Representation of Nye’s Lattice Curvature Tensor by Log Angles*1

Ryosuke Matsutan*2 and Susumu Onaka*3

Department of Materials Science and Engineering, School of Materials and Chemical Technology, Tokyo Institute of Technology, Yokohama 226-8502, Japan

The log angles of a rotation matrix are three independent elements of the logarithm of the rotation matrix. Nye’s lattice curvature tensor \( \kappa \) is discussed by using the log angles. For the change in a crystal orientation \( \Delta \mathbf{R} \) with the change in a position \( \Delta \mathbf{x} \), it is shown that the elements of \( \kappa \) are written as \( \kappa_{ij} = \Delta \omega_{ij}/\Delta x \) using the log angles \( \Delta \omega_{ij} \) 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]

(Received February 22, 2019; Accepted March 22, 2019; Published April 19, 2019)

Keywords: crystal orientation, rotation matrix, log angles, axis/angle pair, logarithm of matrix, lattice curvature tensor, electron backscatter diffraction

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 \( \kappa \). Using the \( x_1 - x_2 - x_3 \) orthogonal coordinate system, this lattice curvature tensor \( \kappa \) describes the orientation change \( \Delta \mathbf{x} \) in the crystal as \( \kappa_{ij} = \delta \omega_{ij}/\Delta x \), 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 \( \Delta \omega_{ij} \) 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 \( 3 \times 3 \) orthogonal matrix whose determinant is 1. The logarithm \( \ln \mathbf{R} \) of \( \mathbf{R} \) is a \( 3 \times 3 \) 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.4,6,8) The three elements of \( \ln \mathbf{R} \) called the log angles \( \omega_{ij} \) by Hayashi et al.9) and Onaka and Hayashi9,10) which are utilized as the characteristic angles of \( \mathbf{R} \). They have discussed geometrical meanings of the log angles \( \omega_{ij} \) and applied these to the analysis of crystal rotations.3,9,10)

When a crystal orientation changes as much as \( \Delta \mathbf{R} \) with the change in a position \( \Delta \mathbf{x} \), the elements of the lattice curvature tensor \( \kappa \) are written as \( \kappa_{ij} = \Delta \omega_{ij}/\Delta x \), the log angles \( \Delta \omega_{ij} \) 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 \( \kappa \) from data of crystal orientations as those given by the SEM/EBSD method. Measurements of the lattice curvature tensor \( \kappa \) 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 as \(^{1}\)

\[
\exp x = 1 + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \ldots = \lim_{p \to \infty} \left( 1 + \frac{x}{p} \right)^p .
\]  

Using \( y = \exp x \) (\( y > 0 \)), this relationship is rewritten by the logarithmic function as \(^2\)

\[
y = \lim_{p \to \infty} \left( 1 + \frac{\ln y}{p} \right)^p .
\]
When \( N \) is a sufficiently large positive integer, we have
\[
y \approx \left(1 + \frac{\ln y}{N}\right)^N.
\] (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 \( \lambda \) showing the length ratio before and after deformation is
\[
\lambda = L/L_0 = (L_0 + \Delta L)/L_0. \quad \text{(4)}
\]
This \( \lambda > 0 \) is written as \( \lambda = 1 + e \).

