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On representing rotations by Rodrigues parameters in non-orthonormal reference systems

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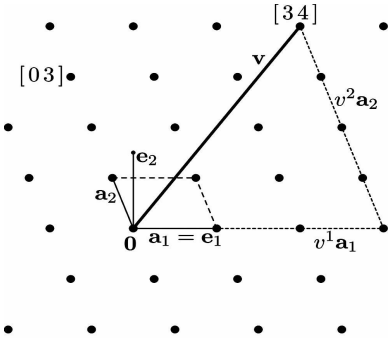
A Rodrigues vector is a triplet of real numbers used for parameterizing rotations or orientations in three-dimensional space. Because of its properties (*e.g.* simplicity of fundamental regions for misorientations) this parameterization is frequently applied in analysis of orientation maps of polycrystalline materials. By conventional definition, the Rodrigues parameters are specified in orthonormal coordinate systems, whereas the bases of crystal lattices are generally non-orthogonal. Therefore, the definition of Rodrigues parameters is extended so they can be directly linked to non-Cartesian bases of a crystal. The new parameters are co- or contravariant components of vectors specified with respect to the same basis as atomic positions in a unit cell. The generalized formalism allows for redundant crystallographic axes. The formulas for rotation composition and the relationship to the rotation matrix are similar to those used in the Cartesian case, but they have a wider range of applicability: calculations can be performed with an arbitrary metric tensor of the crystal lattice. The parameterization in oblique coordinate frames of lattices is convenient for crystallographic applications because the generalized parameters are directly related to indices of rotation-invariant lattice directions and rotation-invariant lattice planes.

1. Introduction

The notion of rotation is fundamental in the field of crystallography. It arises in various contexts: from the theory of crystal symmetry in pure crystallography, to analysis of orientation relationships and crystallographic textures in applied crystallography. Proper rotations in three-dimensional space are usually handled using special orthogonal matrices or unit quaternions. Both representations are convenient for calculating compositions of rotations, and also both are redundant as a rotation is uniquely identified by three independent parameters (*e.g.* three Euler angles).

Prominent among non-redundant rotation parameterizations is that by gnomonic projections of unit quaternions. Under the name of Rodrigues parameterization, it is routinely used in analysis of crystal misorientations, in particular, in software supporting orientation mapping systems (Mason & Schuh, 2009). The parameterization has a number of convenient properties. In contrast to Euler angles, it is non-singular at null rotation. The Rodrigues formula for the composition of rotations (Rodrigues, 1840) is relatively simple. With rotations represented in an orthonormal coordinate system having axes gauged by Rodrigues parameters, rotation-space geodesics and surfaces of points equidistant to two rotations have simple forms (see, *e.g.*, Morawiec, 2004). Owing to the latter property, symmetry-induced fundamental regions for crystal misorientations have planar boundaries. The main disadvantage of



the Rodrigues parameterization is that half-turns correspond to infinite parameters.

Parameterizations of proper rotations are usually defined *via* relationships between Cartesian reference systems;[1] see, *e.g.*, the definition of Euler angles (Bunge, 1982; Diamond, 2006). Also, the conventional definition of Rodrigues parameters is based on Cartesian systems (Rodrigues, 1840; Frank, 1988; Mason & Schuh, 2009). On the other hand, by the nature of crystals, bases of crystal lattices are frequently non-orthogonal. Questions arise about referring rotation parameters directly to such oblique frames. By its definition, the triplet of Rodrigues parameters transforms between reference frames like a vector and, accordingly, it is also referred to as a Rodrigues (or Gibbs) vector, but what are the consequences of this vectorial character of Rodrigues parameters? What is the relationship of the space of Rodrigues vectors to the physical space? What are the actual formulas linking Rodrigues parameters given in a non-Cartesian reference system to conventional Rodrigues parameters and other rotation parameters? How can one interpret the properties originally formulated for the Cartesian case? How complicated is the generalization of the Rodrigues parameters to reference frames with redundant crystallographic axes (as in the four-index description of hexagonal crystals)?

This article addresses the above questions and some related issues. It describes rotations in arbitrary lattice bases comprised of linearly independent vectors and in frames with redundant crystallographic axes. The generalized Rodrigues parameters are defined as contra- or covariant components of vectors in the physical space of the crystal. This parameterization of rotations is in a sense more natural than the matrix parameterization because Rodrigues parameters, as contra- or covariant vector components, are directly linked to crystallographic indices of rotation-invariant lattice directions and to indices of invariant lattice planes. Despite that, to our knowledge, the subject of Rodrigues vectors in non-Cartesian reference frames has not been explicitly considered in the crystallographic literature. Also, the concept of redundant crystallographic axes has been dealt with only superficially with an emphasis on the hexagonal case (Frank, 1965; Nicholas & Segall, 1970; Mackay, 1977).

The article is organized as follows. First, the standard matrix formalism for description of rotations in three-dimensional Euclidean space using non-orthogonal reference systems is recapitulated (Shmueli, 2006); this preparatory section also establishes a large part of our notation. Then, in §3, Rodrigues parameters in the non-orthogonal systems are introduced and some of their properties are discussed. Finally, the formalism is generalized to frames consisting of linearly dependent vectors; the whole presentation could be limited to this general scheme as it includes the case considered in §§2 and 3, but the longer step-by-step approach based on analogies with well known methods was chosen as it is more instructive.

[1] To carry out rotations of vectors or tensors, these objects are first transformed to a Cartesian system and then techniques specific to this case are applied.

We use the notation with vectors, tensors and matrices identified by their components; only some vectors are denoted by bold symbols. The summation convention is used: if an index appears in a term twice, as a subscript and a superscript, a summation over its values is implied. The Kronecker delta δ_{ij} is equal to 1 if $i = j$ and it is zero otherwise. Moreover, ε_{ijk} denotes the permutation symbol equal to $+1$ (-1) if (ijk) is an even (odd) permutation of (123) and it is zero otherwise.

