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A NEW CRYSTAL PLASTICITY CONSTITUTIVE EQUATION BASED ON CRYSTALLOGRAPHIC MISORIENTATION THEORY

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Abstract. Since plastic deformation of polycrystal sheet metal is greatly affected by its initial and plastic deformed textures, multi-scale finite element (FE) analysis based on homogenization with considering micro-polycrystal morphology is required [1]. We formulated a new crystal plasticity constitutive equation to introduce not only the effect of crystal orientation distribution, but also the size of crystal grain and/or the effect of crystal grain boundary for the micro-FE analysis. The hardening evolution equation based on strain gradient theory [2], [3] was modified to introduce curvature of crystal orientation based on crystallographic misorientation theory. We employed two-scale structure, such as a microscopic polycrystal structure and a macroscopic elastic/plastic continuum. Our analysis

code predicts the plastic deformation of polycrystal metal in the macro-scale, and simultaneously the crystal texture and misorientation evolutions in the micro-scale. In this study, we try to reveal the relationship between the plastic deformation and the microscopic crystal misorientation evolution by using the homogenized FE procedure with the proposed crystal plasticity constitutive equation. The crystallographic misorientation evolution, which affects on the plastic deformation of FCC polycrystal metal, was investigated by using the multi-scale FE analysis. We confirmed the availability of our analysis code employing the new constitutive equation through the comparison of a uniaxial tensile problem with the numerical result and the experimental one.

1 INTRODUCTION

Recently, multi-scale finite element (FE) analyses code are developed to evaluate macroscopic material properties such as the strength, the yield loci and the formability, by employing a realistic three-dimensional (3D) microscopic polycrystal structure obtained by using the scanning electron microscopy and the electron backscattering diffraction (SEM-EBSD) measurements [4]. The experimental determination, interpretation, and the numerical simulation for polycrystal texture analyses at the micro-scale have been attracting the attention of researchers in the field of sheet metal forming [5-6]. Further, the progress of computer technology, such as parallel computing [7], promises an unprecedented means for a large-scale numerical calculation in this multi-scale analysis for the industrial applications. For the crystal plasticity constitutive equation, the isotropic and kinematical hardening evolutions are introduced [8]. In our two-scale homogenization theory to assess the sheet material formability, a realistic 3D representative volume element (RVE) is employed, which is determined by SEM-EBSD measurement.

Until now, we have found many “virtual” RVE models, such as Voronoi polyhedron grain models, but they do not have the necessary crystal grain characteristic of location, size or orientation in 3D space. Since the deformation and hardening are very much affected by the neighboring crystal grains, orientation and the grain size themselves.

In this study, a new hardening evolution equation is proposed for assessment of crystal orientation rotation and misorientation evolution. Our model is considered misorientation between adjacent regions across a boundary. This involves a model, which assumes a simple geometrical relationship between crystal slip systems responsible for the rotation and misorientation.

2 ELAST/VISCO-CRYSTAL PLASTICITY CONSTITUTIVE EQUATION BASED ON MISORIENTATION THEORY

2.1 Definition of equivalent misorientation

We calculated curvature of crystallographic misorientation to express geometrically necessary (GN) dislocation storage [9]. When the GN dislocation is stored during plastic deformation, sheet metal shows work hardening. Thus, consideration of misorientation into hardening evolution equation is able to analyze sheet metal forming and to assess the deformation characterization accurately.

We defined the three normal orthogonal coordinate systems for calculation of

crystallographic misorientation as shown in Fig. 1. One is the sample coordinate system ($\boldsymbol{e}_i$ - x_i). The second is the crystalline coordinate system ($\boldsymbol{i}_i$ - y_i), and third is (111) plane coordinate system ($\boldsymbol{j}_i$ - θ_i). Relationship between the sample coordinate system and the crystalline coordinate system, the representative (111) plane coordinate system are expressed as $\boldsymbol{i}_i = \Theta_i^j \boldsymbol{e}_j$, $\boldsymbol{j}_i = \Omega_i^j \boldsymbol{e}_j$, where Θ_i^j, Ω_i^j are coordinate transformation matrices.

