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Same Same but Different - Definition and Explicit Notation of an Orientation in Mtex vs. Quasi-Standard

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Abstract. Even though the descriptive definition of orientation is the same in both settings, the explicit notation of a crystallographic orientation as (3×3) matrix in terms of Euler angles featured by the popular Matlab toolbox Mtex differs by an inversion from the quasi-standard notation dated back to the early days of quantitative texture analysis championed by H.-J. Bunge. The origin of this discrepancy is revealed by an enlightening view provided in algebraic terms of a change of basis. Understanding the effect of inversion is instrumental to do proper computations with crystallographic orientations and rotations, e.g. when multiplying with elements of a crystallographic symmetry group, and to compare results of texture analyses accomplished in different settings.

Introduction

The documentation [1] of the popular Matlab [2] toolbox Mtex [3] states that *"For historical reasons MTEX defines orientations in a slightly different way than they have been defined by Bunge."* [4]. In fact, the descriptive definition of orientation is the same in both settings, but the rotation matrices turning orientations operational are inverse of each other. This discrepancy does not originate from history but from mathematics. In accordance with the general definition, orientation in texture analysis refers to the rotational state of a coordinate system attached to a crystallite thought of a variable with respect to a coordinate system attached to a polycrystalline sample thought of as fixed. When the rotation numerically realizing an orientation is parametrized in terms of Euler angles, the discrepancy of the rotation matrices originates from the erroneous derivation of the quasi-standard notation. It seems to be affected by confusion in the maze of intrinsic vs. extrinsic notation, active vs. passive rotation, rotation of vectors vs. transformation of a frame. If there is any historical association at all, it is that the error originated decades before the existence of Mtex.

Unfortunately, this issue was not addressed in [3]; it is completed here. Following is a comprehensive and mathematically detailed presentation of the derivation of rotation matrices corresponding to orientations in terms of Euler angles. Publications contributing to the development of Mtex are listed at [5].

Orientations and Their Corresponding Rotation Matrices in Terms of Euler Angles

Definition of orientation - rotation of frame.

An orientation g is generally defined as rotational displacement of two right-handed Cartesian coordinate systems. It is described and quantified by the rotation that transforms the rotational state of one system into the rotational state of the other [6]. In materials science and geology, the two coordinate systems are usually $K_{\text{sample}} = \langle \mathbf{x}, \mathbf{y}, \mathbf{z} \rangle$ attached to a polycrystalline sample, and $K_{\text{crystallite}} = \langle \mathbf{a}, \mathbf{b}, \mathbf{c} \rangle$ attached to an individual crystallite such that the rotation g makes the sample coordinate system coincide with the crystallite coordinate system, $g : K_{\text{sample}} \mapsto K_{\text{crystallite}}$ by virtue of $g\,\mathbf{x} = \mathbf{a}$, $g\,\mathbf{y} = \mathbf{b}$, $g\,\mathbf{z} = \mathbf{c}$ with unit vectors $\mathbf{x}, \mathbf{y}, \mathbf{z}$ and $\mathbf{a}, \mathbf{b}, \mathbf{c}$, respectively, [7, p. 3], [8, p. 3], [9]. The orientation g describes the rotational state of the coordinate system $K_{\text{crystallite}}$ with respect to the coordinate system K_{sample}.

The matrix of the corresponding rotation is

$$M(g) = \begin{array}{c} \\ \mathbf{x} \\ \mathbf{y} \\ \mathbf{z} \end{array} \left| \begin{array}{c} \begin{array}{ccc} \mathbf{a} & \mathbf{b} & \mathbf{c} \end{array} \\ \begin{pmatrix} \mathbf{xa} & \mathbf{xb} & \mathbf{xc} \\ \mathbf{ya} & \mathbf{yb} & \mathbf{yc} \\ \mathbf{za} & \mathbf{zb} & \mathbf{zc} \end{pmatrix} \end{array} \right. = \begin{array}{c} \begin{array}{ccc} \mathbf{a} & \mathbf{b} & \mathbf{c} \end{array} \\ \begin{pmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{pmatrix} \end{array} = \left. \begin{array}{c} \begin{pmatrix} x'_1 & x'_2 & x'_3 \\ y'_1 & y'_2 & y'_3 \\ z'_1 & z'_2 & z'_3 \end{pmatrix} \\ \\ \end{array} \right| \begin{array}{c} \mathbf{x} \\ \mathbf{y}. \\ \mathbf{z} \end{array} \tag{1}$$

Its columns are the coordinates of the unit basis vectors **a**, **b**, **c** with respect to the sample coordinate system $\langle \mathbf{x}, \mathbf{y}, \mathbf{z} \rangle$, its rows are the coordinates of the unit basis vectors **x**, **y**, **z** with respect to the crystallite coordinate system $\langle \mathbf{a}, \mathbf{b}, \mathbf{c} \rangle$.