2. Rotation matrix in a non-orthogonal coordinate system

2.1. Bases of non-Cartesian coordinate systems

Let $\mathbf{a}_i$ ($i = 1, 2, 3$) denote three linearly independent vectors of a basis of a three-dimensional lattice. The constant scalar products

$$g_{ij} = \mathbf{a}_i \cdot \mathbf{a}_j \tag{1}$$

are covariant components of the metric tensor. The components make a symmetric positive definite matrix. The entries of its inverse are denoted by the same letter with upper indices g^{ij}, *i.e.* one has $g^{ik}g_{kj} = \delta^i_j$. The vectors

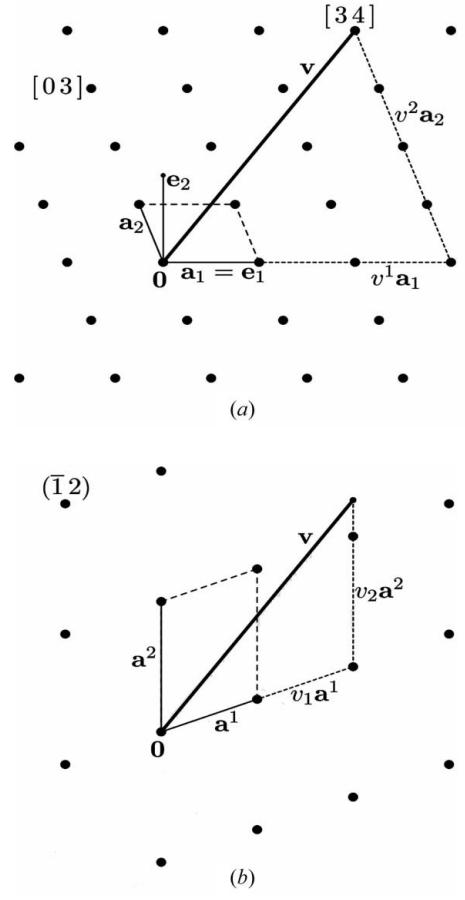


Figure 1
Schematic two-dimensional illustration of decompositions $v^i\mathbf{a}_i$ and $v_i\mathbf{a}^i$ ($i = 1, 2$) of vector $\mathbf{v}$. The basis $\mathbf{a}^i$ in (*b*) is dual to $\mathbf{a}_i$ shown in (*a*). The lattices based on $\mathbf{a}_i$ and $\mathbf{a}^i$ are marked by discs. Primitive cells of the lattices are sketched using long dashes.

$$\mathbf{a}^i = g^{ij}\mathbf{a}_j \tag{2}$$

are linearly independent and constitute a basis dual to $\mathbf{a}_i$. It is easy to verify that

$$g_{ij}\mathbf{a}^j = \mathbf{a}_i,\ \ \mathbf{a}^i \cdot \mathbf{a}_j = \delta^i_j \text{ and } \mathbf{a}^i \cdot \mathbf{a}^j = g^{ij}. \tag{3}$$

A vector can be expressed as a unique linear combination of basis vectors. The contravariant (covariant) components v^i (v_i) of vector $\mathbf{v}$ in the basis $\mathbf{a}_i$ ($\mathbf{a}^i$) are distinguished by upper (lower) indices, *i.e.* $\mathbf{v} = v^i\mathbf{a}_i$ ($\mathbf{v} = v_i\mathbf{a}^i$) (Fig. 1). These components are given by $v^i = v^j\delta_j^{\ i} = v^j\mathbf{a}_j \cdot \mathbf{a}^i = \mathbf{v} \cdot \mathbf{a}^i$ and, similarly, $v_i = \mathbf{v} \cdot \mathbf{a}_i$. The contravariant and covariant components are interrelated by $v^i = \mathbf{v} \cdot \mathbf{a}^i = v_j\mathbf{a}^j \cdot \mathbf{a}^i = g^{ij}v_j$ and $v_i = g_{ij}v^j$. Thus, the metric tensor raises and lowers indices of basis vectors and vector components. The scalar product of vectors $\mathbf{v}$ and $\mathbf{w}$ can be written as $\mathbf{v} \cdot \mathbf{w} = g_{ij}v^iw^j = g^{ij}v_iw_j = v^iw_i = v_iw^i$. In particular, the squared length of $\mathbf{v}$ equals $|\mathbf{v}|^2 = \mathbf{v} \cdot \mathbf{v} = v^iv_i$.

In the crystallographic context, the vectors $\mathbf{a}_i$ can be seen as basis vectors of a direct crystal lattice. Hereafter, for simplicity, the actual basis of the lattice is assumed to be scaled by a divisor with the dimension of length, so the basis vectors $\mathbf{a}_i$ are dimensionless. The vectors $\mathbf{a}^i$ constitute a scaled basis of the crystal reciprocal lattice. The direction indices and direct lattice nodes $[u\ v\ w]$ are contravariant vector components, and the Miller indices $(h\ k\ l)$, which identify nodes of the reciprocal lattice, are covariant vector components (*e.g.* Sands, 2006).

2.2. Transformations between coordinate systems

Entities specified in an orthonormal basis $\mathbf{e}_I$ ($I = 1, 2, 3$) will be distinguished by capital indices. By definition, the orthonormal basis has the metric $\mathbf{e}_I \cdot \mathbf{e}_J = \delta_{IJ}$. With $\mathbf{e}^I = \delta^{IJ}\mathbf{e}_J$, the vectors $\mathbf{e}^I$ of the basis dual to that built of vectors $\mathbf{e}_I$ are identical to $\mathbf{e}_I$. Let the vectors $\mathbf{a}_i$ be related to $\mathbf{e}_I$ by

$$\mathbf{a}_i = T_i^{\ J}\mathbf{e}_J, \tag{4}$$

i.e. $T_i^{\ J} = \mathbf{a}_i \cdot \mathbf{e}^J$ is the Jth component of $\mathbf{a}_i$ in the orthonormal basis. Equation (4) implies the relationship between bases $\mathbf{a}^i$ and $\mathbf{e}^I$ dual to $\mathbf{a}_i$ and $\mathbf{e}_I$, respectively. To carry out this transformation, indices need to be lowered before application of $T_i^{\ J}$ and raised back after the transformation, *i.e.* one has $\mathbf{a}^i = g^{ik}T_k^{\ K}\delta_{KJ}\,\mathbf{e}^J$. This expression can be simplified by defining a new entity $T^i_{\ J} = g^{ik}\,T_k^{\ K}\,\delta_{KJ} = \mathbf{a}^i \cdot \mathbf{e}_J$ with the level of indices switched compared to $T_i^{\ J}$. As defined, $T^i_{\ J}$ is inverse to the transposed $T_i^{\ J}$, *i.e.* $T^i_{\ K}T_j^{\ K} = \delta^i_{\ j}$ and $T_k^{\ I}T^k_{\ J} = \delta^I_{\ J}$. With this new symbol, one has