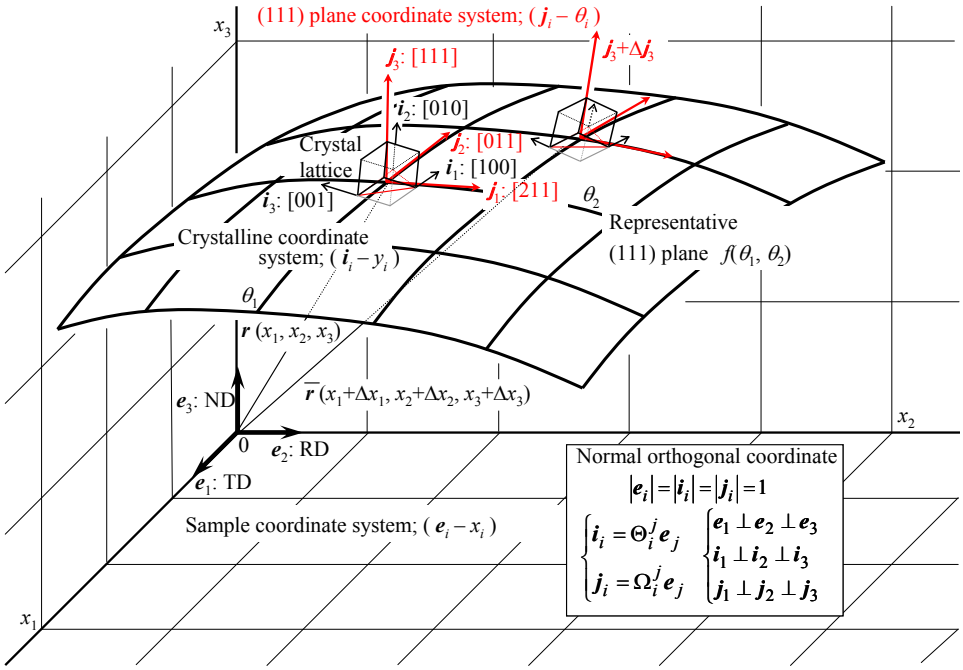

Figure 1: Definition of the three normal orthogonal coordinate systems

In the Fig. 2, $\boldsymbol{j}_1$, $\boldsymbol{j}_2$ and $\boldsymbol{j}_3$ express $[2\bar{1}\bar{1}]$, $[01\bar{1}]$ and $[111]$ vectors on the (111) plane coordinate system ($\boldsymbol{j}_i$ - θ_i), which belongs with the crystalline coordinate system ($\boldsymbol{i}_i$ - y_i). Rate of [111] direction $\Delta\boldsymbol{j}_3$ is defined by using $\boldsymbol{j}_i$ as follow:

$$\Delta \boldsymbol{j}_3 = -b_{\alpha\beta} \boldsymbol{j}_\alpha \Delta\theta_\beta \tag{1}$$

where $b_{\alpha\beta}$ (α, β = 1, 2) is the second fundamental metric tensor, which corresponds to a curvature tensor of crystal orientation, and is expressed as follows:

$$b_{\alpha\beta} = -\frac{\partial \boldsymbol{j}_3}{\partial \theta_\beta} \cdot \boldsymbol{j}_\alpha \tag{2}$$

$$\boldsymbol{b} = b_{\alpha\beta} \boldsymbol{j}_\alpha \otimes \boldsymbol{j}_\beta \tag{3}$$

The curvature tensor $b_{\alpha\beta}$ corresponds to rate of normal direction of tangential plane, and is transformed by the coordinate transformation matrices $\Omega_k^\alpha, \Omega_l^\beta$ to the sample coordinate system as follows:

$$\boldsymbol{b} = b_{\alpha\beta} \Omega_k^\alpha \Omega_l^\beta \boldsymbol{e}_k \otimes \boldsymbol{e}_l = \bar{b}_{kl} \boldsymbol{e}_k \otimes \boldsymbol{e}_l \tag{4}$$

$$\bar{b}_{kl} = -\boldsymbol{j}_{3,l} \cdot \boldsymbol{j}_k \tag{5}$$

where $\bar{b}_{kl}$ is misorientation tensor. Equivalent misorientation K is defined by the second invariant value of $b_{\alpha\beta}$ as follow:

$$K = \sqrt{\frac{1}{2}\bar{b}_{kl}\bar{b}_{kl}} \tag{6}$$

This scalar value K depends on crystal orientation distribution and grain size.

