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Crystal Plasticity Analysis Using Fast Fourier Transform Numerical Scheme

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(1)

Abstract

Crystal plasticity analyses using the fast Fourier transform (FFT) numerical scheme are now receiving much attention with their computer resource advantages over other numerical methods such as finite element since this method does not require a large matrix solution which obviously takes computational time. In this research, the crystal plasticity using FFT is introduced and then its application to a transformation plasticity analysis is conducted. In addition to the transformation plasticity analysis, FFT is used to calculate the texture development formed by a plane strain compression in an fcc metal and the results are discussed.

1. Introduction

Numerical simulations in the steel research field involve several methodologies covering both microscopic and macroscopic scales. The microscopic steel mechanical-metallurgical phenomena have been approached by, for example, first-principles calculations¹⁾ or molecular dynamics²⁾ while the macroscopic approach has been made by the boundary element method (BEM)³⁾ or finite element method (FEM)⁴⁾. The former methods calculate directly individual atoms whereas the latter methods calculate a material deformation based on the framework of continuum mechanics. Bridging these two different scale levels, recently slip deformation in a single crystal is modelled and then extended to the numerical model considering polycrystalline aggregates realizing mesoscopic scale calculations called crystal plasticity.^{5, 6)} Crystal plasticity can be numerically solved by FEM but the major problem involved in applying this method to crystal plasticity is that it requires numerous computational resources and thus only a limited number of crystal aggregates, which is sometimes not enough to describe the entire behavior of the mechanistic nature of polycrystals, is employed to avoid the computation time.

Alternatively, Moulinec and Suquet have proposed the fast Fourier transform (FFT) numerical scheme to apply elasto-plastic mechanical problems allowing precise computation with limited computer resources.⁷⁾ Although only a periodic boundary condition can be adopted in FFT computation, this method allows a fast computation using limited memory space as the most time-consuming matrix computation. In addition, Lebensohn attempted to extend the FFT numerical framework to the crystal plasticity analyses, revealing its efficiency. $^{\$)}$

Thus, in this study, analyses using crystal plasticity fast Fourier transform (CPFFT) are conducted to solve the two complicated phenomena, namely transformation plasticity and texture development by deformation, and the calculated results are discussed.

2. Crystal Plasticity Formulation by Fast Fourier Transform

Under periodic boundary conditions, displacement at local position x in a representative volume element (RVE) is divided into the average part and the fluctuation part such that

 $u(x) = u'(x) + \overline{\varepsilon}x,$

where, u'(x) is a periodic fluctuation displacement. Using this, strain is obtained as:

$$\varepsilon(u(x)) = \varepsilon(u'(x)) + \overline{\varepsilon}.$$
 (2)

As u'(x) is the fluctuation term, its volume average (hereafter represented by <>) in an RVE is null, i.e. $<\varepsilon(u'(x))>=0$.

The thermo-elasto-plastic constitutive equation considering phase transformation can be written as follows in a rate form:

 $\dot{\sigma}(x) = C(x): \dot{\varepsilon}^{e}(x) = C(x): (\dot{\varepsilon}(x) - \dot{\varepsilon}^{p}(x) - \dot{\varepsilon}^{m}(x)),$ (3) where, C(x) is an elastic tensor in $x. \varepsilon^{e}, \varepsilon, \varepsilon^{p}, \varepsilon^{th}$ and ε^{m} are respectively elastic strain, total strain, plastic strain, thermal strain, and transformation strain. Using polarization tensor τ , Eq. (3) can be re-

$$\dot{\sigma}(\mathbf{x}) = C(\mathbf{x}): \dot{\varepsilon}(\mathbf{x}) + \dot{\tau}^{p}(\mathbf{x}) + \dot{\tau}^{thm}(\mathbf{x}), \qquad (4)$$
where

written as:

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$$\dot{\tau}^p(\mathbf{x}) \equiv -\mathbf{C}(\mathbf{x}) : \dot{\varepsilon}^p(\mathbf{x}) \text{ and } \dot{\tau}^{thm}(\mathbf{x}) \equiv -\mathbf{C}(\mathbf{x}) : (\dot{\varepsilon}^{th}(\mathbf{x}) + \dot{\varepsilon}^m(\mathbf{x})).(5)$$