$$\mathbf{a}^i = T^i_{\ J}\mathbf{e}^J.$$

Based on $v_i = \mathbf{v} \cdot \mathbf{a}_i = \mathbf{v} \cdot (T_i^{\ J}\mathbf{e}_J) = T_i^{\ J}(\mathbf{v} \cdot \mathbf{e}_J)$, the covariant components v_i of $\mathbf{v}$ in the basis $\mathbf{a}^i$ are linked to the components $v_J = \mathbf{v} \cdot \mathbf{e}_J$ in the basis $\mathbf{e}^J$ *via*

$$v_i = T_i^{\ J}v_J. \tag{5}$$

Similarly, the contravariant components are transformed according to

$$v^i = T^i_{\ J}\,v^J. \tag{6}$$

Analogous transformation rules apply to higher-rank tensors. In particular, one has

$$g_{ij} = T_i^{\ K}\,T_j^{\ L}\,\delta_{KL} \quad \text{and} \quad g^{ij} = T^i_{\ K}\,T^j_{\ L}\,\delta^{KL}. \tag{7}$$

These relationships reflect the fact that the considered transformations are isometries. It follows from equation (7) that the determinant of g_{ij} equals V^2, where V is the determinant of $T_i^{\ J}$.

A comment is in place that the geometry of the lattice is determined by its metric tensor, and the link to the Cartesian reference frame *via* $T_i^{\ J}$ and $T^i_{\ J}$ is only auxiliary. The matrices are used below to derive general formulas applicable in non-Cartesian systems. These matrices are also of practical importance as they are applied (in various forms) in codes for processing of experimental data; the best known crystallographic example of such an array is the **B** matrix of Busing & Levy (1967).

2.3. The rotation matrix

The special orthogonal matrix representing the rotation about $\mathbf{n} = n^I\mathbf{e}_I$ by the angle θ in the Cartesian system has the entries (*e.g.* Shmueli, 2006)

$$R^I_{\ J} = \delta^I_{\ J}\cos\theta + n^In_J(1 - \cos\theta) + \delta^{IK}\varepsilon_{KJL}n^L\,\sin\theta. \tag{8}$$

The active[2] rotation of vector $\mathbf{v} = v^I\mathbf{e}_I$ gives the vector $\mathbf{w} = w^I\mathbf{e}_I$ with components $w^I = R^I_{\ J}v^J$. In the basis $\mathbf{a}_i$, the contravariant components of vector $\mathbf{w}$ obtained by rotating $\mathbf{v}$ are $w^i = T^i_{\ I}w^I = T^i_{\ I}R^I_{\ J}v^J = T^i_{\ I}R^I_{\ J}T_j^{\ J}v^j$. Thus, with

$$w^i = R^i_{\ j}v^j, \tag{9}$$

the rotation matrix $R^i_{\ j}$ in the basis $\mathbf{a}_i$ is related to $R^I_{\ J}$ describing the rotation in the Cartesian system *via* $R^i_{\ j} = T^i_{\ I}T_j^{\ J}R^I_{\ J}$. By this transformation rule and equation (8), the rotation matrix in the non-Cartesian system is $R^i_{\ j} = \delta^i_{\ j}\cos\theta + n^i\,n_j\,(1 - \cos\theta) + g^{ik}\,\varepsilon_{kjl}\,n^l\,V\,\sin\theta$, where $n_i = T_i^{\ J}n_J$ and $n^i = T^i_{\ J}n^J$ are, respectively, co- and contravariant components of $\mathbf{n}$ in the non-Cartesian frame. There are a number of ways to integrate the determinant V into this expression. The formula can be left unchanged (Shmueli, 2006), or V can be moved to the transformation rule of n^l making it a pseudovector (Morawiec, 2004). The approach used below relies on the tensor $\epsilon_{ijk} = \varepsilon_{ijk}V$ (Sands, 2006). By definition of the matrix determinant, ϵ_{ijk} in the non-Cartesian reference system is obtained by transforming $\epsilon_{IJK} = \varepsilon_{IJK} \times 1$ from the Cartesian system, *i.e.* $\epsilon_{ijk} = T_i^{\ I}\,T_j^{\ J}\,T_k^{\ K}\epsilon_{IJK}$. The same tensor with raised indices is $\epsilon^{uvw} = g^{ui}g^{vj}g^{wk}\epsilon_{ijk} = \varepsilon^{uvw}/V$. With the as-defined ϵ_{ijk}, the rotation matrix has the form

$$R^i_{\ j} = \delta^i_{\ j}\cos\theta + n^i\,n_j\,(1 - \cos\theta) + g^{ik}\,\epsilon_{kjl}\,n^l\,\sin\theta. \tag{10}$$

The trace of the rotation matrix is linked to the rotation angle in the same way as in the Cartesian case, $R^i_{\ i} = R^I_{\ I} = 2\cos\theta + 1$.

The rotation matrix $R^i_{\ j}$ was defined above using contravariant vector components. To carry out the same transformation of $\mathbf{v}$ to $\mathbf{w}$ using their covariant components, indices of

[2] This convention is used to avoid adding more reference frames.

the latter need to be raised before application of $R^i{}_j$ and lowered afterwards, *i.e.* one has

$$w_i = R_i{}^j v_j, \tag{11}$$

where $R_i{}^j = g_{ik} R^k{}_l g^{lj}$. The matrix $R_i{}^j$ is inverse to the transposed $R^i{}_j$, *i.e.* $R_j{}^k R^i{}_k = \delta_j{}^i = R^i_k R^k_j$. The rotation matrices satisfy

$$g_{ij} R^i{}_k R^j{}_l = g_{kl} \quad \text{and} \quad g^{kl} R^i_k R^j_l = g^{ij}. \tag{12}$$

These relationships reflect the fact that the rotations are isometries.

2.4. Direction and Miller indices

The direction indices $[u\,v\,w]$ and Miller indices $(h\,k\,l)$ are transformed according to the rules of contra- and covariant components of vectors, respectively. Accordingly, to calculate indices of rotated directions and planes, one needs to use equations (9) and (11), respectively. Moreover, under the rotation about $\mathbf{n} = n^i \mathbf{a}_i = n_i \mathbf{a}^i$, the lattice directions $[u\,v\,w] \propto [n^1\,n^2\,n^3]$ and the lattice planes $(h\,k\,l) \propto (n_1\,n_2\,n_3)$ remain invariant.

