Representation of Nye's Lattice Curvature Tensor by Log Angles^{*1}

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The log angles of a rotation matrix are three independent elements of the logarithm of the rotation matrix. Nye's lattice curvature tensor κ_{ij} is discussed by using the log angles. For the change in a crystal orientation $\Delta\mathbf{R}$ with the change in a position Δx_i , it is shown that the elements of κ_{ij} are written as $\kappa_{ij} = \Delta\omega_i / \Delta x_j$ using the log angles $\Delta\omega_i$ of $\Delta\mathbf{R}$. The log angles for the crystal rotation given by the axis/angle pair are also discussed. [doi:10.2320/matertrans.M2019049]

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1. Introduction

To obtain an essential understanding of the strength of materials, it is necessary to know development and non-uniformity of plastic deformation in crystals, which are caused by motion and arrangement of dislocations. Since orientations of crystals change as a function of position when dislocation structures are formed in the crystals, efforts have been made to show dislocation structures after plastic deformation by considering such orientation changes. Pioneering work of the efforts is the theoretical study by Nye.¹⁾ Nye has shown that the dislocation density in a crystal can be quantitatively treated when orientation changes in the crystal are evaluated by using the lattice curvature tensor κ . Using the $x_1 - x_2 - x_3$ orthogonal coordinate system, this lattice curvature tensor κ describes the orientation change $\delta\phi_i$ around the x_i axis with the change in a position δx_j in the crystal as $\kappa_{ij} = \delta\phi_i / \delta x_j$.

As shown by Nye,¹⁾ the theoretical framework to discuss dislocation structures using orientation changes in crystal grains have been presented about half a century ago. On the other hand, experimental measurements of changes in crystal orientations for a wide area, with a high accuracy and in a short time have been performed recently only after a rapid development of SEM/EBSD (scanning electron microscopy/electron back scattering diffraction) method. However, the procedure to determine values of $\kappa_{ij} = \delta\phi_i / \delta x_j$ from data obtained by SEM/EBSD method has not been shown clearly in previous studies. When the orientation change in a crystal is given by the rotation angle $\Delta\Phi$ around the unit vector n_i , Pantleon²⁾ and He *et al.*³⁾ have shown that the product $\Delta\Phi n_i$ of n_i and $\Delta\Phi$ is also a vector and the components $\Delta\Phi n_i$ are the components of the rotation angle around the x_i axes. However, it should be noted that, in successive rotations around different axes such as the Euler angles, resultant rotations generally depend on the order of the rotations even if the rotation angle around each axis is the same.⁴⁾ This means that it is not obvious that the components of $\Delta\Phi n_i$ are

the components of rotation around the x_i axes, but the reason is not shown in their papers.^{2,3)} It is hence significant to show the reason if the components of $\Delta\Phi n_i$ can be treated as the components of the rotation angle around the x_i axes.

A crystal orientation can be described by using a rotation matrix $\mathbf{R}$ with respect to a reference coordinate system. The matrix $\mathbf{R}$ is a 3×3 orthogonal matrix whose determinant is 1. The logarithm $\ln \mathbf{R}$ of $\mathbf{R}$ is a 3×3 skew-symmetric matrix with three independent elements of real numbers.⁴⁻⁷⁾ The logarithm $\ln \mathbf{R}$ of $\mathbf{R}$ has been discussed in previous studies to discuss crystal orientations.^{4,6-10)} The three elements of $\ln \mathbf{R}$ are called the log angles ω_i by Hayashi *et al.*⁴⁾ and Onaka and Hayashi,^{9,10)} which are utilized as the characteristic angles of $\mathbf{R}$. They have discussed geometrical meanings of the log angles ω_i and applied these to the analysis of crystal rotations.^{4,9,10)}

When a crystal orientation changes as much as $\Delta\mathbf{R}$ with the change in a position Δx_i , the elements of the lattice curvature tensor κ are written as $\kappa_{ij} = \Delta\omega_i / \Delta x_j$ using the log angles $\Delta\omega_i$ of $\Delta\mathbf{R}$. We will show this in the present paper. This knowledge enables us to understand the procedure to determine the lattice curvature tensor κ from data of crystal orientations as those given by the SEM/EBSD method. Measurements of the lattice curvature tensor κ for plastically deformed metals and evaluation of densities or structures of dislocations from an experimental point of view will be shown in our future work based on the present study.

