and 100$. $\Omega^{(mn)}$ is a weighting matrix, which represents the interaction between the moving and the stored dislocations, and can be represented by six kinds of parameters $w_0, w_1, w_2, w_3, w_3'$, and $w_4$. Here, considering that dislocations stored in the self-slip system and the coplanar slip system do not contribute to the capture of motional dislocations, it is assumed that $w_0 = w_1 = 0, w_2 = w_3 = w_3' = w_4 = 1.0$.

Due to the contribution of the density of GN dislocations having dimension dependence on $L^{(a)}$, the GN dislocations concern the storage of the SS dislocations [refer to equation (9)]. As a result, the dimension effect occurs in the critical resolved shear stress and the
strain hardening characteristics [refer to equations (11) and (12)].

3.4 Increment analysis

The present analysis consists of three parts, that is, analysis of deformation by the finite element method described in section 3.1, calculation of the dislocation density described in section 3.2, and evaluation of strain hardening described in section 3.3. At first, the constitutive equation of elastic deformation is determined from the elastic compliance and the crystal orientation. And the elastic deformation before yield point in accordance with the boundary condition is analyzed. Next, an active slip system is selected by the Schmid law, the strain hardening coefficient is determined from the initial dislocation density, etc., the constitutive equation is modified, and the slip deformation is analyzed. Since strain hardening occurs in every slip system accompanying the advancement of deformation, it is necessary to dynamically modify the constitutive equation. For the analysis of the non-linear phenomenon, in the present analysis, the increment analysis is performed by dividing time into steps each time the slip system starts to act and terminates, and the SS dislocation density \( \rho_S^{(m)} \) and the GN dislocation density norm \( \| \rho_G^{(m)} \| \) serve as internal state variables for determining the constitutive equation in the next time step.

4. Analysis result and consideration

4.1 Relationship between stress and strain

The averaged value \( \bar{\sigma}_{yy} \) of normal stress \( \sigma_{yy} \) of all the elements in Models A and B and the change in its standard deviation \( \sigma \) are shown in Fig. 4. As to \( \bar{\sigma}_{yy} \), as shown in Figs. 4(a) and (b), the difference in the results of Models A and B is extremely slight and cannot be discriminated from the figure. In other words, the macroscopic mechanical properties of Models A and B are almost the same. It is known from either result that the smaller the value of \( c^* \), the larger is the strain hardening and that the difference in the results by the dimension \( l \) is so small that it cannot be discriminated from the figures.

![Fig. 4](image_url)

Fig. 4 (a), (b), Averaged value of normal stress \( \bar{\sigma}_{yy} \), and (c), (d), its standard deviation \( \sigma \) during tensile deformation.
As to the standard deviation $S$, as shown in Figs. 4(c) and (d), the results are different between Models A and B; in Model A, irrespective of the value of $c^*$ and the dimension $l$, $S$ remains at 0 after deformation and the stress distribution inside the model is uniform. On the other hand, in Model B, from the initial stage of deformation, accompanying the increase in the average tensile strain $\overline{\varepsilon}_{yy}$, $S$ develops and a non-uniform stress field is produced inside the model.

The result of the development of the non-uniform stress field in Model B differs depending on the value of $c^*$, and the smaller the value of $c^*$, the more steeply the non-uniformity develops. When the value of $c^*$ is 1, irrespective of the dimension $l$, $S$ develops almost linearly. When the values of $c^*$ are 15 and 100, the results are different depending on the dimension $l$; in the results when the dimension $l$ is 2,000 $\mu$m and 200 $\mu$m, the development of $S$ is relaxed accompanying the advancement of deformations, however, in the result when the dimension $l$ is 20 $\mu$m, $S$ develops linearly. In other words, the smaller the dimension, the more the non-uniformity of the stress distribution state inside the model develops accompanying the advancement of deformations.