3. Rodrigues parameters in non-orthonormal coordinate systems

Let the Rodrigues parameters be defined in two mutually related forms:

$$r^i = n^i \tan(\theta/2) \quad \text{and} \quad r_i = n_i \tan(\theta/2). \tag{13}$$

Since each of the triplets r^i and r_i carries complete information about the direction of the rotation axis and the rotation angle, each of them is a parameterization of rotations. They are components of a true vector in the systems based on $\mathbf{a}_i$ and $\mathbf{a}^i$, *i.e.* they are transformed between reference frames according to the rules (5) and (6), and there occurs $r_i = g_{ij} r^j$.

The vector with components r^i and r_i will be denoted by $\mathbf{r}$. Clearly, the null rotation corresponds to $\mathbf{r} = \mathbf{0}$, and half-turns correspond to Rodrigues vectors of infinite magnitude. Moreover, it is easy to see that the rotation inverse to the rotation represented by $\mathbf{r}$ is represented by $-\mathbf{r}$. By substitution of n^i and n_i, the relationship (10) is transformed to

$$R^i{}_j = \frac{1}{1 + r^k r_k} \left[\delta^i{}_j \left(1 - r^k r_k\right) + 2 r^i r_j + 2 g^{ik} \epsilon_{kjl} r^l \right].$$

The formulas for Rodrigues parameters expressed *via* the rotation matrix are

$$r^i = \epsilon^{ijk} g_{jl} R^l{}_k / (1 + R^k_k) \quad \text{and} \quad r_i = \epsilon_{ilj} g^{jk} R^l{}_k / (1 + R^k_k). \tag{14}$$

Corresponding relationships for $R_i{}^j$ can be easily obtained based on $R_i{}^j = g_{il} R^l{}_k g^{kj}$.

The rotation being a composition of the rotation represented by the matrix $P^i{}_j$ with the rotation represented by $S^i{}_j$ is represented by the product $S^i{}_k P^k_j$. Direct calculation shows that if the matrices $P^i{}_j$ and $S^i{}_j$ correspond *via* the first of equations (14) to the Rodrigues vectors p^i and s^i, respectively, then the matrix $R^i{}_j = S^i{}_k P^k_j$ corresponds to the Rodrigues vector:

$$r^i = \frac{p^i + s^i + g^{ij} \epsilon_{jkl} p^k s^l}{1 - g_{kl} p^k s^l}. \tag{15}$$

Similarly, the composition of rotations represented by p_i and s_i corresponds to

$$r_i = \frac{p_i + s_i + g_{ij} \epsilon^{jkl} p_k s_l}{1 - g^{kl} p_k s_l}. \tag{16}$$

The formulas (15) and (16) for composing rotations in Rodrigues parameterization will be jointly written as[3]

$$\mathbf{r} = \mathbf{p} \circ \mathbf{s}.$$

Clearly, the operation $\circ$ is associative but not commutative. It follows directly from equations (15) and (16) that $\mathbf{0} \circ \mathbf{s} = \mathbf{s} = \mathbf{s} \circ \mathbf{0}$ and $-(\mathbf{p} \circ \mathbf{s}) = (-\mathbf{s}) \circ (-\mathbf{p})$. The rotation represented by $\mathbf{r}$ transforms vector $\mathbf{v}$ to

$$\mathbf{w} = (-\mathbf{r}) \circ \mathbf{v} \circ \mathbf{r}. \tag{17}$$

In this short component-free notation, vector relationships are identical to those used in the Cartesian case, but they are more general in explicit forms which allow for an arbitrary metric tensor and have convenient crystallographic interpretations applicable to arbitrary crystal lattices. If a calculation is carried out using contravariant components, the expression (17) gives directly indices of a lattice direction rotated by $\mathbf{r}$. If a calculation is carried out using covariant components, it gives Miller indices of a rotated lattice plane. For a real ξ, the rotation by $\mathbf{r}$ leaves vectors $\xi\mathbf{r}$ invariant, *i.e.* one has $(-\mathbf{r}) \circ (\xi\mathbf{r}) \circ \mathbf{r} = \xi\mathbf{r}$. Thus, from the crystallographic viewpoint, the rotation represented by $\mathbf{r} = r^i \mathbf{a}_i = r_i \mathbf{a}^i$ leaves the directions $[u\,v\,w] \propto [r^1\,r^2\,r^3]$ and the lattice planes $(h\,k\,l) \propto (r_1\,r_2\,r_3)$ invariant.

In the conventional description of rotations, rotation parameters are frequently ascribed to some loosely defined 'spaces' like, *e.g.*, the 'Rodrigues space' or the 'Euler space' used in texture analysis (Bunge, 1982; Mason & Schuh, 2009). In contrast, the Rodrigues parameters r^i are components of a $\mathbf{0}$-bound vector given in the scaled physical point space, *i.e.* the vector is specified with respect to the same basis as the atomic positions in the crystal unit cell. Some other properties of the Rodrigues parameterization are considered in Appendix *A*.

4. Rotation representations based on overcomplete sets of vectors

Planes and directions of hexagonal and rhombohedral lattices are conveniently described using the standard symmetry-based four-index schemes of Miller–Bravais (Bravais, 1866) and Weber (1922). The formalism of previous sections does not admit redundant crystallographic axes, but it can be generalized so both three- and four-index cases are taken into account.

[3] The difference in the order of factors ($S^i{}_k P^k_j$ *versus* $\mathbf{p} \circ \mathbf{s}$) gives expressions conforming with the convention used for quaternions without the addition of extra minus signs.