Let the elastic tensor C^0 in a reference medium be substituted with the local elastic tensor in Eq. (4), and the following is obtained:

$$\dot{\boldsymbol{\tau}}(\boldsymbol{x}) = \boldsymbol{C}^{0}: \dot{\boldsymbol{\varepsilon}}(\boldsymbol{x}) + (\boldsymbol{C}(\boldsymbol{x}) - \boldsymbol{C}^{0}): \dot{\boldsymbol{\varepsilon}}(\boldsymbol{x}) + \dot{\boldsymbol{\tau}}^{p}(\boldsymbol{x}) + \dot{\boldsymbol{\tau}}^{thm}(\boldsymbol{x})$$

$$= C^0$$
: $\dot{arepsilon}(x) + \dot{ au}(x)$

 $\forall x \in V, \partial \dot{\sigma} / \partial x = 0 \quad \forall x \in V, \dot{u}' \#, \dot{\sigma} \cdot n - \#,$ (6) where, $\dot{\tau}(x)$ is a polarization tensor derived from the heterogeneity in the RVE. Equation (6) in the Fourier space can be written as:

$$\dot{\sigma}(\xi) = i\mathbf{C}^0: (\dot{u}'(\xi) \otimes \xi) + \dot{\tau}(\xi), \quad i\dot{\sigma}(\xi) \cdot \xi = 0,$$
 (7)
where, ξ is frequency and non-Italic i is an imaginary number. E

where, $\boldsymbol{\xi}$ is frequency and non-Italic i is an imaginary number. By eliminating $\hat{\boldsymbol{\sigma}}$ from Eq. (7), the following is obtained:

$$\hat{\boldsymbol{u}}'(\boldsymbol{\xi}) = \frac{1}{2} \left(N^0 \otimes \boldsymbol{\xi} + \boldsymbol{\xi} \otimes N^0 \right) \hat{\boldsymbol{\tau}}(\boldsymbol{\xi}), \tag{8}$$

with

$$N^{0}(\boldsymbol{\xi}) = \boldsymbol{K}^{0}(\boldsymbol{\xi})^{-1}, \, \boldsymbol{K}^{0}(\boldsymbol{\xi}) = \boldsymbol{C}^{0}: (\boldsymbol{\xi} \otimes \boldsymbol{\xi}), \tag{9}$$

$$\hat{\varepsilon}(\boldsymbol{\xi}) = \frac{1}{2} \left(\boldsymbol{\xi} \otimes \hat{\boldsymbol{u}}'(\boldsymbol{\xi}) + \hat{\boldsymbol{u}}'(\boldsymbol{\xi}) \otimes \boldsymbol{\xi} \right) = -\hat{\boldsymbol{\Gamma}}^0(\boldsymbol{\xi}) : \hat{\boldsymbol{\tau}}(\boldsymbol{\xi}), \tag{10}$$

$$\hat{F}^{0}(\xi) = \frac{1}{4} \left(N_{li}^{0} \xi_{j} \xi_{k} + N_{ki}^{0} \xi_{j} \xi_{l} + N_{lj}^{0} \xi_{i} \xi_{k} + N_{kj}^{0} \xi_{i} \xi_{l} \right).$$
(11)

 $\hat{\Gamma}^0$ is a periodic green's operator. The strain rate distribution in a heterogeneous medium can be obtained by taking the inverse Fourier transformation of Eq. (10).

An iterative approach is taken to numerically solve the above equations (strain rate and stress rate), such that:

Initialization: $\dot{\epsilon}^0 = \dot{\epsilon}^n(\mathbf{x}), \forall \mathbf{x} \in V$ Iteration: (n+1): $\dot{\epsilon}^n(\mathbf{x})$ and $\dot{\sigma}^n(\mathbf{x})$ are known (a) $\hat{\sigma}^n = FFT(\dot{\sigma}^n)$