2. Log Angles

2.1 Logarithmic function

Here we explain characteristics of the logarithmic function before summarizing the log angles. For a real number x , the relationship between x and the exponential function $\exp x$ is well-known as¹¹⁾

$$\exp x = 1 + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \dots = \lim_{p \rightarrow \infty} \left(1 + \frac{x}{p}\right)^p. \quad (1)$$

Using $y = \exp x$ ($y > 0$), this relationship is rewritten by the logarithmic function as

$$y = \lim_{p \rightarrow \infty} \left(1 + \frac{\ln y}{p}\right)^p. \quad (2)$$

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Fig. 1 Schematic illustration showing one-dimensional deformation of a bar. The lengths L_0 and $L = L_0 + \Delta L$ are those before and after the deformation.

When N is a sufficiently large positive integer, we have

$$y \approx \left(1 + \frac{\ln y}{N}\right)^N. \quad (3)$$

This equation gives us better understanding on variables describing various changes.

Figure 1 shows the schematic illustration of deformation of a rod-like material along the longitudinal direction. The upper figure shows the state before deformation with the initial length L_0 and the state after uniform deformation with the length $L = L_0 + \Delta L$ is shown in the lower one. The nominal strain e is defined as $e = \Delta L/L_0$ and the definition of the stretch λ showing the length ratio before and after deformation is

$$\lambda = L/L_0 = (L_0 + \Delta L)/L_0. \quad (4)$$

This λ of $\lambda > 0$ is written as $\lambda = 1 + e$.

From (3), we have

$$\lambda \approx \left(1 + \frac{\ln \lambda}{N}\right)^N \quad (5a)$$

and this equation is rewritten from (4) as

$$L \approx L_0 \left(1 + \frac{\ln \lambda}{N}\right)^N. \quad (5b)$$

Since the logarithmic strain ε is

$$\varepsilon = \ln(1 + e) = \ln \lambda, \quad (6)$$

using a sufficiently large integer N , from (6) and (5b), the relationship among L_0 , L and ε is given by

$$L \approx L_0 \left(1 + \frac{\varepsilon}{N}\right)^N. \quad (7)$$

This eq. (7) shows a characteristic of the logarithmic strain ε as an appropriate measure to describe large deformation. Even for large deformation where $|\varepsilon| \ll 1$ is not satisfied, if we divide the large deformation into small deformation of N -times, we can reasonably treat the large deformation as an extension of the concept of infinitesimal deformation. That is to say, $\varepsilon = (\varepsilon/N) \times N$ and this ε is understood as the sum of N -times repeated small strain ε/N . This is an interpretation of the logarithmic strain ε given by (7). A similar interpretation can be put on (5a): the stretch λ is the quantity describing the deformation as it occurred, but its logarithm $\ln \lambda$ is a measure to show the extent of the deformation.

2.2 Outline of log angles

The relationship between the 3×3 orthogonal matrix $\mathbf{R}$ and its logarithm $\ln \mathbf{R}$ is written as¹²⁾

$$\mathbf{R} = \lim_{p \rightarrow \infty} \left(\mathbf{E} + \frac{\ln \mathbf{R}}{p} \right)^p, \quad (8)$$

where $\mathbf{E}$ is the 3×3 unit matrix. This is given from (2) by expanding the concept of numbers to matrices. The logarithm $\ln \mathbf{R}$ is the skew-symmetric matrix with elements of real numbers.^{5-7,12)} The log angles ω_i of $\mathbf{R}$ are the elements of $\ln \mathbf{R}$ and are written as^{4,9,10)}

$$\ln \mathbf{R} = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix}. \quad (9)$$

A calculation method to obtain $\ln \mathbf{R}$ from $\mathbf{R}$ will be shown later in this paper.

As well as the discussion made in 2.1, using a sufficiently large positive integer N , from (8) we have

$$\mathbf{R} \approx \left(\mathbf{E} + \frac{\ln \mathbf{R}}{N} \right)^N. \quad (10)$$

This equation can be rewritten from (9) as

$$\mathbf{R} \approx (\delta \mathbf{R})^N, \quad (11a)$$

where

$$\delta \mathbf{R} = \mathbf{E} + \left(\frac{\ln \mathbf{R}}{N} \right) = \begin{pmatrix} 1 & -(\omega_3/N) & (\omega_2/N) \\ (\omega_3/N) & 1 & -(\omega_1/N) \\ -(\omega_2/N) & (\omega_1/N) & 1 \end{pmatrix}. \quad (11b)$$