### 4.2 Development of SS and GN dislocation densities

The development of the average value of the density of SS dislocations $\rho_{S}^{SS}$ accumulated in the primary slip systems of all the elements of Models A and B, and the development of the average value of the GN dislocation density $\rho_{G}^{GN}$ are shown in Fig. 5. As shown in Figs. 5(a) to (c), $\rho_{S}^{SS}$ linearly increases accompanying the increase in the average tensile strain $\overline{\varepsilon}_{yy}$ both in Model A and in Model B. The order of $\rho_{S}^{SS}$ differs depending on the value of the material constant $c^*$ and the smaller the value of $c^*$, the higher is the order. The difference in the results between Models A and B and the difference in the results by dimension are so extremely slight that they cannot be discriminated from the figures.

As to $\rho_{G}^{GN}$, as shown in Figs. 5(d) to (f), the results are different between Models A and B. In Model A, irrespective of the values of dimension $l$ and $c^*$, the GN dislocation does not occur even after deformation. This indicates that Model A deforms uniformly.

![Fig. 5](image_url)

**Fig. 5** (a), (b), (c), Average density of statistically stored dislocations on primary slip system $\rho_{S}^{SS}$ and (d), (e), (f), density of norm of geometrically necessary dislocations on primary slip system $\rho_{G}^{GN}$ during tensile deformation.
On the other hand, the GN dislocation occurs from the initial stage of deformation in Model B and the density increases accompanying the increase in the average tensile strain $\varepsilon_{yy}$.

The density of GN dislocations that have occurred in Model B has dimension dependence and the smaller the dimension $l$, the higher the order is as to the relationship with the value of $c^*$, as shown in Figs. 5(d) and (e), when the dimension $l$ is 2,000 $\mu$m and 200 $\mu$m, the density linearly increases accompanying the advancement of deformation, and the smaller the value of $c^*$, the larger the gradient. When the dimension $l$ is 20 $\mu$m, as shown in Fig. 5(f), the tendency of increase differs depending on the value of $c^*$.

When $l$ is 20 $\mu$m and the values of $c^*$ are 15 and 100 [Fig. 5(f)], after $\varepsilon_{yy}$ is 0.4%, the dislocation density exhibits a rapid increase. The GN dislocation density has dimension dependence and the SS dislocation density largely depends on the value of $c^*$, and therefore, under the analysis condition that the dimension $l$ is small and the value of $c^*$ is large, there may be the case where the order of the GN dislocation density reaches the order of the SS dislocation density [Figs. 5(b), (c), (f)]. In this case, the contribution of the GN dislocation density to the average mean free path $L^{(n)}$ of the motional dislocation appears remarkably and it is made easier for the motional dislocation to stop in the area where the GN dislocations are accumulated. At the place at which the motional dislocation stops, a spatial gradient of plastic shear strain occurs, and this is the GN dislocation itself. Because of this, it is thought that the GN dislocation density has increased rapidly.

### 4.3 Density distribution of GN dislocation

![Graphs showing density distribution of GN dislocation](image)

Fig. 6 Density distribution of norm of geometrically necessary dislocations when $\varepsilon_{yy} = 0.1\%$. Unit of dislocation density is $m^{-2}$. 
As to Model B, in which the GN dislocation occurs from the initial stage of deformation, the distribution of the GN dislocation density norm $\|\rho^{(\text{GN})}_G\|$ in the stage at which the average tensile strain $\bar{\varepsilon}_{yy}$ is 0.1% is shown in Fig. 6. The GN dislocations form a structure in which the dislocations accumulate in a high density in the band-like area that has developed in the inward direction of the crystal grain from the vicinity of the intersection line of the model top plane and the grain boundary. In other words, it is known that the “GN dislocation band” is formed. Incidentally, irrespective of the dimension $l$ and the value of the material constant $c^*$, the place at which the “GN dislocation band” is formed and the direction of development remain the same.

The distribution of the GN dislocation density norm $\|\rho^{(\text{GN})}_G\|$ after pulling until the average tensile strain $\bar{\varepsilon}_{yy}$ reaches 1% is shown in Fig. 7. As is obvious from Figs. 6 and 7, even when deformation advances, the place of formation of the GN dislocation band and the direction of development do not change or a new “GN dislocation band” is not formed under the present analysis condition.