Accounting for crystallographic symmetries and considering symmetrically equivalent rotations provide the notion of crystallographic orientation.

Change of basis - coordinate transform.
Let the unit vector **v** have coordinates (r_x, r_y, r_z) with respect to K_{sample}, and coordinates (h_a, h_b, h_c) with respect to $K_{\text{crystallite}}$ such that

$$r_x \, \mathbf{x} + r_y \, \mathbf{y} + r_z \, \mathbf{z} = h_a \, \mathbf{a} + h_b \, \mathbf{b} + h_c \, \mathbf{c}, \tag{2}$$

which is referred to as change of basis in linear algebra [10], [11, pp. 87–94]. If the crystallite coordinate system $K_{\text{crystallite}}$ is rotationally displaced with respect to the sample coordinate system K_{sample} by the orientation g, i.e., $g : K_{\text{sample}} \mapsto K_{\text{crystallite}}$, the coordinate vectors $\mathbf{h} = (h_a, h_b, h_c)^{\mathsf{T}}$ and $\mathbf{r} = (r_x, r_y, r_z)^{\mathsf{T}}$ are related as

$$g \, \mathbf{h} = \mathbf{r}, \tag{3}$$

i.e., the orientation g transforms the crystallographic direction **h** into the sample direction **r**.

Since *"The reader must realize that indiscriminate use of any matrix quoted in group theory can lead into mortal trouble: One must know precisely on what basis and in what form the matrix is supposed to operate."* [12, p. 69], here we discriminate rotation, e.g.

$$\begin{pmatrix} \mathbf{xa} & \mathbf{xb} & \mathbf{xc} \\ \mathbf{ya} & \mathbf{yb} & \mathbf{yc} \\ \mathbf{za} & \mathbf{zb} & \mathbf{zc} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}_{K_{\text{sample}}} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}_{K_{\text{sample}}} = \mathbf{a} \tag{4}$$

staying in the sample coordinate system, and transformation converting from the crystallite to the sample coordinate system, e.g.

$$\begin{pmatrix} \mathbf{xa} & \mathbf{xb} & \mathbf{xc} \\ \mathbf{ya} & \mathbf{yb} & \mathbf{yc} \\ \mathbf{za} & \mathbf{zb} & \mathbf{zc} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}_{K_{\text{crystallite}}} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}_{K_{\text{sample}}} = \mathbf{a}. \tag{5}$$

Given any two unit vectors **h** and **r**, Eq. 3 does not define a unique orientation g. The on-line documentation [13] is erroneous.

Given a pair $(\mathbf{h}, \mathbf{r})$ of unit vectors, the set $G(\mathbf{h}, \mathbf{r})$ of all orientations satisfying Eq. 3 is called fiber, fibers are the geodesics of $\mathrm{SO}(3)$ [14]. Fibers are crucial for the definition of the bi-directional probability density function ("pole figures") $P(\mathbf{h}, \mathbf{r})$ that the crystallographic direction **h** or any of its symmetrically equivalents is converted to coincide with the sample direction **r**. Integration of a function along the geodesics of its domain is referred to as Radon transform of the function [15].

Parametrization in terms of Euler angles: Intrinsic vs. extrinsic notation.
To parametrize the orientation g, Bunge [7, p. 5, Eq. (2.3)], [8, p. 4, Eq. (2.1)] uses the triplet of Euler angles $(\varphi_1, \phi, \varphi_2)$ according to the **zx′z″** or, equivalently, **zxz** convention:

- first rotation $R(\varphi_1, \mathbf{z})$ by $\varphi_1 \in [0, 2\pi)$ about the sample **z**–axis,