Instead of three linearly independent basis vectors, we consider a set (frame) of $M \geq 3$ vectors:

$$\mathbf{a}_\mu = T_\mu^{\ J}\mathbf{e}_J, \quad \mu = 1, 2, \ldots, M.$$

It is assumed here that no two vectors $\mathbf{a}_\mu$ are collinear and the rank of the matrix $T_\mu^{\ J} = \mathbf{a}_\mu \cdot \mathbf{e}^J$ equals 3. Thus, the vectors $\mathbf{a}_\mu$ span the three-dimensional vector space and an arbitrary vector can be expressed as a linear combination of $\mathbf{a}_\mu$. Let the matrix $T_J^{\ \mu}$ be the transposed pseudoinverse[4] of $T_\mu^{\ J}$. With the full rank of $T_\mu^{\ J}$, one has $T_\mu^{\ I} T_J^{\ \mu} = \delta^I_{\ J}$, but the products with summation over capital Latin indices

$$T_\mu^{\ J}\, T_J^{\ \nu} = g_\mu^{\ \nu} \quad \text{and} \quad T_J^{\ \mu}\, T_\nu^{\ J} = g^\mu_{\ \nu}$$

are generally different from the Kronecker delta. These matrices satisfy the symmetry condition $g_\mu^{\ \nu} = g^\nu_{\ \mu}$, they are idempotent ($g_\mu^{\ \kappa} g_\kappa^{\ \nu} = g_\mu^{\ \nu}$ and $g^\mu_{\ \kappa} g^\kappa_{\ \nu} = g^\mu_{\ \nu}$) and $g_\mu^{\ \mu} = 3$. Using $T_J^{\ \mu}$, we define the dual frame,

$$\mathbf{a}^\mu = T_J^{\ \mu}\mathbf{e}^J,$$

and the analogue of the metric tensor,

$$g_{\mu\nu} = \mathbf{a}_\mu \cdot \mathbf{a}_\nu \quad \text{and} \quad g^{\mu\nu} = \mathbf{a}^\mu \cdot \mathbf{a}^\nu.$$

Based on the above definitions, it can be shown that $g^{\mu\nu}$ is the pseudoinverse of $g_{\mu\nu}$. Moreover, one has

$$\begin{aligned} &g^\mu_{\ \nu}\mathbf{a}^\nu = \mathbf{a}^\mu, \quad g_\mu^{\ \nu}\mathbf{a}_\nu = \mathbf{a}_\mu, \\ &g_{\mu\nu}\mathbf{a}^\nu = \mathbf{a}_\mu, \quad g^{\mu\nu}\mathbf{a}_\nu = \mathbf{a}^\mu, \\ &\mathbf{a}_\mu \cdot \mathbf{a}^\nu = g_\mu^{\ \nu} \quad \text{and} \quad g_{\mu\rho}\, g^{\rho\nu} = g_\mu^{\ \nu}. \end{aligned}$$

If $M > 3$, the set of vectors $\mathbf{a}_\mu$ is not a basis, and the decomposition of a given vector into a linear combination of $\mathbf{a}_\mu$ is ambiguous. It is made unique by additional constraints which follow from a particular designation of vector components. With $v^J\mathbf{a}_J = \mathbf{v} = v_J\mathbf{a}^J$, and vector components v^μ and v_μ defined as

$$v^\mu = T_J^{\ \mu}\, v^J \quad \text{and} \quad v_\mu = T_\mu^{\ J} v_J,$$

one has a set of relationships analogous to those given for linearly independent basis vectors:

$$v^\mu \mathbf{a}_\mu = \mathbf{v} = v_\mu \mathbf{a}^\mu, \tag{18}$$

$$v^\mu = \mathbf{v} \cdot \mathbf{a}^\mu, \quad v_\mu = \mathbf{v} \cdot \mathbf{a}_\mu, \tag{19}$$

$$g_{\mu\nu}v^\nu = v_\mu, \quad g^{\mu\nu}v_\nu = v^\mu, \tag{20}$$

and the additional conditions

$$g^\kappa_{\ \nu}v^\nu = v^\kappa, \quad g_\kappa^{\ \nu}v_\nu = v_\kappa. \tag{21}$$

The properties (21) are general in the sense that they are applicable to other tensor quantities, *e.g.* $g_{\mu\kappa}g^\kappa_{\ \nu} = g_{\mu\nu}$, $g^{\mu\kappa}g_\kappa^{\ \nu} = g^{\mu\nu}$, $g_\mu^{\ \nu}T_\nu^{\ J} = T_\mu^{\ J}$ and $g^\mu_{\ \nu}T_J^{\ \nu} = T_J^{\ \mu}$. The relationships (18)–(21) are illustrated in Fig. 2

[4] A reader unfamiliar with generalized matrix inverses is referred to Ben-Israel & Greville (2003).

4.1. Generalized Rodrigues parameters

Proceeding as in §3, with $w^I = R^I_{\ J}v^J$ and $w^\mu = T_I^{\ \mu}w^I = T_I^{\ \mu}R^I_{\ J}T_\nu^{\ J}v^\nu$, one has $w^\mu = R^\mu_{\ \nu}v^\nu$ where $R^\mu_{\ \nu} = T_I^{\ \mu}T_\nu^{\ J}R^I_{\ J}$. Hence, based on equation (8), the rotation by θ about $n^\mu = T_J^{\ \mu}n^J$ is represented by

$$R^\mu_{\ \nu} = g^\mu_{\ \nu}\cos\theta + n^\mu n_\nu(1-\cos\theta) + g^{\mu\kappa}\epsilon_{\kappa\nu\rho}n^\rho \sin\theta, \tag{22}$$

where $\epsilon_{\kappa\mu\nu} = T_\kappa^{\ I}T_\mu^{\ J}T_\nu^{\ K}\epsilon_{IJK}$. The contravariant version of this tensor is given by $\epsilon^{\kappa\mu\nu} = T^\kappa_{\ I}T^\mu_{\ J}T^\nu_{\ K}\epsilon^{IJK} = g^{\kappa\alpha}g^{\mu\beta}g^{\nu\gamma}\epsilon_{\alpha\beta\gamma}$. Both $\epsilon_{\kappa\mu\nu}$ and $\epsilon^{\kappa\mu\nu}$ are antisymmetric in each pair of indices. Moreover, $\epsilon_{\kappa\mu\nu}$ ($\epsilon^{\kappa\mu\nu}$) is equal to the signed volume of the parallelepiped spanned on vectors $\mathbf{a}_\kappa$, $\mathbf{a}_\mu$, $\mathbf{a}_\nu$ ($\mathbf{a}^\kappa$, $\mathbf{a}^\mu$, $\mathbf{a}^\nu$). In particular, if vectors $\mathbf{a}_\kappa, \mathbf{a}_\mu, \mathbf{a}_\nu$ are linearly dependent, so are $\mathbf{a}^\kappa$, $\mathbf{a}^\mu$, $\mathbf{a}^\nu$, and one has $\epsilon_{\kappa\mu\nu} = 0 = \epsilon^{\kappa\mu\nu}$. The product of $\epsilon_{\mu\nu\kappa}$ and $\epsilon^{\mu\nu\kappa}$ has some properties analogous to those of the permutation symbol; especially useful are $\epsilon^{\mu\nu\kappa}\epsilon_{\sigma\rho\kappa} = g^\mu_{\ \sigma}g^\nu_{\ \rho} - g^\mu_{\ \rho}g^\nu_{\ \sigma}$ and $\epsilon^{\mu\nu\kappa}\epsilon_{\sigma\nu\kappa} = 2g^\mu_{\ \sigma}$.