The distributions of the edge dislocation density component $\rho^{(\text{GN})}_{\text{edge}}$ and the screw dislocation density component of the GN dislocation in the stage at which 0.1% of average tensile strain $\bar{\varepsilon}_{yy}$ has occurred in the model whose value of $c^*$ is 15 and dimension $l$ is 200 $\mu$m are shown in Figs. 8(a) and (b). From the comparison of these aspects and the densities, it is known that the “GN dislocation band” that occurs in Figs. 6 and 7 is formed to an almost perfect edge dislocation.

![Fig. 7 Density distribution of norm of geometrically necessary dislocations when $\bar{\varepsilon}_{yy} = 1\%$. Unit of dislocation density is m$^{-2}$](image-url)
Fig. 8  Density distribution of edge and screw components of geometrically necessary dislocations when $\varepsilon_{yy} = 0.1\%$, $l = 200\mu m$, $c^* = 15$. Unit of dislocation density is $m^{-2}$

4.4 Relationship between mechanical boundary condition and slip restriction of crystal grain

The distributions of the plastic shear strain $\gamma^{(0k)}$ in the stage at which 0.1% of average tensile strain has occurred in the model whose value of $c^*$ is 15 and dimension $l$ is 200 µm and after pulling until 1% is reached are shown in Figs. 9(a) and (b).

![Image](a) $\rho_{G,\text{edge}}^{(0k)}$
(b) $\rho_{G,\text{screw}}^{(0k)}$

Fig. 8  Density distribution of edge and screw components of geometrically necessary dislocations when $\varepsilon_{yy} = 0.1\%$, $l = 200\mu m$, $c^* = 15$. Unit of dislocation density is $m^{-2}$

Fig. 9  Distribution of slip strain $\gamma^{(0k)}$ on primary slip system $l = 200\mu m$, $c^* = 15$.

It is known that the structure of the deformation field (such as the strain concentrated portion, etc.) does not change even if deformation advances. Because of this, it is known that the GN dislocation density, which is the spatial gradient of $\gamma^{(0k)}$, only increases even if deformation advances and the structure does not change. Further, from the result, it is thought that the fact that the “GN dislocation band” occurs from the vicinity of the intersection line of the grain boundary plane and the model top plane is determined from the stage of setting the initial conditions. In this case, it is thought that the boundary condition (as to forced displacement and the constraint of displacement) imposed on the top and bottom planes and the initial crystal orientation are involved in order to cause tensile deformation to occur.

Figs. 10(a) and (b) schematically show slip deformation that takes place when a forced tensile strain displacement is given to Models A and B.

![Image](a) Model A  (b) Model B

Fig. 10  Schematic illustration of constriction condition of slip deformation under tensile deformation.
In Model A, the side plane of the model is a free surface and no restriction is imposed on the slip in the primary slip system, and therefore, as shown in Fig. 10(a), it is possible for two crystal grains to uniformly deform into a parallelepiped. Because of this, it is thought that GN dislocation has not occurred even in the stage at which deformation has advanced.

On the other hand, in Model B, as shown in Fig. 10(b), it is not possible for two crystal grains to deform into a parallelepiped because the top and bottom planes of the model and the grain boundary plane maintain the perpendicular relationship even after deformation. The change in shape accompanying the slip in the primary slip system is constrained by the top and bottom planes of the model and the grain boundary plane and free slips in the primary slip system are restricted. Because of this, it is thought that the “GN dislocation band” has been formed as well as the GN dislocation has occurred.

From the above, it has been found that even in “compatible type” bicrystals, the non-uniform deformation takes place, the GN dislocations are accumulated, and the “GN dislocation band” is formed when the restriction imposed on the slip in the primary slip system differs depending on how the load is applied and the slip is restricted.

5. Conclusion

Crystal plasticity analysis of the deformation and accumulation of dislocations accompanying tensile in symmetric type bicrystals of the “compatible type” was conducted. The results of discussing the formation of the “GN dislocation band” were as follows.

(1) Even in the “compatible type” symmetric bicrystals, in some cases non-uniform deformation may take place depending on how the load is applied from the outside and the “GN dislocation band” is formed inside the model.

(2) The cause of the “GN dislocation band” is thought to be the restriction that acts on the free slip in the primary slip system under the imposed mechanical boundary condition, not the constraint of deformation that works interactively between the crystal grains through the crystal grain boundary.

References


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