From (11a) and (11b), the meanings of the log angles ω_i are understood as well as the case of the logarithmic strain ε . The third side of (11b) shows that $\delta \mathbf{R}$ is a small-angle rotation matrix since $|\omega_i/N| \ll 1$ is satisfied for the sufficiently large N .⁴⁾ This $\delta \mathbf{R}$ is interpreted as the result of three successive rotations composed of the angle ω_1/N around the x_1 axis, the angle ω_2/N around the x_2 axis and the angle ω_3/N around the x_3 axis.⁴⁾ Since the rotation angles around the axes are small, any orders of the successive rotations give the same result given by the third side of (11b) by neglecting the second and higher terms of the elements.⁴⁾ This shows that the log angles ω_i are treated as the characteristic angles and the components of $\mathbf{R}$ in the sense that the angles ω_i are the sum of the divided rotation angles around the x_i axes.⁴⁾

3. Change of Orientation with Change of Position in Crystal

As shown in Fig. 2, we assume that a crystal orientation changes as much as $\Delta \mathbf{R}$ with the change of a position from x_i to $x_i + \Delta x_i$. Moreover we assume that the change $\Delta \mathbf{R}$ is written as $\Delta \mathbf{R} \approx (\delta \mathbf{R})^N$ and $\Delta \mathbf{R}$ is given by the N -time successive rotations of $\delta \mathbf{R}$. This treatment means that the change of orientation between the positions x_i and $x_i + \Delta x_i$ is assumed to be uniform and $\delta \mathbf{R}$ corresponds to the orientation change with the position change as much as $\delta x_i = \Delta x_i/N$ between x_i and $x_i + \Delta x_i$.

When the small-angle rotation $\delta \mathbf{R}$ is composed of the rotation angles $\delta \phi_i$ around the x_i axes as shown in Fig. 2,

Fig. 2 The change in a crystal orientation as much as $\Delta \mathbf{R}$ with the change in a position from (x_1, x_2, x_3) to $(x_1 + \Delta x_1, x_2 + \Delta x_2, x_3 + \Delta x_3)$. $\delta \mathbf{R}$ is a small-angle rotation which satisfies $\Delta \mathbf{R} \approx (\delta \mathbf{R})^N$ where N is a sufficiently large positive integer. The relationship $\Delta \mathbf{R} \approx (\delta \mathbf{R})^N$ means that the N -times successive rotations of $\delta \mathbf{R}$ with an interval of $\delta \mathbf{x} = (\Delta x_1/N, \Delta x_2/N, \Delta x_3/N)$ is equivalent to $\Delta \mathbf{R}$. The angles $\delta \phi_i$ are the small rotation angles of $\delta \mathbf{R}$ around the x_i axes.

using the log angles $\Delta \omega_i$ of $\Delta \mathbf{R}$, from (9) and (11b) we have

$$\delta \phi_i = \Delta \omega_i / N. \quad (12)$$

Hence the relationship between the changes $\delta \phi_i$ and δx_i is given by

$$\delta \phi_i / \delta x_j = \Delta \omega_i / \Delta x_j. \quad (13)$$

This relationship means that using $\Delta \omega_i$ of $\Delta \mathbf{R}$ with the position change from x_i to $x_i + \Delta x_i$, the average lattice curvature tensor κ for the region is given by

$$\kappa_{ij} = \Delta \omega_i / \Delta x_j, \quad (14a)$$

which is rewritten as

$$\kappa = \begin{pmatrix} \Delta \omega_1 / \Delta x_1 & \Delta \omega_1 / \Delta x_2 & \Delta \omega_1 / \Delta x_3 \\ \Delta \omega_2 / \Delta x_1 & \Delta \omega_2 / \Delta x_2 & \Delta \omega_2 / \Delta x_3 \\ \Delta \omega_3 / \Delta x_1 & \Delta \omega_3 / \Delta x_2 & \Delta \omega_3 / \Delta x_3 \end{pmatrix}. \quad (14b)$$

4. Log Angles for Rotation Matrix Given by the Axis/Angle Pair

The matrix $\mathbf{R}$ for the rotation given by the rotation angle Φ ($0 \leq \Phi \leq \pi$) around the unit vector n_i is written as^{9,13)}

$$\mathbf{R} = \begin{pmatrix} (1 - n_1^2) \cos \Phi + n_1^2 & n_1 n_2 (1 - \cos \Phi) - n_3 \sin \Phi & n_3 n_1 (1 - \cos \Phi) + n_2 \sin \Phi \\ n_1 n_2 (1 - \cos \Phi) + n_3 \sin \Phi & (1 - n_2^2) \cos \Phi + n_2^2 & n_2 n_3 (1 - \cos \Phi) - n_1 \sin \Phi \\ n_3 n_1 (1 - \cos \Phi) - n_2 \sin \Phi & n_2 n_3 (1 - \cos \Phi) + n_1 \sin \Phi & (1 - n_3^2) \cos \Phi + n_3^2 \end{pmatrix}. \quad (15)$$