Analogously to the 3×3 matrices $R^i_{\ j}$ of §2, the $M \times M$ matrices $R^\mu_{\ \nu}$ of equation (22) constitute a faithful representation of proper rotations. If $M > 3$, this is a singular-matrix representation. The null rotation is represented by $R^\mu_{\ \nu} = g^\mu_{\ \nu}$. Like in the previous section, one can define $R_\mu^{\ \nu} = g_{\mu\kappa}R^\kappa_{\ \sigma}g^{\sigma\nu}$. The matrix $R_\mu^{\ \nu}$ is the transposed pseudoinverse of $R^\mu_{\ \nu}$. The matrices $R^\mu_{\ \nu}$ and $R_\mu^{\ \nu}$ satisfy conditions analogous to equation (11) with Latin indices replaced by Greek indices: $g_{\kappa\rho}R^\kappa_{\ \mu}R^\rho_{\ \nu} = g_{\mu\nu}$ and $g^{\kappa\rho}R_\kappa^{\ \mu}R_\rho^{\ \nu} = g^{\mu\nu}$. Moreover, one has $g^\mu_{\ \kappa}R^\kappa_{\ \nu} = R^\mu_{\ \nu} = R^\mu_{\ \kappa}g^\kappa_{\ \nu}$ and corresponding relationships for $R_\mu^{\ \nu}$.

Similarly to equation (13), let the generalized Rodrigues parameters be defined as

$$r^\mu = n^\mu \tan(\theta/2) \quad \text{and} \quad r_\mu = n_\mu \tan(\theta/2).$$

They satisfy conditions (20)–(21) and $r^\mu r_\mu = \tan^2(\theta/2)$. The null rotation corresponds to the parameters $r^\mu = 0 = r_\mu$. Moreover, the rotation matrix (22) is related to the generalized Rodrigues parameters by

$$R^\mu_{\ \nu} = \frac{1}{1 + r^\kappa r_\kappa}\left[g^\mu_{\ \nu}(1 - r^\kappa r_\kappa) + 2r^\mu r_\nu + 2g^{\mu\kappa}\epsilon_{\kappa\nu\rho}r^\rho\right].$$

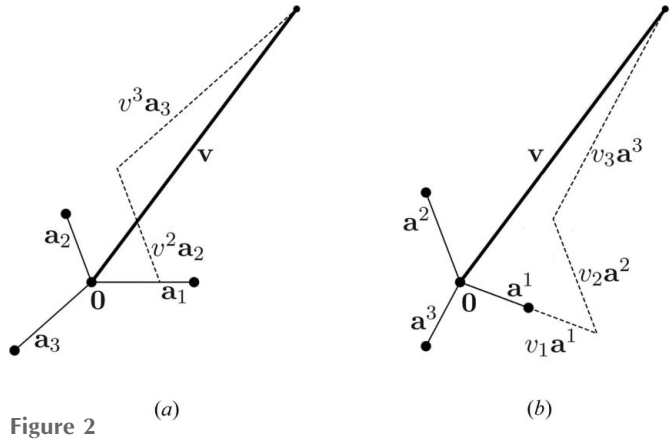


Figure 2
Schematic two-dimensional illustration of decompositions $v^\mu\mathbf{a}_\mu$ and $v_\mu\mathbf{a}^\mu$ ($\mu = 1, 2, 3$) of vector $\mathbf{v}$. Vectors $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{v}$ are the same as in Fig. 1. The set of vectors $\mathbf{a}^\mu$ in (*b*) is dual to $\mathbf{a}_\mu$ shown in (*a*) in the sense described in §4. The coefficients v^μ and v_μ satisfy the relationships (21).

The formulas for Rodrigues parameters r^μ and r_μ expressed *via* the elements $R^\mu_{\ \nu}$ of the rotation matrix are analogous to equation (14):

$$r^\mu = \epsilon^{\mu\nu\kappa}\, g_{\nu\rho}\, R^\rho_{\ \kappa}/(1 + R^\sigma_{\ \sigma}), \quad r_\mu = \epsilon_{\mu\rho\nu}\, g^{\nu\kappa}\, R^\rho_{\ \kappa}/(1 + R^\sigma_{\ \sigma}). \tag{23}$$

The formulas for composition of rotations are analogous to equations (15) and (16):

$$r^\mu = \frac{p^\mu + s^\mu + g^{\mu\nu}\,\epsilon_{\nu\kappa\rho}\, p^\kappa\, s^\rho}{1 - g_{\alpha\beta}\, p^\alpha\, s^\beta}, \quad r_\mu = \frac{p_\mu + s_\mu + g_{\mu\nu}\,\epsilon^{\nu\kappa\rho}\, p_\kappa\, s_\rho}{1 - g^{\alpha\beta}\, p_\alpha\, s_\beta}. \tag{24}$$

With the last two expressions written jointly as $\mathbf{r} = \mathbf{p} \circ \mathbf{s}$, the brief formula for the vector $\mathbf{w}$ resulting from the rotation of $\mathbf{v}$ by $\mathbf{r}$ is identical to equation (17): $\mathbf{w} = (-\mathbf{r}) \circ \mathbf{v} \circ \mathbf{r}$.

4.2. Vectors $\mathbf{a}_\mu$ and a lattice

The formalism relying on M vectors $\mathbf{a}_\mu$ was introduced without referring to a lattice. Not every set of vectors $\mathbf{a}_\mu$ naturally induces a lattice; for some sets, integer combinations of vectors $\mathbf{a}_\mu$ can be arbitrarily close to each other. Even if the latter is not the case, the relationship between the vectors $\mathbf{a}_\mu$ and the lattice is not unique and needs to be explicitly specified.

