J Math Chem (2016) 54:1686–1695
DOI 10.1007/s10910-016-0644-5

ORIGINAL PAPER

# Interpretation of elements of the logarithm of a rotation matrix as rotation components around coordinate axes of a reference frame

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Received: 21 February 2016 / Accepted: 11 May 2016 / Published online: 23 May 2016


**Abstract** Crystal orientation is an important factor when we consider microstructures in materials. With respect to a reference frame, certain crystal orientation can be expressed by a rotation angle $\Phi$ around a unit vector $\mathbf{n} = (h,\ k,\ l)$. Partitioning of $\Phi$ into rotation components around coordinate axes of the reference frame is discussed. For a rotation matrix $\mathbf{R}$ corresponding to the axis/angle pair, its logarithm $\ln \mathbf{R}$ is a skew symmetric tensor with three independent elements, $h\Phi$, $k\Phi$ and $l\Phi$. It is shown that these elements can be interpreted to be sums of the divided rotation angles around the coordinate axes. The elements $h\Phi$, $k\Phi$ and $l\Phi$ of $\ln \mathbf{R}$ called the log angles can be used as the rotation components to evaluate crystal orientation in materials.

**Keywords** Crystal orientation · Rotation angle · Rotation matrix · Logarithm of matrix · Microstructure · Dislocation

## 1 Introduction

Crystal orientation and how it varies is important when describing microstructures of materials [1–6]. When assessing structures that can vary their crystal orientation (dislocations, for example), it is often necessary to partition a rotation angle of the crystal orientation into components [7–9]. However, an established method for partitioning has not been shown in previous microstructural analyses. In this work, we discuss the partitioning of the rotation angle and show that the components around the coordinate axes are given by the elements of the logarithm of a rotation matrix. We also show examples of applications of the rotation components.

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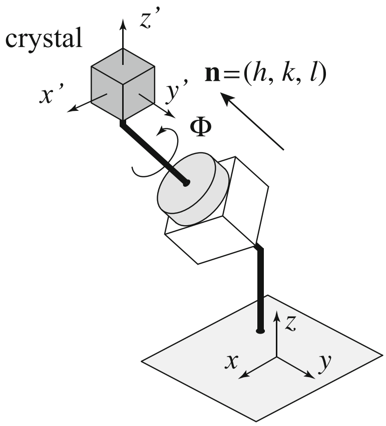


**Fig. 1** A model showing the rotation of a crystal with respect to the $x-y-z$ reference frame given by the axis/angle pair ($\mathbf{n}$, $\Phi$)

# 2 Analysis

## 2.1 The axis/angle pair

With respect to the $x-y-z$ reference frame, certain crystal orientation can be expressed by a rotation angle $\Phi$ around a unit vector $\mathbf{n} = (h, k, l)$ [10]. The set of $\mathbf{n}$ and $\Phi$ is the well-known axis/angle pair. Figure 1 shows a model demonstrating the crystal rotation given by the axis/angle pair. A crystal with the $x'$, $y'$ and $z'$ coordinate axes is located on the top of the model and the axis/angle pair determines the primed axes with respect to the reference frame. The primed and the unprimed axes are parallel when $\Phi$ is null.

The crystal orientation can also be expressed by a rotation matrix $\mathbf{R}$. Matrix notation of Rodrigues' formula gives the elements of $\mathbf{R}$ corresponding to the axis/angle pair ($\mathbf{n}$, $\Phi$) [10,11]:

$$\mathbf{R} = \begin{pmatrix} (1-h^2)\cos\Phi + h^2 & hk(1-\cos\Phi) - l\sin\Phi & lh(1-\cos\Phi) + k\sin\Phi \\ hk(1-\cos\Phi) + l\sin\Phi & (1-k^2)\cos\Phi + k^2 & kl(1-\cos\Phi) - h\sin\Phi \\ lh(1-\cos\Phi) - k\sin\Phi & kl(1-\cos\Phi) + h\sin\Phi & (1-l^2)\cos\Phi + l^2 \end{pmatrix}. \tag{1}$$

