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Determination of volume fraction of the texture components in the Rodrigues fundamental region

Jae-Hyung Cho *

Sangnam 66, Korea Institute of Machinery and Materials, Changwon, Kyungnam 641-010, South Korea

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Abstract

The fundamental region of Rodrigues space was discretized with finite elements as Euler space was discretized with 5° cell structures. Texture components were modeled with Gaussian distributions in the Rodrigues fundamental region. Spherical texture components are described by a sphere with a Gaussian distribution centered at its ideal position. Ideal fiber orientations are represented by a straight line or a skeleton line in Rodrigues space. The usual fiber textures are represented by a tube with a Gaussian distribution centered along a fiber line in Rodrigues space. The volume fractions of typical texture components can be collected by misorientation approach. The volume collections of spherical components of interest begin with the calculation of misorientation angles between the ideal components and their adjacent orientations. The radius of the orientation sphere is an angular distance. Adjacent components with smaller misorientation angles than a given criterion or a cut-off value locate inside the sphere and contribute to the volume fraction of the spherical component. For fibers, angular distances between the orientations along a skeleton line and adjacent orientations are compared with a cut-off. In addition, discretization effects of the Rodrigues fundamental region on the ODF and texture analysis were investigated. The volume fractions of texture components measured from a cold-rolled gold sheet and bonding wire were analyzed using the misorientation approach proposed.

Keywords: Rodrigues space; ODF; Spherical/fiber textures; Volume fraction

1. Introduction

Orientation distribution function (ODF, $f(g)$) is the probability density function of orientations in a polycrystalline material. Quantitative texture analysis is based on the calculation of ODF in orientation space. The ODF consists of normalized positive values and its summation over the entire orientation space is unity [1–3].

In order to describe an orientation, g, several mathematical parameters can be used. These include rotation matrices, Miller indices, Euler angles, angle-axis pair, Rodrigues vector and unit quaternions. All of these are used for a description of different aspects of macrotexture and microtexture analysis [4]. Misorientation can be used as a useful measure or relationship between two orientation components. Since Mackenzie [5] and Handcomb [6] calculated misorientation distributions in a randomly oriented cubic material, the distribution profiles of misorientation have been reported for crystallites with different symmetries [7–9]. Euler angle has been widely used to describe orientations in Euler space for quantitative texture analysis, although its disadvantages have also been recognized. The unique representation of an orientation in Euler space would only be possible in a subspace having curved boundaries. A degeneracy of the invariant volume element at second Euler angle, $\Phi = 0$ are also found. An alternative to the Euler space is a class of axis-angle parameterizations [10,11] or Rodrigues vector. The geometrical differences between Rodrigues and Euler spaces can be summarized as follows [12–14]:

- A multiplicity of an orientation results in several equivalent positions in Euler space when using a standard mapping, while an orientation appears only once in the Rodrigues fundamental region.
- A fiber component is represented by a curved line in Euler space, while, Rodrigues space has rectilinear geometry and fiber texture is a straight line in the Rodrigues space.
- Some boundaries of Euler space are curved surfaces, while boundaries of Rodrigues space are planes due to its rectilinear property.

* Tel.: +82 10 8222 3306; fax: +82 55 280 3599.
E-mail address: jhcho@kmail.kimm.re.kr.

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Recently, ODF based on finite element scheme in Rodrigues space was proposed [15–17]. The finite element representation of ODF space has some advantages resulting from usage of piecewise polynomial interpolating functions. Interpolating functions are given by simple forms and perform well even for a strong texture component due to their local support. The various texture transformations, such as differencing, interpolation and projection are also easily constructed for the ODFs in finite element scheme.

Texture components in real materials often have Gauss-shaped distributions when measured using a diffraction method. The Gauss-shaped distributions have a bell shape with a FWHM (full width at half maximum), b, and maximum ODF at the ideal position of g_0. When considering the volume fractions of texture components, it is useful to define a window around g_0 based on a difference in orientations measured by misorientation angles between g_0 and its surrounding components. All of the ODF, $f(g)$ within the acceptance angle or cut-off can be assumed to be a part of the ideal texture component, g_0. It has been found that the misorientation angle is a useful measure of distance from a texture component to others to calculate its volume fraction in Euler space [18].

Here, to help understand characteristics of Rodrigues space and orientation representation using it, various model texture components with the shape of spheres and fibers and experimental texture components were investigated in Rodrigues space. The volume fractions of texture components are calculated with misorientation angle approach. The basic idea for the misorientation angle approach is first to find misorientation angles between the ideal orientation component and its surrounding orientations and then to compare them with a cut-off. The orientation components with a smaller misorientation angle than the cut-off are considered to be part of the targeting orientation. Effects of mesh discretization on the ODF and volume fractions in Rodrigues space were also discussed using model texture components.