Assuming a *canonical* case, when all integer combinations of vectors $\mathbf{a}_\mu$ constitute a lattice, what are the requirements on $\mathbf{a}_\mu$ for this lattice to be based on a certain three linearly independent vectors $\mathbf{a}_i$? Each $\mathbf{a}_\mu$ must be an integer combination of vectors $\mathbf{a}_i$, *i.e.* $\mathbf{a}_\mu = T_\mu^{\ i}\mathbf{a}_i$, with $T_\mu^{\ i} = \mathbf{a}_\mu \cdot \mathbf{a}^i$ being integers. This implies that an arbitrary integer combination of the vectors $\mathbf{a}_\mu$ can be expressed as an integer combination of the vectors $\mathbf{a}_i$. On the other hand, also the vector $k^i\mathbf{a}_i$ with integer k^i must be expressible as an integer combination of the vectors $\mathbf{a}_\mu$. Thus, the system of three linear Diophantine equations $\sum_\mu T_\mu^{\ i} x^{(\mu)} = k^i$ must be solvable with respect to integer $x^{(\mu)}$ for all k^i.[5] This means that all three elementary divisors of the integer matrix $T_\mu^{\ i}$ must be equal to 1. Moreover, let $T_i^{\ \mu}$ be the transposed pseudoinverse of $T_\mu^{\ i}$. With integer $T_\mu^{\ i}$, the matrix $T_i^{\ \mu}$ is rational. Since $T_\mu^{\ i}\, T^\nu_{\ i} = g_\mu^{\ \nu}$, for $\mathbf{a}_\mu$ to determine a lattice in the above sense, the matrix $g_\mu^{\ \nu}$ must be rational. With the full rank of $T_\mu^{\ i}$, there occurs $T_\mu^{\ i} T^\mu_{\ j} = \delta^i_{\ j}$ and, hence, $\mathbf{a}_i = \mathbf{a}_\mu T_i^{\ \mu}$. Thus, some lattice vectors with integer components k^i in the basis $\mathbf{a}_i$ may have rational (*i.e.* not necessarily integer) components k^μ when expressed as $k^\mu\mathbf{a}_\mu$. [By definition of the canonical case, these vectors are linear combinations of $\mathbf{a}_\mu$ with integer coefficients, but such coefficients may not satisfy conditions (21).]

Other consequences of assuming the canonical scheme concern the $\mathbf{a}^i$-based reciprocal lattice. It is easy to see that the vector $\mathbf{a}^\mu = g^{\mu\nu}\mathbf{a}_\nu$ may not necessarily be a vector of the reciprocal lattice (see Fig. 3). The key observation is that the reciprocal lattice based on vectors $\mathbf{a}^i$ is identical with the lattice $k_\mu\mathbf{a}^\mu$, where k_μ are integer vector components satisfying $k_\mu = g_\mu^{\ \nu} k_\nu$. More explicitly, there occurs:

(i) With integer k_i, the vector $k_i\mathbf{a}^i$ of the reciprocal lattice can be represented as $k_\mu\mathbf{a}^\mu$ with integer components k_μ satisfying $k_\mu = g_\mu^{\ \nu} k_\nu$.

(ii) If k_μ are integers satisfying $k_\mu = g_\mu^{\ \nu} k_\nu$ then $k_\mu\mathbf{a}^\mu$ is a vector of the lattice based on $\mathbf{a}^i$, *i.e.* it is equal to $k_i\mathbf{a}^i$ with integer k_i.

The first part follows immediately. The second one can be proved using the Smith normal form of the matrix $T_\mu^{\ i}$, by taking into account that its elementary divisors are all equal to 1.

Summarizing, in the canonical scheme, the direct lattice based on vectors $\mathbf{a}_i$ is identical to the lattice constructed of all integer combinations of $\mathbf{a}_\mu$, and the reciprocal lattice based on

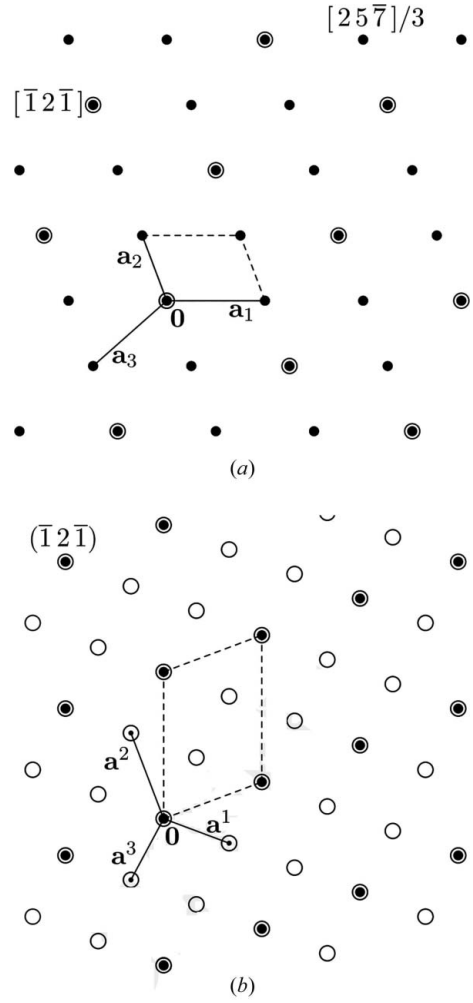


Figure 3
Schematic two-dimensional illustration of canonical configuration for the vectors $\mathbf{a}_\mu$ shown in Fig. 2. In both (*a*) and (*b*), the actual lattices are depicted using discs, and their primitive cells are sketched using dashed lines. (*a*) Direct lattice comprised of all integer combinations of $\mathbf{a}_\mu$. The particular nodes $k^\mu\mathbf{a}_\mu$ with integer k^μ satisfying $k^\mu = g^\mu_{\ \nu} k^\nu$ are marked by circles. (*b*) Reciprocal lattice built of the combinations $l_\mu\mathbf{a}^\mu$ with integer l_μ satisfying $l_\mu = g_\mu^{\ \nu} l_\nu$. Circles mark points corresponding to all integer combinations of $\mathbf{a}^\mu$. [In both (*a*) and (*b*), the circles indicate nodes of lattices constructed using the 'dual-to-canonical' scheme.]

[5] A different indexing is used to indicate that $x^{(\mu)}$ generally do not satisfy the conditions (21).

vectors $\mathbf{a}^i$ is reproduced by linear combinations of $\mathbf{a}^\mu$ with integer coefficients satisfying conditions (21).

Clearly, one may consider another natural relationship between the set of vectors $\mathbf{a}_\mu$ and a lattice which is in a sense dual to the canonical scheme, with the roles of lattices reversed: the direct lattice based on vectors $\mathbf{a}_i$ is identical to the linear combinations of $\mathbf{a}_\mu$ with integer coefficients satisfying the conditions (21), and the reciprocal lattice based on vectors $\mathbf{a}^i$ overlaps with linear combinations of $\mathbf{a}^\mu$ with arbitrary integer coefficients. It is self-evident that if $M = 3$, the canonical scheme and its dual lead to the same lattices.