## 2.2 The Euler angles

Any $\mathbf{R}$ can be written as a product of appropriate successive rotations around coordinate axes. Here we consider the rotation matrices $\mathbf{R}_x$, $\mathbf{R}_y$, and $\mathbf{R}_z$ which are those around the coordinate axes $x$, $y$ and $z$ as much as $\theta$, $\phi$ and $\psi$, respectively. When $\mathbf{R}$ is a product of $\mathbf{R}_x$, $\mathbf{R}_y$ and $\mathbf{R}_z$ in the order given by

$$\mathbf{R} = \mathbf{R}_x(\theta)\,\mathbf{R}_y(\phi)\,\mathbf{R}_z(\psi), \tag{2}$$

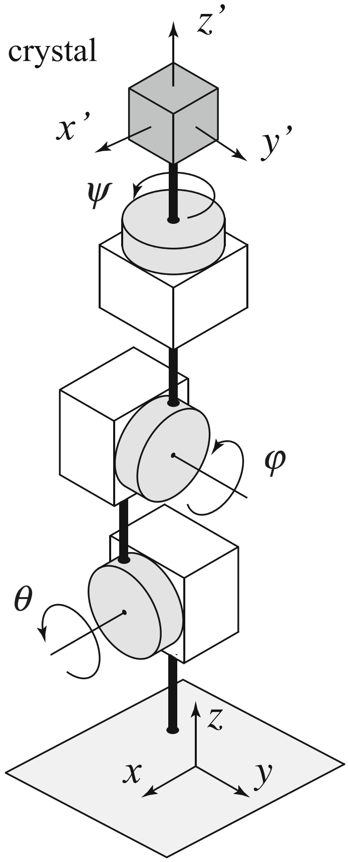


**Fig. 2** A goniometer-stage model showing the rotation of a crystal with respect to the $x-y-z$ reference given by (2) with the rotation angles $\theta$, $\phi$ and $\psi$

we have Fig. 2 as a graphical or mechanical representation of **R** [12]. The model in Fig. 2 consists of three rotation parts showing $\mathbf{R}_x$, $\mathbf{R}_y$, and $\mathbf{R}_z$ connected in series. Note the correspondence between the right-hand-side of (2) and the order of the rotation parts in Fig. 2. Similar models have been considered by Onaka et al. [13] as a goniometer-stage model, which is convenient to understand the combination of rotations [12]. Equation (2) and the model shown in Fig. 2 are a set of expressions for the same **R**. The matrix notation of **R** corresponding to the model shown in Fig. 1 is derived in "Appendix 1".

Equation (2) and Fig. 2 represent successive rotations around coordinate axes given by the concept of the Euler angles. However, the product of matrices is not commutative generally. Even if the angles $\theta$, $\phi$ and $\psi$ are fixed, the value of the product of $\mathbf{R}_x$, $\mathbf{R}_y$, and $\mathbf{R}_z$ depends on the order of the three rotations. In addition to that shown by (2) and Fig. 2, many kinds of the Euler angles exist, depending on the selection of the rotation axes and their order [14]. For example, the Bunge Euler angles, or the Euler angles due to Bunge, used for texture analysis, are those given by the successive rotations in the order of $\mathbf{R}_z$, $\mathbf{R}_x$ and $\mathbf{R}_z$. When we treat a set of the angles in the framework of the Euler angles, it is necessary to specify the rotation axes and their order.

### 2.3 Logarithm lnR of rotation matrix R

Exponential and logarithmic functions of matrices are necessary tools to consider rotations in the framework of the group theory [15–17]. The logarithm $\ln \mathbf{R}$ of the rotation matrix $\mathbf{R}$ is a skew symmetric tensor and $\ln \mathbf{R}$ of $\mathbf{R}$ given by (1) is written as [16]

$$\ln \mathbf{R} = \begin{pmatrix} 0 & -l\Phi & k\Phi \\ l\Phi & 0 & -h\Phi \\ -k\Phi & h\Phi & 0 \end{pmatrix}. \tag{3}$$