(b) Check convergence

$$e^{n} = \left| \sqrt{\langle \| \operatorname{div}(\dot{\boldsymbol{\sigma}}^{n}) \|^{2} \rangle} - \sqrt{\langle \| \operatorname{div}(\dot{\boldsymbol{\sigma}}^{n-1}) \|^{2} \rangle} \right|$$
$$= \left| \sqrt{\langle \| \boldsymbol{\xi} \cdot \hat{\boldsymbol{\sigma}}^{n}(\boldsymbol{\xi}) \|^{2} \rangle} - \sqrt{\langle \| \boldsymbol{\xi} \cdot \hat{\boldsymbol{\sigma}}^{n-1}(\boldsymbol{\xi}) \|^{2} \rangle} \right| < \epsilon$$

and

 $e^n = \sqrt{\langle \| \operatorname{div}(\dot{\boldsymbol{\sigma}}^n) \|^2 \rangle} = \sqrt{\langle \| \boldsymbol{\xi} \cdot \hat{\boldsymbol{\sigma}}^n(\boldsymbol{\xi}) \|^2 \rangle} < \epsilon$ if no macroscopic stress is imposed

$$e^{n} = \frac{\sqrt{\langle ||\operatorname{div}(\check{\sigma}^{n})||^{2}\rangle}}{\sqrt{||\langle \check{\sigma}^{n} \rangle||^{2}}} = \frac{\sqrt{\langle ||\check{\xi} \cdot \hat{\sigma}^{n}(\xi)||^{2}\rangle}}{||\check{\sigma}^{n}(0)||} < \epsilon \quad \text{otherwise}$$
(c) $\hat{\varepsilon}^{n+1}(\xi) = \hat{\varepsilon}^{n}(\xi) - \hat{\Gamma}^{0}(\xi) : \hat{\sigma}^{n}(\xi) \quad \forall \xi \neq 0 \quad \text{and} \quad \hat{\varepsilon}^{n+1}(0) = \hat{\varepsilon}$
(d) $\dot{\varepsilon}^{n+1} = FFT^{-1}(\hat{\varepsilon}^{n+1})$
(e) $\dot{\sigma}^{n+1}(\mathbf{x}) = g(\dot{\varepsilon}^{n+1}(\mathbf{x})) \quad \forall \mathbf{x} \in V,$

where, q is a constitutive relation.

Then, plastic strain rate $\dot{\varepsilon}^p$ is modelled below by the crystal plasticity framework. Plastic strain of a crystalline metal derives from deformations in the slip directions on the slip surfaces. This slip surface and the slip direction are mostly determined by the crystal structure, and this combination is called the slip system. Twelve slip systems are present in fcc metal and 48 main slip systems are present in bcc metal. The following uses 12 slip systems of {111}<110>, which is a representative slip system of the fcc metal. Let the slip rate in the α slip system be written as \dot{y}^{α} , and the plastic strain rate can be expressed as the sum of slip deformation in all slip systems such that:

$$\dot{\varepsilon}^{p} = \sum_{\alpha} p^{\alpha} \dot{\gamma}^{\alpha}, \tag{12}$$

where, p^{α} is the Schmid tensor in the α slip system, which takes the following form using slip direction vector s^{α} and vector m^{α} normal to the slip surface:

$$\boldsymbol{p}^{\alpha} = \frac{1}{2} \left(\boldsymbol{s}^{\alpha} \otimes \boldsymbol{m}^{\alpha} + \boldsymbol{m}^{\alpha} \otimes \boldsymbol{s}^{\alpha} \right).$$
(13)

Resolved shear stress applied to the slip surface can be calculated from the stress tensor by Schmid's law. When this resolved shear stress exceeds the elastic limit, plastic deformation takes place. This elastic limit is called Critical Resolved Shear Stress (CRSS), which is expressed as g^{α} as follows, and is obtained as a tensor product of the Schmid tensor and stress tensor, such that:

$$|\tau^{\alpha}| = |\boldsymbol{p}^{\alpha}:\boldsymbol{\sigma}| = g^{\alpha}. \tag{14}$$

Considering the symmetry and the incompressibility of the plastic strain rate, the degree of freedom of the plastic strain rate is five whereas the fcc crystal has 12 slip systems. In this case, the solution of the slip rates on each slip system in order to obtain the plastic strain rate $\dot{\epsilon}^p$ cannot be uniquely obtained because of the singularity. To avoid the problem, application of the viscoplastic-type constitutive equation (all slip systems are active) is widely used.⁹⁻¹²⁾