From (3), we have
\[
\lambda \approx \left(1 + \frac{\ln \lambda}{N}\right)^N \quad \text{(5a)}
\]
and this equation is rewritten from (4) as
\[
L \approx L_0 \left(1 + \frac{\ln \lambda}{N}\right)^N. \quad \text{(5b)}
\]
Since the logarithmic strain \( \varepsilon \) is
\[
\varepsilon = \ln(1 + e) = \ln \lambda,
\]
using a sufficiently large integer \( N \), from (6) and (5b), the relationship among \( L_0, L \) and \( \varepsilon \) is given by
\[
L \approx L_0 \left(1 + \frac{\varepsilon}{N}\right)^N. \quad \text{(7)}
\]
This eq. (7) shows a characteristic of the logarithmic strain \( \varepsilon \) 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 \( \varepsilon \) is understood as the sum of \( N \)-times repeated small strain \( \varepsilon/N \). This is an interpretation of the logarithmic strain \( \varepsilon \) given by (7). A similar interpretation can be put on (5a): the stretch \( \lambda \) 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 \( 3 \times 3 \) orthogonal matrix \( R \) and its logarithm \( \ln R \) is written as\(^{12}\)
\[
R = \lim_{p \to \infty} \left(E + \frac{\ln R}{p}\right)^p,
\]
where \( E \) is the \( 3 \times 3 \) unit matrix. This is given from (2) by expanding the concept of numbers to matrices. The logarithm \( \ln R \) is the skew-symmetric matrix with elements of real numbers.\(^5-7,12\) The log angles \( \alpha_i \) of \( R \) are the elements of \( \ln R \) and are written as\(^{4,9,10}\)
\[
\ln R = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix}.
\]
(9)
A calculation method to obtain \( \ln R \) from \( R \) 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
\[
R \approx \left(E + \frac{\ln R}{N}\right)^N. \quad \text{(10)}
\]
This equation can be rewritten from (9) as
\[
R \approx (\delta R)^N, \quad \text{(11a)}
\]
where
\[
\delta R = E + \left(\frac{\ln R}{N}\right) = \begin{pmatrix} 1 & -(\omega_3/N) & (\omega_2/N) \\ (\omega_3/N) & 1 & -(\omega_1/N) \\ -(\omega_2/N) & (\omega_1/N) & 1 \end{pmatrix}.
\]
(11b)
From (11a) and (11b), the meanings of the log angles \( \alpha_i \) are understood as well as the case of the logarithmic strain \( \varepsilon \). The third side of (11b) shows that \( \delta R \) is a small-angle rotation matrix since \( |\alpha_i/N| \ll 1 \) is satisfied for sufficiently large \( N \).\(^4\) This \( \delta R \) is interpreted as the result of three successive rotations of the angle \( \alpha_i/N \) around the \( x_i \) axis, the angle \( \omega_2/N \) around the \( x_2 \) axis and the angle \( \omega_3/N \) 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 \( \alpha_i \) are treated as the characteristic angles and the components of \( R \) in the sense that the angles \( \alpha_i \) 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 \( \Delta R \) with the change of a position from \( x_i \) to \( x_i + \Delta x_i \). Moreover, we assume that the change \( \Delta R \) is written as \( \Delta R = \delta R \) and \( \Delta R \) is given by the \( N \)-time successive rotations of \( \delta R \). 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 \( \delta R \) 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 \( \delta R \) is composed of the rotation angles \( \delta \phi_i \) around the \( x_i \) axes as shown in Fig. 2,
using the log angles \( \Delta \omega_j \) of \( \Delta R \), from (9) and (11b) we have

\[
\delta \Phi_i = \Delta \omega_i / N.
\]

Hence the relationship between the changes \( \delta \Phi_i \) and \( \delta x_i \) is given by

\[
\delta \Phi_i / \delta x_j = \Delta \omega_i / \Delta x_j.
\]

This relationship means that using \( \Delta \omega_i \) of \( \Delta R \) with the position change from \( x_i \) to \( x_i + \Delta x_i \), the average lattice curvature tensor \( \kappa \) for the region is given by

\[
\kappa_{ij} = \Delta \omega_i / \Delta x_j, \tag{14a}
\]

which is rewritten as

\[
\kappa = \left( \begin{array}{ccc}
\Delta \omega_1 / \Delta x_1 & \Delta \omega_1 / \Delta x_2 & \Delta \omega_1 / \Delta x_3 \\
\Delta \omega_2 / \Delta x_1 & \Delta \omega_2 / \Delta x_2 & \Delta \omega_2 / \Delta x_3 \\
\Delta \omega_3 / \Delta x_1 & \Delta \omega_3 / \Delta x_2 & \Delta \omega_3 / \Delta x_3
\end{array} \right). \tag{14b}
\]