The relationship between $\mathbf{R}$ and $\ln \mathbf{R}$ is generally given by [17]

$$\mathbf{R} = \lim_{p\to\infty} \left( \mathbf{E} + \frac{\ln \mathbf{R}}{p} \right)^p, \tag{4}$$

where $\mathbf{E}$ is a unit matrix. From (3) and (4), we have

$$\mathbf{R} \approx (\delta \mathbf{R})^N \tag{5}$$

and

$$\delta \mathbf{R} = \mathbf{E} + \frac{\ln \mathbf{R}}{N} = \begin{pmatrix} 1 & -l\Phi/N & k\Phi/N \\ l\Phi/N & 1 & -h\Phi/N \\ -k\Phi/N & h\Phi/N & 1 \end{pmatrix}, \tag{6}$$

where $N$ is a sufficiently large positive integer. Equation (5) means that the $N$ ($\gg 1$) times successive operations of $\delta\mathbf{R}$ are equivalent to $\mathbf{R}$. Hence, we have Fig. 3 as a graphical representation of $\mathbf{R}$ given by (5), where spherical units corresponding to $\delta\mathbf{R}$ are stacked $N$ times.

The operation $\delta\mathbf{R}$ given by the third side of (6) can be represented by the three parts connected in series in the spherical unit in Fig. 3. This is because when the off-diagonal elements in the third side of (6) are small, we have

$$\begin{aligned} &\mathbf{R}_x(\delta\theta)\,\mathbf{R}_y(\delta\phi)\,\mathbf{R}_z(\delta\psi) \\ &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\delta\theta) & -\sin(\delta\theta) \\ 0 & \sin(\delta\theta) & \cos(\delta\theta) \end{pmatrix} \begin{pmatrix} \cos(\delta\phi) & 0 & \sin(\delta\phi) \\ 0 & 1 & 0 \\ -\sin(\delta\phi) & 0 & \cos(\delta\phi) \end{pmatrix} \\ &\quad \begin{pmatrix} \cos(\delta\psi) & -\sin(\delta\psi) & 0 \\ \sin(\delta\psi) & \cos(\delta\psi) & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ &\approx \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & -\delta\theta \\ 0 & \delta\theta & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & \delta\phi \\ 0 & 1 & 0 \\ -\delta\phi & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & -\delta\psi & 0 \\ \delta\psi & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ &\approx \begin{pmatrix} 1 & -\delta\psi & \delta\phi \\ \delta\psi & 1 & -\delta\theta \\ -\delta\phi & \delta\theta & 1 \end{pmatrix}. \end{aligned} \tag{7}$$

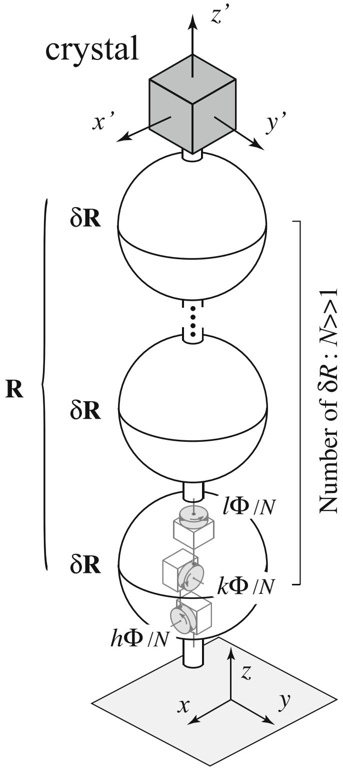


**Fig. 3** A goniometer-stage model showing the rotation of a crystal with respect to the $x-y-z$ reference given by (5) and (6) with the log angles $h\Phi$, $k\Phi$ and $l\Phi$

The third and fourth sides of (7) are the results obtained by neglecting higher-order terms of infinitesimal $\delta\theta$, $\delta\phi$ and $\delta\psi$. Equation (5) is satisfied even if the third side of (6) is replaced with the product of matrices given by the type of second or third side of (7). Moreover, the order of the three parts in the spherical units in Fig. 3 can be changed since we can consider the product $\mathbf{R}_x\ (\delta\theta)\ \mathbf{R}_y\ (\delta\phi)\ \mathbf{R}_z\ (\delta\psi)$ commutative for infinitesimal $\delta\theta$, $\delta\phi$ and $\delta\psi$.