In contrast, the strain rate independent model has been developed by Hutchinson,⁹⁾ which limits the maximum number of slip systems that can simultaneously be active. This model allows the non-singular solution as described below. Let the shear force applied to the active slip surface be written as:

$$\dot{\tau}^{\alpha} = \operatorname{sgn}(\tau^{\alpha})\dot{g}^{\alpha},\tag{15}$$

and by assuming the small deformation theory, the following equation is satisfied:

$$\dot{\boldsymbol{\sigma}}: \boldsymbol{p}^{\alpha} = \sum_{\beta} h^{\alpha\beta} \dot{\gamma}^{\beta}. \tag{16}$$

Work hardening is a consequence of the pile up of slip deformation on each slip system, such that:

$$\dot{g}^{\alpha} = \sum_{\beta} h^{\alpha\beta} |\dot{\gamma}^{\beta}|, \tag{17}$$

where, $h^{\alpha\beta}$ is a work hardening parameter. Here, a simple model that describes the work hardening behavior can be written using parameter H_0 , initial yield shear stress τ_0 , and saturation stress τ_s ,¹³⁾ such that:

$$h^{\alpha\alpha} = h = H_0 \operatorname{sech}^2 \left[\frac{H_0 \Sigma_{\beta} \gamma^{\beta}}{\tau_s - \tau_0} \right]$$
(18)

$$h^{\alpha\beta} = qh + (1-q)h\delta_{\alpha\beta}, \tag{19}$$

where, q decides the ratio of self-hardening and latent-hardening, whose value varies from 1.0 to 1.4.

By eliminating plastic strain from the constitutive equation using Eq. (16), the following is obtained:

$$\dot{\sigma}: p^{\alpha} = C: (\dot{\varepsilon} - \dot{\varepsilon}^{\mu} - \dot{\varepsilon}^{ih} - \dot{\varepsilon}^{m}): p^{\alpha}$$

$$= C: (\dot{\varepsilon} - \dot{\varepsilon}^{ih} - \dot{\varepsilon}^{m}): p^{\alpha} - \sum_{\beta} p^{\alpha}: C: p^{\beta} \dot{\gamma}^{\beta}$$

$$= \sum_{\beta} h^{\alpha\beta} \dot{\gamma}^{\beta}.$$
(20)

The slip rate in slip system α can thus be calculated: $\dot{y}^{\alpha} = f^{\alpha}: (\dot{\epsilon} - \dot{\epsilon}^{th} - \dot{\epsilon}^{m})$ with $f^{\alpha} = \sum_{\alpha} Y^{\alpha\beta} C: p^{\beta}$, (21)

where $(2 - \beta)^{-1} = (2 - \beta)^{-1}$

$$Y^{\alpha\beta} = (X^{\alpha\beta})^{-1} \text{ and } X^{\alpha\beta} = h^{\alpha\beta} + p^{\alpha}: C: p^{\beta}.$$
(22)

The direct discretization of Eq. (21) may not give a correct solution for an elastic to elasto-plastic transient state¹⁴ because this causes incompatibility between pre- $(|\tau^{\alpha}| < g^{\alpha})$ and post- $(|\tau^{\alpha}=g^{\alpha})$ in a one-time step. In this case, proper hardening in finite time increments should be taken into account, such that:

$$\tau^{\alpha} + \Delta \tau^{\alpha} = \operatorname{sgn}(\tau^{\alpha})(g^{\alpha} + \Delta g^{\alpha}).$$
(23)

Therefore, Eq.(16) can be rewritten in an incremental form as follows:

$$(\boldsymbol{\sigma} + \Delta \boldsymbol{\sigma}): \boldsymbol{p}^{\alpha} = \operatorname{sgn}(\tau^{\alpha}) g^{\alpha} + \sum_{\beta} h^{\alpha\beta} \Delta \gamma^{\beta}.$$
(24)

Finally, the following equation should be solved numerically.

$$\Delta \gamma^{\alpha} = \sum_{\beta} Y^{\alpha\beta} \Big(\boldsymbol{\sigma} : \boldsymbol{p}^{\beta} + \boldsymbol{p}^{\beta} : \boldsymbol{C} : (\Delta \boldsymbol{\varepsilon} - \Delta \boldsymbol{\varepsilon}^{ih} - \Delta \boldsymbol{\varepsilon}^{m}) - \operatorname{sgn}(\tau^{\beta}) g^{\beta} \Big).$$
(25)

When the state is elastoplastic at the beginning of the step, the critical resolved shear stress is equal to the stress on the slip surface. In this case, Eq. (25) coincides with Eq. (21).