- second rotation $R(\phi, \mathbf{x}')$ by $\phi \in [0, \pi]$ about the *rotated* sample **x**–axis,
- third rotation $R(\varphi_2, \mathbf{z}'')$ by $\varphi_2 \in [0, 2\pi)$ about the *twice rotated* sample **z**–axis,

resulting in the notation

$$g(\varphi_1, \phi, \varphi_2) = R(\varphi_2, \mathbf{z}'')\ R(\phi, \mathbf{x}')\ R(\varphi_1, \mathbf{z}) \tag{6}$$

as intrinsic rotation. Elaborating on

$$\begin{aligned} &R(\varphi_2, \mathbf{z}'')\ R(\phi, \mathbf{x}')\ R(\varphi_1, \mathbf{z}) = \\ &\quad R\Big(\varphi_2, R\big(\phi, R(\varphi_1, \mathbf{z})\,\mathbf{x}\big)\ R(\varphi_1, \mathbf{z})\,\mathbf{z}\Big)\ R\Big(\phi, R(\varphi_1, \mathbf{z})\,\mathbf{x}\Big)\ R(\varphi_1, \mathbf{z}) \end{aligned} \tag{7}$$

leads straightforward to the notation as extrinsic rotation

$$g(\varphi_1, \phi, \varphi_2) = R(\varphi_1, \mathbf{z})\ R(\phi, \mathbf{x})\ R(\varphi_2, \mathbf{z}) \tag{8}$$

justifying the label **zxz** convention.

Matrices $g_{\text{MTEX}}(\varphi_1, \phi, \varphi_2)$ and $g_{\text{Bunge}}(\varphi_1, \phi, \varphi_2)$.
Explicitly in terms of (3×3) matrices of SO(3) it is

$$\begin{aligned} &R(\varphi_1, \mathbf{z})\ R(\phi, \mathbf{x})\ R(\varphi_2, \mathbf{z}) \\ &= \begin{pmatrix} \cos\varphi_1 & -\sin\varphi_1 & 0 \\ \sin\varphi_1 & \cos\varphi_1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\phi & -\sin\phi \\ 0 & \sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} \cos\varphi_2 & -\sin\varphi_2 & 0 \\ \sin\varphi_2 & \cos\varphi_2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} \cos\varphi_1\cos\varphi_2 - \sin\varphi_1\cos\phi\sin\varphi_2 & -\cos\varphi_1\sin\varphi_2 - \sin\varphi_1\cos\phi\cos\varphi_2 & \sin\varphi_1\sin\phi \\ \sin\varphi_1\cos\varphi_2 + \cos\varphi_1\cos\phi\sin\varphi_2 & -\sin\varphi_1\sin\varphi_2 + \cos\varphi_1\cos\phi\cos\varphi_2 & -\cos\varphi_1\sin\phi \\ \sin\phi\sin\varphi_2 & \sin\phi\cos\varphi_2 & \cos\phi \end{pmatrix} \end{aligned} \tag{9}$$

$$= M(\varphi_1, \phi, \varphi_2) = g_{\text{MTEX}} \tag{10}$$

as used in Mtex.
For whatever reason, Bunge [8, p. 21, Eq. (2.50)] set

$$\begin{aligned} &g_{\text{Bunge}}(\varphi_1, \phi, \varphi_2) = \\ &\begin{pmatrix} \cos\varphi_1\cos\varphi_2 - \sin\varphi_1\cos\phi\sin\varphi_2 & \sin\varphi_1\cos\varphi_2 + \cos\varphi_1\cos\phi\sin\varphi_2 & \sin\phi\sin\varphi_2 \\ -\cos\varphi_1\sin\varphi_2 - \sin\varphi_1\cos\phi\cos\varphi_2 & -\sin\varphi_1\sin\varphi_2 + \cos\varphi_1\cos\phi\cos\varphi_2 & \sin\phi\cos\varphi_2 \\ \sin\varphi_1\sin\phi & -\cos\varphi_1\sin\phi & \cos\phi \end{pmatrix} \end{aligned} \tag{11}$$

which results from taking the inverse of the right hand side of Eq. 8

$$g_{\text{Bunge}}(\varphi_1, \phi, \varphi_2) = \Big(R(\varphi_1, \mathbf{z})\ R(\phi, \mathbf{x})\ R(\varphi_2, \mathbf{z})\Big)^{-1} = R(-\varphi_2, \mathbf{z})\ R(-\phi, \mathbf{x})\ R(-\varphi_1, \mathbf{z}). \tag{12}$$