From the model of $\mathbf{R}$ shown in Fig. 3, the elements $h\Phi$, $k\Phi$ and $l\Phi$ of $\ln \mathbf{R}$ are interpreted as the sums of the divided rotation angles around the coordinate axes. The elements $h\Phi$, $k\Phi$ and $l\Phi$ that can be called the log angles are determined uniquely for certain $\mathbf{R}$. Hence, we can treat the log angles $h\Phi$, $k\Phi$ and $l\Phi$ as the rotation components of $\Phi$ around the coordinate axes $x$, $y$ and $z$.

Using the elements $h\Phi$, $k\Phi$ and $l\Phi$, we can construct a vector $\mathbf{w}$ written as

$$\mathbf{w} = (h\Phi,\ k\Phi,\ l\Phi)\,. \tag{8}$$

Since $h$, $k$ and $l$ are the components of the unit vector $\mathbf{n}$, the norm $|\mathbf{w}|$ is equal to the angle $\Phi$. $\mathbf{R}$ and its logarithm $\ln \mathbf{R}$ can also be written as [16]

$$\mathbf{R} = \exp\left(\hat{\mathbf{w}}\right) \tag{9}$$

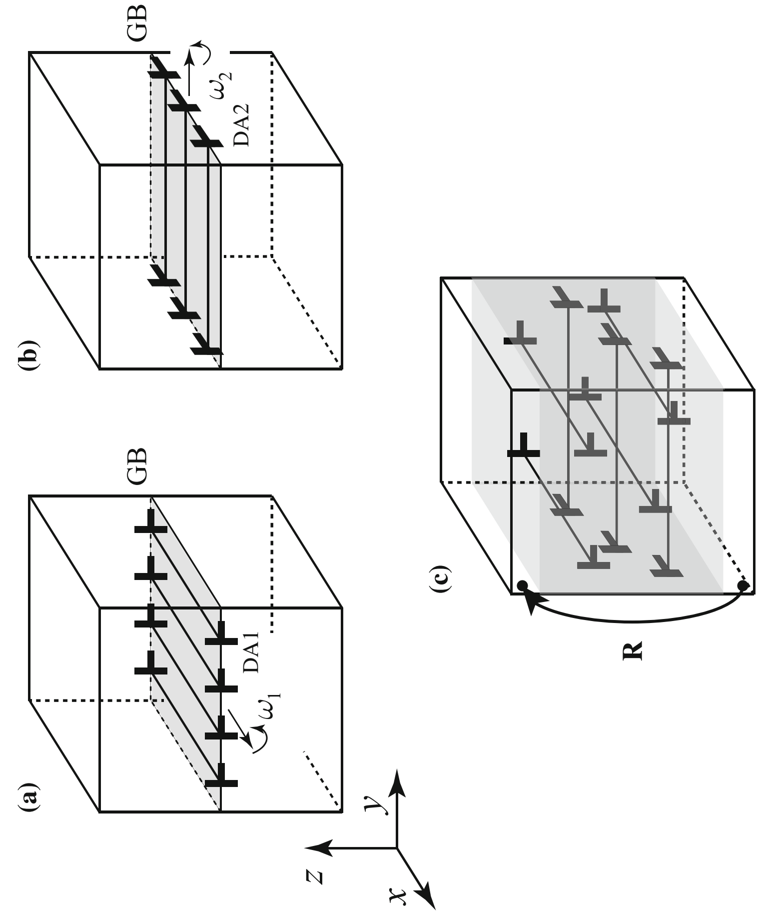


**Fig. 4** Schematic illustration showing materials containing grain boundaries composed of **a** the array of dislocations DA1 and **b** the array of dislocations DA2 that cause the rotations of the upper grain with respect to the lower grain as much as $\omega_1$ around the $x$-axis and $\omega_2$ around the $y$-axis, respectively. **c** A grain containing both of the dislocations of DA1 and DA2 dispersed in a local region. The rotation angles $\omega_1$ and $\omega_2$ are the log angles of the rotation matrix **R** giving the orientation change above and below the region shown in (**c**)