3. Transformation Plastic Strain Analysis

Stress applied to a steel material in phase transformation can cause large plastic deformation even when the stress is smaller than the yield stress. This phenomenon is called transformation plasticity supplement plastic strain is called transformation plastic strain. Transformation plastic strain significantly affects the residual stress and shape after heat treatment, so this type of phenomenon needs to be considered in heat treatment simulations. Greenwood and Johnson have created a model in which transformation plastic strain is linked with volume changes during transformation supposing that transformation plasticity is caused by the accommodation of strain difference due to volume changes during transformation.¹⁵

Meanwhile, Magee has presumed that load stress affects the selection of variants during diffusionless transformation, which causes transformation plastic strain.¹⁶ In addition, Otsuka et al. have shown that volume change plays an important role in the occurrence of transformation plastic strain in diffusionless transformation as well.¹⁷⁾ Leblond has solved analytically, based on the Greenwood-Johnson mechanism, elasto-plastic deformation in a mother phase (soft layer) when a spherical new phase (hard layer that is not supposed to deform plastically) is formed from the matrix of the mother phase involving transformation strain, and formulated transformation plastic strain.¹⁸⁾ This study is based on the Greenwood-Johnson mechanism as the purpose of present study is to calculate transformation plasticity during diffusion transformation. In this case, crystal plasticity analysis schemes using the FEM19) and aforementioned FFT¹⁴) can be used without introducing an artificial term, namely transformation plastic strain, since transformation plastic strain can be derived from classic elasto-plasticity constitutive frameworks.²⁰⁾

Next, the inside of an RVE that is the calculation target is divided into polycrystals. In FEM, the crystal orientation is determined for each integration point (or element). However, in crystal plasticity analysis using FFT, a crystal orientation is given to each of the lattice points placed at regular intervals in the region and the stress and strain are calculated at each point. These lattices are assigned to crystal grains using Voronoi tessellation. In this study, it is supposed that in one crystal grain, the initial orientations are the same. Therefore, it can be supposed that there are grain boundaries between the lattice points, each of which has a different initial orientation. Usually, a transformation nucleus is formed from a grain boundary. However, this study supposes for simplification that the nuclei of new grains would form randomly. In addition, random crystal orientations are given to the initial microstructure. Figure 1(a) shows the initial polycrystal in which 100 crystal grains are placed in a $64 \times$ 64×64 lattice and Fig. 1(b) for which new 100 phases are formed from the initial texture. Table 1 lists the parameters used in this study.

For the new phases, it is assumed that nuclei with crystal orientations that satisfy the K-S relation with the mother phases would form at the same time. These nuclei spread isotopically (spherically) and transformation strain ($\varepsilon^{m}(x)$) occurs on the phase-transformed lattice points. Hereinafter, the average in the RVE is referred to as "macroscopic" and the value at each lattice point as "microscopic".

In order to validate the proposed numerical model, simulation of phase transformation under the stress-free condition is considered. Macroscopic transformation strain from the start of the transforma-



(b) During phase transformation

Fig. 1 Sample Voronoi tessellation and phase transformation: 100 grains in 64³ cubic space

Table 1 Parameters for crystal plasticity calculation

	Parent phase	Daughter phase
Bulk modulus (GPa)	135833	150 000
Shear modulus (GPa)	62 692	69 2 3 1
H_0 (MPa)	10	550
τ_0 (MPa)	30	100
τ_s (MPa)	40	130
q	1.0	1.0
Number of grains	100	100

tion to its end can be theoretically expressed with the equation below: $^{21)} \label{eq:21}$

m o	(0.0)
$\varepsilon = \varepsilon'' = K_7$	(26)
$v v p_2$	(20)

where, $\bar{\varepsilon}$ is macroscopic strain without load, so it matches the transformation strain ($\bar{\varepsilon}^m$) and it is in a linear relation with the volume fraction of the transformed phase (z) that has a transformation expansion coefficient (β). To allow Eq. (26) to strictly hold, the material needs to be isotropic. Therefore, in this verification of the appropriateness only, isotropic elastic constant is used which is independent of crystal orientations.