2.2 Introducing equivalent misorientation into crystal plasticity constitutive equation

In this study, the equivalent misorientation caused by crystal orientation distribution is introduced into the crystallographic homogenized multi-scale FE procedure, which is based on the dynamic explicit scheme [1]. The strain rate dependent crystal plasticity constitutive equation [2, 8] is employed to the micro-FE analysis. The crystalline viscoplastic shear strain rate $\dot{\gamma}^{(a)}$ of the power law form defined on the slip system (a) is expressed as follow:

$$\dot{\gamma}^{(a)} = \dot{\gamma}_0^{(a)} \left[\frac{\tau^{(a)}}{g^{(a)}} \right] \left[\left| \frac{\tau^{(a)}}{g^{(a)}} \right| \right]^{\frac{1-m}{m}} \tag{7}$$

where $\tau^{(a)}$ is the resolved shear stress, $g^{(a)}$ is the reference shear stress, $\dot{\gamma}_0^{(a)}$ is the reference shear strain rate, and m is the coefficient of strain rate sensitivity. In this study, $\dot{\gamma}_0^{(a)} = 0.033$ and $m = 0.01$ are employed for FCC metal, respectively.

The equivalent misorientation K is introduced into the hardening evolution equation as follow:

$$\dot{g}^{(a)} = \left\{ \frac{1}{\tanh C_2} \tanh\left(C_1 |K| + C_2\right) \right\} \sum_{b=1}^{N} h_{ab} \left| \dot{\gamma}^{(b)} \right| \tag{8}$$

where N is the total number of slip systems for the FCC crystal $N = 12$, C_1 and C_2 are constants of hardening parameters. The hardening coefficient h_{ab} for the nth power equation is expressed as follows:

$$h_{ab} = q_{ab} h(\gamma) + (1 - q_{ab}) h(\gamma) \delta_{ab} \tag{9}$$

$$h(\gamma) = h_0 n C \{ C(\gamma_0 + \gamma) \}^{n-1} \tag{10}$$

where the matrix q_{ab} is introduced to describe the self and latent hardenings. The γ is the accumulated shear strain over all the slip systems, h_0 is the initial hardening modulus, and n and C are the hardening exponent and the hardening coefficient, respectively. These values including C_1 and C_2 in Eq. (8) are determined by the parameter identification calculation through the comparison with the experimental results.

When $K = 0$, which is uniform crystal orientation distribution condition, the hardening evolution equation (8) becomes the conventional equation as follow:

$$\dot{g}^{(a)} = \sum_{b=1}^{N} h_{ab} \left| \dot{\gamma}^{(b)} \right| \tag{11}$$

3 NUMERICAL RESULTS

3.1 Material parameter identification by using 3D-EBSD measured polycrystal model

We obtained distribution of crystal orientation in a 3D parallelepiped box region of the aluminum alloy sheet metal A5182-O by SEM-EBSD measurement, which is a material of the NUMISHEET 2008 benchmark problem [10], and developed a RVE-FE model as shown in Fig. 2. The RVE-FE model is 5×5×5 voxel FEs by using 8-node solid element with 1000 Gaussian integration points. The crystal orientation distribution of the sheet metal measured by SEM-EBSD is assigned into the integration points on the RVE-FE model.

Figure 3 shows comparison of stress-strain curves obtained by the experiment of the rolling direction (RD) tensile test and its multi-scale FE analyses by using identified parameters as summarized in Table 1. In the multi-scale FE analyses, proportional loading is applied to macro-FE model, which consists of one 8-node solid element, combined with the micro RVE-FE model to obtain the homogenized stress. It is good agreement of stress-strain relationships between the experiment and FE analyses. In the multi-scale FE result by misorientation theory, the critical (initial) resolved shear stress (CRSS) τ_0 and the initial hardening modulus h_0 are smaller than conventional ones due to effect the misorientation hardening parameters C_1 and C_2.