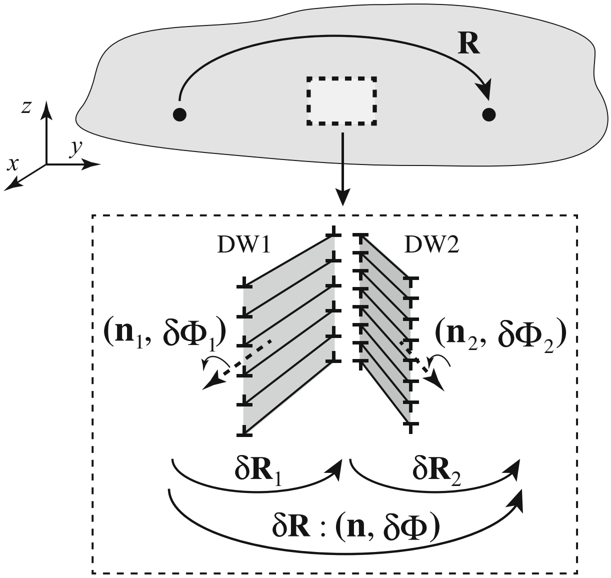


**Fig. 5** Schematic illustration showing the changes of crystal orientations in a grain caused by dislocation walls DW1 and DW2

and

$$\ln \mathbf{R} = \hat{\mathbf{w}}, \tag{10}$$

where $\hat{\mathbf{w}}$ is the skew symmetric tensor of the right-hand-side of (3) and called the hat map of $\mathbf{w}$ [16]. The vector $\mathbf{w}$ is different from Rodrigues' vector $\mathbf{v}$ [10,11,18]. The definition of Rodrigues' vector $\mathbf{v}$ and $\mathbf{R}$ expressed by $\mathbf{v}$ are shown in the "Appendix 2".

## 3 Examples of applications

### 3.1 Changes caused by dislocations in materials

Crystal orientation changes when defects such as dislocations are included in materials. Figure 4 show materials containing dislocations. There are grain boundaries composed of arrays of dislocations [19]. Figure 4a, b show materials having grain boundaries between two grains composed of the arrays of dislocations DA1 and DA2. As shown in these figures, here we assume that the effects of DA1 and DA2 are respectively the rotations of the upper grain with respect to the lower grain as much as $\omega_1$ around the $x$-axis and $\omega_2$ around the $y$-axis when they exist solely. When both of the dislocations of DA1 and DA2 are dispersed in a local region in a grain as shown in Fig. 4c, crystal orientation changes above and below the region. When $\mathbf{R}$ is the rotation matrix giving the orientation change above and below the region, we can consider that the rotation angles $\omega_1$ and $\omega_2$ are the log angles of $\mathbf{R}$. To discuss such rotations of crystal orientation caused by many defects in materials, the log angles considering the sums of the divided rotation angles may be significant. In other words, the log angles can be used as measures to discuss structures of defects in materials. Comparing other parameters to describe rotations such as the Euler angles or the axis/angle pair [20], this is a unique characteristic of the log angles.

### 3.2 Changes caused by dislocation walls in a grain

Dislocation walls in grains cause orientation changes across the walls [2,3]. Figure 5 shows two dislocation walls DW1 and DW2 and the orientation changes $\delta\mathbf{R}_1 : (\mathbf{n}_1,\ \delta\Phi_1)$ and $\delta\mathbf{R}_2 : (\mathbf{n}_2,\ \delta\Phi_2)$ across DW1 and DW2, respectively. When the rotation angles $\delta\Phi_1$ and $\delta\Phi_2$ are small, the product of $\delta\mathbf{R}_1$ and $\delta\mathbf{R}_2$ are commutative and we have

$$\delta\mathbf{R} \approx \delta\mathbf{R}_1\delta\mathbf{R}_2 \approx \delta\mathbf{R}_2\delta\mathbf{R}_1 \tag{11}$$

and

$$\ln\delta\mathbf{R} \approx \ln\delta\mathbf{R}_1 + \ln\delta\mathbf{R}_2. \tag{12}$$