Figure 2 compares macroscopic strain calculated from the numerical scheme and the strain (normalized with β) calculated from Eq. (26) when β is 1.536×10^{-3} . The numerical results in the graph show that macroscopic strain occurs linearly with the volume fraction coinciding with the theoretical equation.

Figure 3 shows the volume fraction of the phase and plastic strain in each of the mother and daughter phase. In transformation expansion due to phase transformation, macroscopic and isotropic expansion occurs, so it seems nothing is happening at a glance, but plastic deformation actually occurs in the vicinity of new grain



Fig. 2 Evolution of the macroscopic strain with the volume fraction of transformed phase (no applied stress, isotropic polycrystal)









results using Table 1 show that plastic deformation occurs in the daughter phase as well.

Next, the calculation results of a case where stresses are applied in phase transformation are discussed. Tensile or compressive stress is applied before the phase transformation begins and is retained until the phase transformation completes. **Figure 4** (a) shows the strain changes under several stress levels clearly exhibit the strain dependence on applied stress. Here, deducting the strain at no stress from that with stress applied at the transformation end produces transformation plastic strain. Figure 4 (b) shows the transformation plastic strain obtained for each stress value. These results show that when the load stress is from -50 to 50 MPa, the transformation plastic strain is in a linear relation with the applied stress.^{15, 18, 20}

Meanwhile, when the absolute value of the applied stress exceeds 50 MPa which is the linear relationship between transformation plastic strain and applied stress no longer conforms which is approximately one half of the yield stress of the mother phase. This behavior matches the values shown in the papers.^{15, 22)} The transformation plasticity coefficient (K_p) calculated from the linear relation at the low load stress (-50 to 50 MPa) in Fig. 4(b) is 2.20×10^{-5} MPa⁻¹. This result almost correlates with the result from the Leblond model (K_p =2.17×10⁻⁵ MPa⁻¹).

4. Deformation Texture Analyses

This section discusses a deformation texture analysis scheme in the crystal plasticity framework using FFT and its application to plane strain compression calculation. Deformation involves local rotation, so deformation texture is formed, which affects the anisotropy and other material properties. Some schemes have been proposed for crystal plasticity deformation texture analyses: Analyses using FEM,²³ FFT,⁸ and the self-consistent method.⁸ In these papers, viscoplastic constitutive equations are used, but how the strain rate sensitivity exponent (hereinafter, "*m*-value") and other parameters affect the calculation results have not been clarified. Therefore, this study examines the impact of the *m*-value on the texture formation by using strain rate-dependent constitutive equations.

In this section, for the sake of simplicity, the constitutive model uses the infinitesimal deformation theory. In addition, it is assumed that the calculation points are fixed despite the deformation.

A spin tensor is used to calculate crystal rotation. That is to say, when considering elasto-plasticity analysis of the velocity gradient shown below:

$$\boldsymbol{L} = \boldsymbol{L}^* + \boldsymbol{L}^p, \tag{27}$$

the slip direction, slip plane, and Euler angle changes in each step can be expressed as follows using elastic spin (W^*): $\dot{\sigma} = W^* \sigma$, $\dot{w} = W^* w$. (28)

$$s = w s, \ m = w m$$

$$\dot{\phi}_{1} = -(W_{23}^{*} \sin \varphi_{1} - W_{31}^{*} \cos \varphi_{1}) \cot \phi + W_{12}^{*}$$

$$\dot{\phi} = W_{31}^{*} \sin \varphi_{1} + W_{23}^{*} \cos \varphi_{1}$$

$$\dot{\phi}_{2} = \frac{W_{23}^{*} \sin \varphi_{1} - W_{31}^{*} \cos \varphi_{1}}{\sin \phi}, \qquad (29)$$

where, Euler angles are in Bunge notation. The elastic spin is the anti-symmetrical part of the elastic velocity gradient tensor:

$$W^* = \frac{1}{2} (L^* - L^{*T}).$$
(30)

$$\boldsymbol{w}^{a} = \frac{1}{2} \left(\boldsymbol{s}^{a} \otimes \boldsymbol{m}^{a} - \boldsymbol{m}^{a} \otimes \boldsymbol{s}^{a} \right), \tag{31}$$

the plastic spin can be expressed as follows:

$$W^{p} = \sum_{\alpha} w^{\alpha} \dot{\gamma}^{\alpha}. \tag{32}$$

Thereby, once the spin is determined, elastic spin can be easily calculated. As is the case with Eqs.(10) and (11), using the polarization tensor, elastic spin can be calculated from the spin tensor in a Fourier space:

$$\widehat{W}(\xi) = \frac{1}{4} \left(\xi \otimes \hat{u}'(\xi) - \hat{u}'(\xi) \otimes \xi \right) = -\widehat{\Gamma}'^{0}(\xi) : \hat{\tau}(\xi),$$
(33)

$$\hat{\Gamma}^{\prime 0}(\xi) = \frac{1}{4} \left(-N_{li}^{0} \xi_{j} \xi_{k} + N_{ki}^{0} \xi_{j} \xi_{l} - N_{lj}^{0} \xi_{i} \xi_{k} + N_{kj}^{0} \xi_{i} \xi_{l} \right).$$
(34)

In this case, the polarization tensor itself needs to be calculated. As a viscoplastic crystal plasticity model, the equation below is employed using the strain rate sensitivity exponent (m):^{9–12)}

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left(\frac{\tau^{\alpha}}{g^{\alpha}}\right) \left| \frac{\tau^{\alpha}}{g^{\alpha}} \right|^{\frac{1}{m}-1},\tag{35}$$

where, although all slip systems become active, when the *m*-value is sufficiently small, it approaches the strain rate independent constitutive equation.

Placed in the RVE consisting of 128^3 lattice points (Fig. 5) are 2000 crystal grains to calculate the deformation texture after plane strain compression. Initial crystal orientations are randomly given to the 2000 crystal grains, the average strain in the *y* direction (width direction) is determined as 0, and 30% compressive strain is given in the *z* direction. Calculation results for this texture under these conditions are shown below.

Figure 6(a) to 6(e) show ODF ($\varphi_2=45^\circ$) when the *m* in Eq. (35) is varied from 0.05 to 0.5. Figure 6(f) is ODF calculated using Eq. (21). These results show that typical rolling texture at the thickness center for the Copper and Brass orientations is developed under all the conditions. This is because strain from rolling at the center of the thickness is close to that under plane strain compression.

Meanwhile, the development of the texture varies depending on the m-value. When the m-value is 0.05, although the texture is weak



Fig. 5 Voronoi tessellation (2000 grains in 128³ cubic space)



Fig. 6 Strain rate sensitivity exponent dependence on ODF ($\phi_2 = 45^\circ$)

on the whole, the Copper orientation is stronger than the Brass orientation. In addition, as the *m*-value increases, the Brass orientation becomes stronger and the Copper orientation tends to become weaker. When the strain rate independent constitutive equation is used, the Copper orientation is stronger than the Brass orientation, similar to when the *m*-value is small. This matches the characteristic of the constitutive Eq. (35) that shows when the *m*-value is smaller, the strain rate dependency is smaller. These changes in the *m*-value can be understood as the materials' temperature dependency (when the *m*-value is small, the temperature is low and when it is large, the temperature is high): The relation between the work hardening behavior by changes in the *m*-value and the texture formation matches the influence of stacking fault energy qualitatively, so they may be related.

5. Conclusions

This study proposed a crystal plasticity analysis scheme using

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FFT and discussed its application to transformation plasticity and texture analyses. The crystal plasticity analysis scheme using FFT can handle only periodic boundary conditions, unlike schemes using FEM. However, it can perform mathematical operations with very small computation resources and is capable of large-scale analyses.

The transformation plasticity analysis using this scheme has enabled analysis of transformation plastic strain through numerical computation and the result matched that from Leblond's analytical model. In addition, nonlinearity of transformation plastic strain under high stress could be naturally calculated from the classical elasto-plasticity constitutive equation.

Furthermore, this scheme can be applied to the calculation of deformation texture. Texture at 30% plane strain compression was analyzed to investigate the influence of the strain rate sensitivity exponent (*m*-value) on the texture. The results show that when the *m*-value is smaller and the strain rate independent constitutive equation is used, the Copper orientation is strong and the Brass orientation is weak; and when the *m*-value is large (sensitive to strain rate), the Brass orientation is strong and the Copper orientation is weaker.

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