2. Orientations and Rodrigues space

The orientation of a crystal coordinate K_B in regard to sample K_A can be described by three successive rotations. It is given by a symbol, $g=\{\phi_1, \Phi, \phi_2\}$ or $g=\{\alpha, \beta, \gamma\}$ in Euler space, which is Bunge Euler angles or Roe Euler angles, respectively. Orientations in Euler angle space usually represent the transformation of K_A into K_B, and the orientation space, G is finite [1,3], $G{:}0 \leq \phi_1, \phi_2 < 2\pi;\ 0 \leq \Phi \leq \pi$:

$$g : [K_A \to K_B] \quad \text{or} \quad g^{-1} = g^T : [K_B \to K_A]. \tag{1}$$

The space element or volume element in Euler space is

$$dg = d\phi_1 \sin\Phi \, d\Phi \, d\phi_2. \tag{2}$$

The ODF, $f(g)$, in the orientation space is normalized to satisfy

$$V(g) = \frac{1}{8\pi^2}\int_G f(g)\,dg = 1. \tag{3}$$

Among various rotation representations, Rodrigues parameters can be constructed by scaling the axis of rotation as

$$\mathbf{r} = \mathbf{n}\tan\frac{\phi}{2}, \tag{4}$$

where $\mathbf{n}$ and ϕ are rotation axis and angle, respectively. They are providing a set of parameters that are symmetric relative to the sample axes. The Rodrigues parameter $\mathbf{r}$ and rotation matrix $\mathbf{R}$ is related [11], as follows:

$$\mathbf{R} = \frac{1}{1+\mathbf{r}\cdot\mathbf{r}}(\mathbf{I}(1-\mathbf{r}\cdot\mathbf{r}) + 2(\mathbf{r}\otimes\mathbf{r} + \mathbf{I}\times\mathbf{r})). \tag{5}$$

A multiplication rule for Rodrigues parameters is useful for Rodrigues operations and it is given

$$\mathbf{ab} = \frac{1}{1-\mathbf{a}\cdot\mathbf{b}}(\mathbf{a}+\mathbf{b}+\mathbf{a}\times\mathbf{b}), \tag{6}$$

where $\mathbf{ab}$ refers to the orientation that results when rotation $\mathbf{b}$ is followed by rotation $\mathbf{a}$. The volume element in Rodrigues space is given by

$$dv = \sqrt{\det g_{ij}}\,dr^1\,dr^2\,dr^3, \quad \text{where}$$
$$g_{ij} = \frac{1}{(1+r^k r^k)^2}\{(1+r^k r^k)\delta^{ij} - r^i r^j\}. \tag{7}$$

Here, g_{ij} is the metric over the Rodrigues space. The ODF, $f(g)$, in the Rodrigues fundamental region (RF) is normalized to satisfy

$$V_{RF}(\mathbf{R}) = \frac{24}{\pi^2}\int_{RF} f(\mathbf{R})\,dv = 1. \tag{8}$$

Using 24 cubic symmetric operations, Rodrigues space can be reduced into the fundamental region [7,19]. The fundamental region in Rodrigues space is expressed by

$$(2^{1/2}-1) \geq \pm r_i, \quad i = 1, 2, 3, \tag{9}$$

$$1 \geq \pm r_1 \pm r_2 \pm r_3. \tag{10}$$

The cubic-reduced unique Rodrigues vector of any cubic orientation exists within a cube in Rodrigues vector space. This cube is truncated at its corners by (1 1 1) type planes. The length of its edges is $(2^{1/2}-1)$. The maximum rotation angle is corresponding to the Rodrigues vector $(2^{1/2}-1,\ 2^{1/2}-1,\ 3-2\times 2^{1/2})$. The cubic fundamental region of Rodrigues space is shown in Fig. 1(a). The fundamental region can be discretized into cell structure using finite elements. Fig. 1(b)–(e) shows the different number of discretization meshes of the fundamental region. Table 1 shows the summary of the different discretization cases. Independent nodes are the unique positions in the fundamental

Table 1
Various discretization of the Rodrigues fundamental region

Discretization	Total nodes	Independent nodes	Dependent nodes	Total elements
Type 1	145	76	69	448
Type 2	849	600	249	3,584
Type 3	5,729	4,784	945	28,672
Type 4	41,921	38,240	3681	229,376