Then, among the following $\mathbf{w}$ vectors giving the log angles for each crystal rotation:

$$\begin{aligned} \mathbf{w} &= \mathbf{n}\delta\Phi = \delta\Phi\,(h, k, l) \ \text{ for } \delta\mathbf{R}, \\ \mathbf{w}_1 &= \mathbf{n}_1\delta\Phi_1 = \delta\Phi_1\,(h_1, k_1, l_1) \ \text{ for } \delta\mathbf{R}_1, \\ \mathbf{w}_2 &= \mathbf{n}_2\delta\Phi_2 = \delta\Phi_2\,(h_2, k_2, l_2) \ \text{ for } \delta\mathbf{R}_2, \end{aligned} \tag{13}$$

we have the relationship

$$\mathbf{w} = \mathbf{w}_1 + \mathbf{w}_2. \tag{14}$$

These equations can be used to analyze crystal rotations caused by certain dislocation walls. For example, when we know crystallographic directions $\mathbf{n}_1$ and $\mathbf{n}_2$, we can evaluate the ratio of the contributions of DW1 and DW2 from $\mathbf{w}$.

## 4 Conclusions

With respect to a reference frame, certain crystal orientation can be expressed by a rotation angle $\Phi$ around a unit vector $\mathbf{n} = (h,\ k,\ l)$. We have discussed partitioning of $\Phi$ into rotation components around coordinate axes of the reference frame. For a rotation matrix $\mathbf{R}$ corresponding to the axis/angle pair, its logarithm $\ln\mathbf{R}$ is a skew symmetric tensor with three independent elements, $h\Phi$, $k\Phi$ and $l\Phi$. We have shown that these elements can be interpreted to be sums of the divided rotation angles around the coordinate axes. The elements $h\Phi$, $k\Phi$ and $l\Phi$ of $\ln\mathbf{R}$, called the log angles can be used as the rotation components to evaluate crystal orientation in materials.

**Acknowledgments** This work was supported by a Grand-in-Aid for Scientific Research C (16K06703) through the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan.

## Appendix 1

The rotation matrix **R** corresponding to the model shown in Fig. 1 is written by the successive rotations as

$$\mathbf{R} = \mathbf{M}\mathbf{R}_x(\Phi)\,{}^t\mathbf{M}, \tag{15}$$

where

$$\mathbf{R}_x(\Phi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\Phi & -\sin\Phi \\ 0 & \sin\Phi & \cos\Phi \end{pmatrix}, \tag{16}$$

**M** is the rotation matrix giving the transformation

$$\begin{pmatrix} h \\ k \\ l \end{pmatrix} = \mathbf{M}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \tag{17}$$

and ${}^t\mathbf{M}$ is the transpose of **M**. Since **M** is the orthogonal matrix with determinant 1, the elements of **R** given by (15) can be written as a function of $h, k, l$ and $\Phi$. Calculating the right-hand-side of (15) from (16) and (17), we find it is the same with the right-hand-side of (1).

## Appendix 2

The definition of Rodrigues' vector **v** for the axis/angle pair $\mathbf{n} = (h,\ k,\ l)\,/\Phi$ is [10,11,18]

$$\mathbf{v} = \tan(\Phi/2)\,\mathbf{n} = \tan(\Phi/2)\begin{pmatrix} h \\ k \\ l \end{pmatrix}.$$

Using Rodrigues' vector **v**, the rotation matrix **R** corresponding to this axis/angle pair is given by [11]

$$\mathbf{R} = \frac{1}{1 + {}^t\mathbf{v}\mathbf{v}}\left[\left(1 - {}^t\mathbf{v}\mathbf{v}\right)\mathbf{E} + 2\mathbf{v}\,{}^t\mathbf{v} + 2\hat{\mathbf{v}}\right],$$

where ${}^t\mathbf{v}$ is the transpose of **v** and $\hat{\mathbf{v}}$ the hat map of **v**.

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