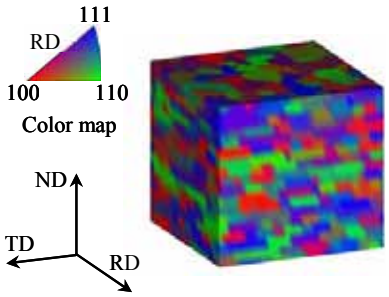

Figure 2: RVE-FE model of A5182-O (111×111×111μm^3)

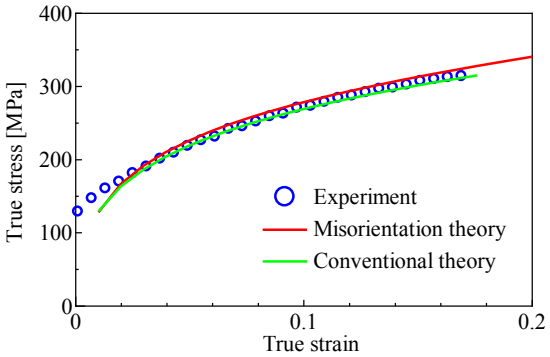

Figure 3: Relationships between true stress and true strain of experimental and identification results

Table 1: Material parameters obtained by multi-scale FE analysis

	n	τ_0 [MPa]	h_0 [MPa]	C	γ_0 [MPa]	C_1	C_2
Misorientation	0.19	13.0	49.0	17.0	0.10	5.0	0.8
Conventional	0.19	15.0	72.0	17.0	0.10	–	–

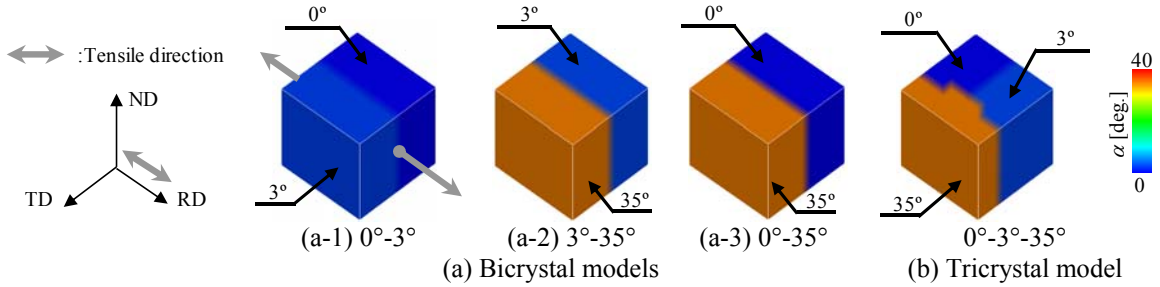

Figure 4: Initial crystal orientation angle α distributions of micro-models

Table 2: Euler angle (φ_1, Φ, φ_2) and crystal orientation angle α

	φ_1	Φ	φ_2	α
Grain 1	–12.3°	54.5°	44.7°	0.3°
Grain 2	12.5°	57.7°	43.3°	3.2°
Grain 3	89.6°	69.0°	8.84°	34.7°

3.2 Multi-scale analysis by using bicrystal and tricrystal micro-models

In order to consider the newly developed constitutive equation based on misorientation theory, simple initial crystal models, such as bicrystal and tricrystal models are employed to the micro-FE analysis, as shown in Fig. 4. Three crystal orientations are selected from the SEM-EBSD crystal orientation distribution of A5182-O sheet metal as summarized in Table 2. Micro-FE model is $111\times111\times111\mu m^3$ volume with $5\times5\times5$ FEs, which is same as the polycrystal A5182-O RVE-FE model. A crystal orientation angle α is defined as angle between crystal [111] direction and normal direction (ND) of sheet metal. Consequently, a low tilt angle boundary model as shown in Fig. 4 (a-1) and high tilt angle boundary models as shown in Fig. 4 (a-2) and (a-3) are constructed in the bicrystal models, respectively. In addition, tricrystal model as shown in Fig. 4 (b) is also constructed. It has mixed with low and high tilt angle boundaries. Figure 5 shows initial equivalent misorientation distribution on the center cross-section surface of the ND direction (ND = 55.5μm) of micro-models. The tilt angle is clearly described by the equivalent misorientation distribution.

Figure 6 shows comparison of stress-strain curves obtained by the multi-scale FE analyses of the RD tensile problem by using three types of bicrystal models and the tricrystal model. The material parameters of A5182-O polycrystal sheet metal are used for these models. In the tilt angle 0°-3° bicrystal model, the highest stress is achieved because the model has larger amount of active slip systems by smaller α value than the others, which means the crystal

(111) plane coincides with sheet plane. The 35° single crystal model is the lowest stress. The high tilt 0°-35° and 3°-35° bicrystal models, and the 0°-3°-35° tricrystal model are combination behavior between the low tilt model and the 35° single crystal model.