In fact, the matrices [8, p. 21, Eqs. 2.47, 2.48, 2.49] have been confused with the matrices of the three elementary rotations according to the **zxz** convention , e.g. the matrix

$$\begin{pmatrix} \cos\varphi_1 & \sin\varphi_1 & 0 \\ -\sin\varphi_1 & \cos\varphi_1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{13}$$

[8, p. 21, Eqs. 2.47] is mistaken as matrix of the rotation by φ_1 about $\mathbf{z}$. However, it is either the matrix of the rotation by $-\varphi_1$ about $\mathbf{z}$ or of the rotation by φ_1 about $-\mathbf{z}$ [12, p. 69, Eq. (14)]. Moreover, Bunge [8] uses the same symbol $g(\varphi_1, \phi, \varphi_2)$ to denote both the orientation as defined informally in terms of rotational displacement of coordinate systems in [8, p. 4, Eq. (2.1)] and its inverse as derived as (3×3) matrix of Euler angles in [8, p. 21, Eq. (2.50)]. Since [8, p. 21, Eq. (2.50)], this communication's Eq. 11, is taken as operative formal definition of orientation throughout theory and practice of crystallographic texture analysis by the Bunge school, their term orientation actually denotes the rotational displacement of the sample coordinate system K_{sample} with respect to the crystallite coordinate system $K_{\text{crystallite}}$ – just the opposite of Bunge's initial definition [7, p. 3], [8, p. 3]). Referring to the notation featured here, $g^{-1}_{\text{Bunge}}(\varphi_1, \phi, \varphi_2) = g_{\text{MTEX}}(\varphi_1, \phi, \varphi_2)$, and of course $g_{\text{Bunge}}(\varphi_1, \phi, \varphi_2)\,\mathbf{r} = \mathbf{h}$.

Exemplary implication of inversion.
The relationships $g_{\text{MTEX}}(\varphi_1, \phi, \varphi_2)\,\mathbf{h} = \mathbf{r}$ and $g_{\text{Bunge}}(\varphi_1, \phi, \varphi_2)\,\mathbf{r} = \mathbf{h}$, respectively, indicate an implication of the inversion. For any rotation σ of some crystallographic symmetry group $G_{\text{cs}} \subset \text{SO}(3)$, $g_{\text{MTEX}}\,\mathbf{h} = \mathbf{r}$ implies $g_{\text{MTEX}}\sigma\,\mathbf{h} = \widetilde{\sigma}\mathbf{r}$, i.e., multiplication $g_{\text{MTEX}}\,\sigma$ from the right, where $\widetilde{\sigma}$ denotes the conjugate of rotation σ, i.e., the rotation $\widetilde{\sigma}(\omega, g_{\text{MTEX}}\mathbf{n})$ by the same angle ω about the rotated axis $g_{\text{MTEX}}\mathbf{n}$ of rotation $\sigma(\omega, \mathbf{n})$. The axis $\mathbf{n}$ of rotation $\sigma \in G_{\text{cs}}$ refers to the crystallite coordinate system $K_{\text{crystallite}}$, the rotated axis $g_{\text{MTEX}}\mathbf{n}$ of the conjugate rotation $\widetilde{\sigma}$ refers to the sample coordinate system K_{sample}. In the quasi-standard notation, $g_{\text{Bunge}}\,\mathbf{r} = \mathbf{h}$ implies $\sigma g_{\text{Bunge}}\,\mathbf{r} = \sigma\mathbf{h}$, i.e., multiplication $\sigma\, g_{\text{Bunge}}$ from the left.

Discussion

The same confusion of the three elementary Euler rotations and their inverses and, consequentially, of g and g^{-1} occured in [16, p. 1059, Eqs. 9, 10, 11], and in [17, p. 730, Eq. (5), (6)], but it was supposedly spread by the extended English translation [8] of [7]. Ever since, it has often been perpetuated, e.g. in the textbooks [18, pp. 27-28] and [19, pp. 34-35, Eqs. 2.15, 2.16], where the elementary rotations about the three axes of any Cartesian reference frame are defined as clockwise for non-negative angles of rotations as opposed, i.e., inverse, to the standard definition as anti-clockwise [12, p. 69, Eq. (14)]. The result of their composition agrees of course with g_{Bunge}.