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

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

\[
R = \left( \begin{array}{ccc}
(1 - n_i^2) \cos \Phi + n_i^2 & n_i n_j (1 - \cos \Phi) - n_k \sin \Phi & n_i n_k (1 - \cos \Phi) + n_j \sin \Phi \\
(1 - n_i^2) \cos \Phi + n_i^2 & (1 - n_j^2) \cos \Phi + n_k^2 & n_j n_k (1 - \cos \Phi) - n_i \sin \Phi \\
n_j n_i (1 - \cos \Phi) + n_k \sin \Phi & n_j n_k (1 - \cos \Phi) - n_i \sin \Phi & (1 - n_i^2) \cos \Phi + n_j^2
\end{array} \right). \tag{15}
\]

This is the representation of \( R \) by using the axis/angle pair, \( n_i \) and \( \Phi \). 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 \( \delta R \) of \( \delta \Phi \) around \( n_i \) is written as

\[
\delta R \approx \left( \begin{array}{ccc}
1 & -\delta \Phi n_3 & \delta \Phi n_2 \\
\delta \Phi n_3 & 1 & -\delta \Phi n_1 \\
-\delta \Phi n_2 & \delta \Phi n_1 & 1
\end{array} \right). \tag{16}
\]

When the relationship between \( \Phi \) and \( \delta \Phi \) is given by

\[
\delta \Phi = \Phi / N, \tag{17}
\]

\( R \) of \( \Phi \) around \( n_i \) is the same with the \( N \)-times successive rotations of \( \delta R \). Then, using the relationship \( R \approx (\delta R)^N \) and (9), (11b) and (16), we have the logarithm \( \ln R \) of \( R \) given by \((15)\) is written as\(^{7,6}\)

\[
\ln R = \left( \begin{array}{ccc}
0 & -\Phi n_3 & \Phi n_2 \\
\Phi n_3 & 0 & -\Phi n_1 \\
-\Phi n_2 & \Phi n_1 & 0
\end{array} \right). \tag{18}
\]

This shows that the log angles \( \omega_i \) of \( R \) are

\[
\omega_i = \Phi n_i. \tag{19}
\]

Equation (18) is satisfied even if the rotation angle \( \Phi \) of \( R \) is not small.

The above discussion shows that the log angles \( \omega_i \) of \( R \) with \( \Phi \) around \( n_i \) are given by \( \Phi n_i \). Hence, as shown in the papers by Pantleon\(^2\) and He et al.,\(^{7,8}\) 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 \( R \) and its logarithm \( \ln R \) is given by

\[
\ln R = \frac{\Phi}{2 \sin \Phi} (R - (R)^T), \tag{20}
\]

where \( (R)^T \) is the transposed matrix of \( R \). The proof of (2) is shown in Ref. 14). The angle \( \Phi \) is given by the trace \( \text{Tr} R \) of \( R \) as\(^{13}\)

\[
\cos \Phi = (\text{Tr} R - 1)/2. \tag{21}
\]

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

5. Conclusions

The log angles \( \omega_i \) of a rotation matrix \( R \) are three elements of the logarithm \( \ln R \) of \( R \). Using the log angles \( \omega_i \), we have discussed the operation to obtain the lattice curvature tensor \( \kappa \) from position-dependent changes of crystal orientations in a grain. When the crystal orientation changes as much as \( \Delta R \) with the change in the position \( \Delta x_i \), using the log angles \( \Delta \omega_i \)
of $\Delta R$, the elements of the lattice curvature tensor changes $\kappa$ are given by $\kappa_{ij} = \Delta \alpha_i / \Delta x_j$. When crystal-orientation change is given by the rotation angle $\Delta \Phi$ around the unit vector $n_i$, the log angles $\Delta \lambda_i$ of this orientation change satisfy $\Delta \alpha_i = \Delta \Phi n_i$. Both of $\Delta \alpha_i$ and $\Delta \Phi n_i$ are considered to be the components of the rotation angle around the $x_i$ axes.

Acknowledgment

Funding from the JSPS KAKENHI (Grant Number JP16K06703) is gratefully acknowledged.

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