Figure 7 shows texture evolution on {111} pole figures compared with the initial texture and after 0.5 tensile deformation. The textures are evoluted to toward preferred orientation of tensile deformation such as the Copper orientation {112}<111>. The crystal angle α is also rotated by tensile deformation as shown in Fig. 8. According to crystal angle rotation, equivalent misorientation distribution is also changed as shown in Fig. 9. In the 0°-3° low tilt angle bicrystal model, grain boundary is disappearance and crystal binding each other. In the high title angle bicrystal models 0°-35° and 3°-35°, however, grain boundary has been remained during tensile deformation.

Since there is a triple point in the tricrystal model and interaction of each grain, the subgrain growth and localization of misorientation are occurred as shown in Fig. 9 (b). Figure 10 shows history of crystal angle α rotation of tricrystal model during tensile deformation. While the crystal $\alpha = 35°$ as red solid line did not almost rotate, crystals $\alpha = 0°$ and 3° as blue and purple solid lines rotated toward 15° and then low tilt angle boundary between 0° and 3° is disappeared. It could predict physical evidence that crystal rotations and misorientation effect on material hardening by using our multi-scale analyses with the new hardening evolution equation.

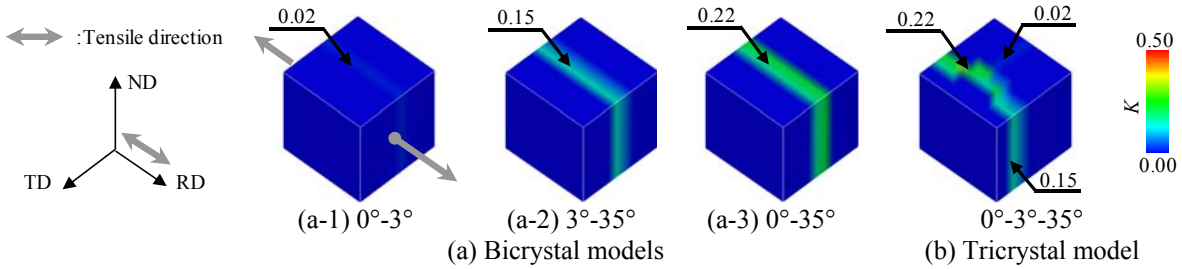

Figure 5: Initial equivalent misorientation distributions of micro models

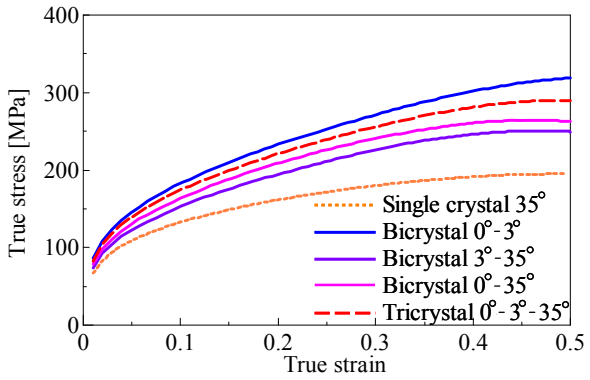

Figure 6: Relationships between true stress and true strain of multi-scale FE analyses