Surprisingly enough, the error to mistake the inverse orientation g^{-1} as orientation g happens in [20] as well. Applying the $\mathbf{zy'z''}$ [20, p. 4, Eqs. 1.4, 1.5, 1.6] or equivalently the $\mathbf{zyz}$ [20, p. 12] convention, respectively, where the former refers to the intrinsic and the latter to the extrinsic notation, the rotational displacement of the crystallite coordinate system $K_{\text{crystallite}}$ with respect to the sample coordinate system K_{sample} is described by the sequence of elementary Euler rotations

$$g(\alpha, \beta, \gamma) = R(\alpha, \mathbf{z})R(\beta, \mathbf{y})R(\gamma, \mathbf{z}) \tag{14}$$

$$= \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & \\ -\sin\beta & 0 & \cos\beta \end{pmatrix} \begin{pmatrix} \cos\gamma & -\sin\gamma & 0 \\ \sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{15}$$

resulting in the orientation matrix [12, p. 69, Eqs. 14, 15].

$$M(g(\alpha, \beta, \gamma)) =$$

$$\begin{pmatrix} \cos\alpha\cos\beta\cos\gamma - \sin\alpha\sin\gamma & -\cos\alpha\cos\beta\sin\gamma - \sin\alpha\cos\gamma & \cos\alpha\sin\beta \\ \sin\alpha\cos\beta\cos\gamma + \cos\alpha\sin\gamma & -\sin\alpha\cos\beta\sin\gamma + \cos\alpha\cos\gamma & \sin\alpha\sin\beta \\ -\sin\beta\cos\gamma & \sin\beta\sin\gamma & \cos\beta \end{pmatrix}, \tag{16}$$

As before, the matrix $M(g(\alpha, \beta, \gamma))$ realizes the transformation converting coordinate vectors from the crystallite to the sample coordinate system, $M(g(\alpha, \beta, \gamma))\mathbf{h}_{K_{\text{crystallite}}} = \mathbf{r}_{K_{\text{sample}}}$, and of course

$M^{-1}(g(\alpha,\beta,\gamma))\mathbf{r}_{K_{\text{sample}}} = M(g^{-1}(\alpha,\beta,\gamma))\mathbf{r}_{K_{\text{sample}}} = \mathbf{h}_{K_{\text{crystallite}}}$. The confusion of $g(\alpha,\beta,\gamma)$ and its inverse takes its course from [20, p. 7, Eq. (20)] onward with matrix $A(g_{\text{MVH}}(\alpha,\beta,\gamma)$ (subscript mvh by this author), the elements of which are defined in [20, p. 7, Eqs. 1.21, ... , 1.30] such that it agrees with $M^{-1}(g(\alpha,\beta,\gamma))$ of Eq. 16; thus $g_{\text{MVH}}(\alpha,\beta,\gamma) = g^{-1}(\alpha,\beta,\gamma)$ of Eq. 16. However, the confusion does not seem like an insurmountable problem [21].

Conclusions

The definition of (crystallographic) orientation as rotational displacement of a Cartesian coordinate system attached to an individual crystallite with respect to a Cartesian coordinate system fixed to the polycrystalline sample is unique. Here, the lasting and annoying confusion about the explicit expression of the orientation of the crystallite coordinate system with respect to the sample coordinate system has been traced back to the early days of quantitative crystallographic texture analysis. It seems to originate to some extent in a rash definition of elementary rotations by Euler angles about convenient axes or in the hasty exchange of an elementary rotation matrix by its inverse by getting signs wrong. However, there may also be a common misconception that the matrix rotating the unit vectors defining the Cartesian sample coordinate system onto the unit vectors defining the Cartesian crystallite coordinate system converts for any given unit vector its coordinate vector with respect to the sample coordinate system into the coordinate vector with respect to the crystallite coordinate system. In fact, this conversion is realized by the inverse of the rotation matrix. Elaborating on the distinction between rotation of vectors and conversion of vectors between rotational displaced coordinate systems, the confusion should be resolved now. Since the early mistake has been perpetuated it remains to note that Bunge's school of crystallographic texture analysis features orientation as rotational displacement of the sample coordinate system with respect to the crysallite coordinate system.

After all, it is a matter of definition. The crystallographic texture community should be aware that there is a quasi-standard parametrization in terms of Euler angles originating from an erroneous derivation dating back to the early days of mathematization of crystallographic texture analysis, and a proper parametrization originating in linear algabra and implemented in Mtex. They need to know the difference to do proper computations involving crystallographic orientations and rotations in either setting, and to compare results accomplished in different settings.

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