This is the representation of $\mathbf{R}$ by using the axis/angle pair, n_i and Φ . When the rotation angle is small and satisfies $|\delta \Phi| \ll 1$, we have

$$\sin \delta \Phi \approx \delta \Phi \text{ and } \cos \delta \Phi \approx 1.$$

Using these approximations, the rotation matrix $\delta \mathbf{R}$ of $\delta \Phi$ around n_i is written as

$$\delta \mathbf{R} \approx \begin{pmatrix} 1 & -\delta \Phi n_3 & \delta \Phi n_2 \\ \delta \Phi n_3 & 1 & -\delta \Phi n_1 \\ -\delta \Phi n_2 & \delta \Phi n_1 & 1 \end{pmatrix}. \quad (16)$$

When the relationship between Φ and $\delta \Phi$ is given by

$$\delta \Phi = \Phi / N, \quad (17)$$

$\mathbf{R}$ of Φ around n_i is the same with the N -times successive

rotations of $\delta \mathbf{R}$. Then, using the relationship $\mathbf{R} \approx (\delta \mathbf{R})^N$ and (9), (11b) and (16), we have the logarithm $\ln \mathbf{R}$ of $\mathbf{R}$ given by (15) is written as^{5,6)}

$$\ln \mathbf{R} = \begin{pmatrix} 0 & -\Phi n_3 & \Phi n_2 \\ \Phi n_3 & 0 & -\Phi n_1 \\ -\Phi n_2 & \Phi n_1 & 0 \end{pmatrix}. \quad (18)$$

This shows that the log angles ω_i of $\mathbf{R}$ are

$$\omega_i = \Phi n_i. \quad (19)$$

Equation (18) is satisfied even if the rotation angle Φ of $\mathbf{R}$ is not small.

The above discussion shows that the log angles ω_i of $\mathbf{R}$ with Φ around n_i are given by Φn_i . Hence, as shown in the papers by Pantleon²⁾ and He *et al.*,³⁾ when the rotation angle is $\Delta \Phi$, the product $\Delta \Phi n_i$ can be treated as the components of the rotation angles around the x_i axes in the sense that these are the sum of the divided rotation angles around the axes.

From (15) and (18), the relationship between the rotation matrix $\mathbf{R}$ and its logarithm $\ln \mathbf{R}$ is given by

$$\ln \mathbf{R} = \frac{\Phi}{2 \sin \Phi} (\mathbf{R} - {}^t \mathbf{R}), \quad (20)$$

where ${}^t \mathbf{R}$ is the transposed matrix of $\mathbf{R}$. The proof of (2) is shown in Ref. 14). The angle Φ is given by the trace $\text{Tr } \mathbf{R}$ of $\mathbf{R}$ as¹³⁾

$$\cos \Phi = (\text{Tr } \mathbf{R} - 1)/2. \quad (21)$$

The logarithm of matrix is generally obtained by the procedure starting from the diagonalization of the matrix. Recent computation programs such as *Mathematica* have a command to calculate the logarithm of matrix. However, for the logarithm $\ln \mathbf{R}$ of the rotation matrix $\mathbf{R}$, (20) and (21) are convenient to calculate the values of $\ln \mathbf{R}$.

5. Conclusions

The log angles ω_i of a rotation matrix $\mathbf{R}$ are three elements of the logarithm $\ln \mathbf{R}$ of $\mathbf{R}$. Using the log angles ω_i , we have discussed the operation to obtain the lattice curvature tensor κ from position-dependent changes of crystal orientations in a grain. When the crystal orientation changes as much as $\Delta \mathbf{R}$ with the change in the position Δx_i , using the log angles $\Delta \omega_i$

of $\Delta \mathbf{R}$, the elements of the lattice curvature tensor changes κ are given by $\kappa_{ij} = \Delta \omega_i / \Delta x_j$. When crystal-orientation change is given by the rotation angle $\Delta \Phi$ around the unit vector n_i , the log angles $\Delta \omega_i$ of this orientation change satisfy $\Delta \omega_i = \Delta \Phi n_i$. Both of $\Delta \omega_i$ and $\Delta \Phi n_i$ are considered to be the components of the rotation angle around the x_i axes.

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