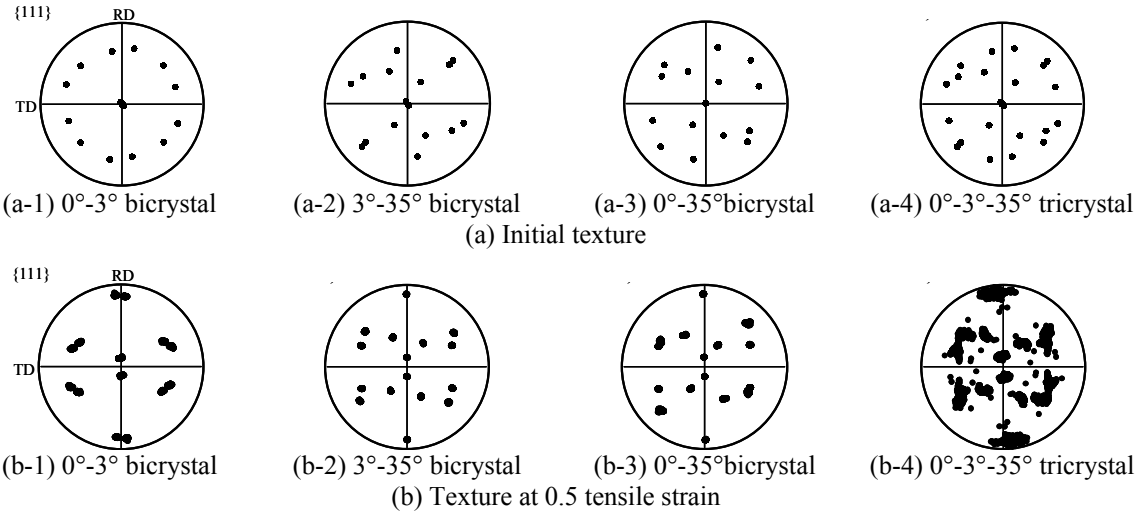

Figure 7: Texture evolution on {111} pole figures

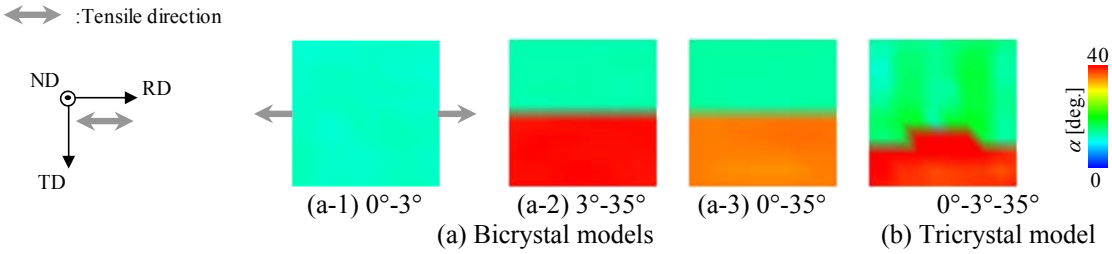

Figure 8: Distributions of Crystal orientation angle α evolutions at 0.5 tensile strain

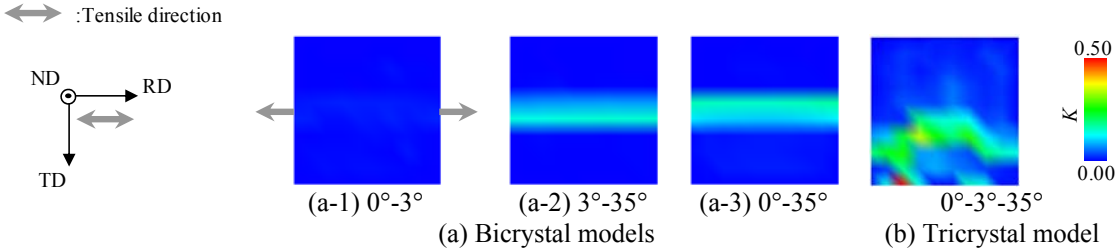

Figure 9: Distributions of equivalent misorientation evolutions at 0.5 tensile strain

4 CONCLUSIONS

We suggest the new hardening evolution equation based on crystallographic misorientation and carried out tensile analyses. Misorientation evolution and forming subgrain boundary were expressed. We conclude that consideration of misorientation is necessary for crystal plastic analysis.

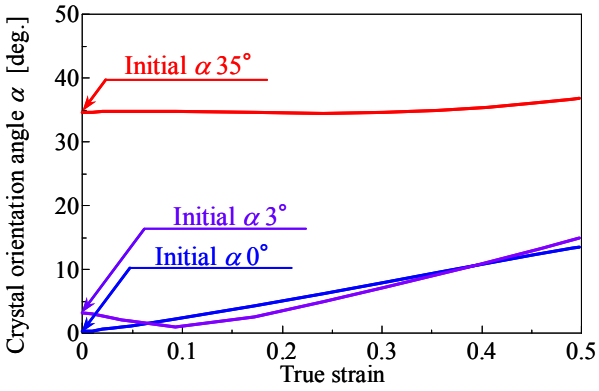

Figure 10: Crystal rotation histories of tricrystal model

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