With the canonical scheme, the generalized Rodrigues parameters of rotations have the simple crystallographic interpretation: if a calculation is carried out using contravariant (covariant) components, it gives indices of a rotated lattice direction (plane). The rotation represented by $\mathbf{r} = r^\mu \mathbf{a}_\mu = r_\mu \mathbf{a}^\mu$ leaves the directions $[u\, v\, \ldots\, w] \propto [r^1\, r^2\, \ldots\, r^M]$ and the lattice planes $(h\, k\, \ldots\, l) \propto (r_1\, r_2\, \ldots\, r_M)$ invariant. As a concrete example, the 'symmetric basis' of the three-dimensional hexagonal lattice is considered in more detail in Appendix *B*.

5. Final remarks

Summarizing, the conventional definition of vectorial Rodrigues parameterization of rotations was extended to non-Cartesian reference frames. The parameters are defined as co- or contravariant components of a vector given in the scaled physical space, *i.e.* the vector specified with respect to the same basis as atomic positions in a unit cell. In its most general form, the construction allows for redundant crystallographic axes. When explicitly written down, the formalism is relatively simple and conforms with intuition. Some formulas can be derived 'automatically' based on the covariance principle by obeying the rules of the summation convention. The expressions for rotation composition and the relationship to the rotation matrix are similar to those used in the Cartesian case, but they are more general: calculations can be performed for an arbitrary metric tensor of the crystal lattice. The Rodrigues parameterization of rotations in non-orthogonal coordinate systems is in a sense more natural than the matrix parameterization because vectorial parameters are directly linked to indices of rotation-invariant lattice directions and invariant lattice planes.

This article focuses on Rodrigues parameters because of their properties and some applications. However, there are a number of other interesting vectorial parameterizations $f(\theta)\,\mathbf{n}$, where f is monotonic in the domain $0 \le \theta \le \pi$; see, *e.g.*, Bauchau & Trainelli (2003) and Morawiec (2004). Parts of the above-described approach can be adapted to such parameterizations in general. The case with $f(\theta) = \sin(\theta/2)$ corresponds to the vector part of a quaternion. The results obtained for Rodrigues parameters can be easily transcribed using quaternions. For completeness, the link between these two approaches is outlined in Appendix *C*.

One may ask about extensibility of the above formalism to spaces of dimension higher than three. In such spaces, there are no analogues of vectorial parameterizations of rotations as the number of independent vector components is too small to contain all rotation parameters. The aspects not related to the vectorial parameterizations, in particular those concerning redundant axes, can be easily generalized to space dimensions other than three.

The subject of having a redundant axis was considered in the crystallographic context by Nicholas & Segall (1970), but our approach is simpler and more general. The formalism described above can also be compared to that with the three-dimensional physical space embedded in an abstract space of higher dimension M (with $g_\mu{}^\nu$ and $g^\mu{}_\nu$ as projection matrices). Such a description of Miller–Bravais and Weber indexing was given in Frank (1965).[6] In our scheme, all vectors and tensors are limited to the physical space, and no explicit references to the abstract space were made. Technically, the formalism with redundant axes belongs to the finite frame theory – the theory of non-orthogonal overcomplete sets of vectors in finite-dimensional inner-product spaces; see, *e.g.*, Casazza *et al.* (2013) and references therein. We did not refer to the frame theory in order to keep the article self-contained, and to use the nomenclature and notation close to that of the *International Tables for Crystallography* (Shmueli, 2006; Sands, 2006).

The choice of reference axes in the hexagonal and rhombohedral lattices is imposed by lattice symmetry, but one may have other motives for having redundant axes. They can be used to facilitate handling of arbitrary symmetries, *e.g.* symmetries of processes. The formalism is very flexible: the restrictions put on the choice of the vectors $\mathbf{a}_\mu$ are weak, the array of these vectors can be highly redundant, and the vectors can fit various geometries. For example, in the description of orientation changes caused by plastic deformation of a crystal by dislocation slip or twinning, the vectors $\mathbf{a}_\mu$ can be chosen based on characteristic directions and/or planes of slip or twinning systems.

This article was written with crystallographic applications in mind, but the methods described here can be used for characterizing rotations or orientations of arbitrary rigid bodies. In particular, the formalism allowing for redundant axes can be useful to account for symmetries or to improve resilience to perturbation of input data.

APPENDIX *A*
Some special properties of Rodrigues parameterization

Two aspects are worth considering because of their applications to crystallographic texture analysis and to research on grain boundaries in polycrystalline materials. Both concern distances in the manifold of rotations. Finite distances

[6] A similar method is used for depiction of quasicrystals with three-dimensional quasilattices considered to be projections of subsets of lattices of higher dimensions (see, *e.g.*, Janssen, 2002).

between orientations are used for determination of fundamental regions in the manifold.[7] For calculation of rotation rate fields, one needs infinitesimally small rotations and the metric tensor in the manifold of rotations (see, *e.g.*, Morawiec, 1990). This tensor also governs geodesics, which in the Rodrigues parameterization have the form of straight lines or arcs of **0**-centred great circles of infinite radius (Morawiec, 2004).

A1. Finite distance between rotations

Since the Rodrigues parameters defined by equation (13) are vector components, distance-based properties observed in the Cartesian case, when expressed using the general frame-independent notation, are held in non-Cartesian systems. The angular distance ω between rotations represented by Rodrigues vectors $\mathbf{p}$ and $\mathbf{r}$ is given by $\omega = 2\arctan|(-\mathbf{p})\circ\mathbf{r}|$. Points equidistant to distinct $\mathbf{r}$ and $\mathbf{p}$ constitute two planes in the Rodrigues 'space' or the **0**-centred sphere of infinite radius. In particular, points equidistant to non-zero finite $\mathbf{r}$ and $-\mathbf{r}$ constitute the plane perpendicular to $\mathbf{r}$ through **0** and the infinite sphere. Points equidistant to **0** and $\mathbf{r}$ constitute two parallel planes of the form $\mathbf{r}_\parallel + \mathbf{r}_\perp$, where $\mathbf{r}_\parallel = \mathbf{r}/[1 \pm (1+|\mathbf{r}|^2)^{1/2}]$ collinear with $\mathbf{r}$ satisfies $\mathbf{r}_\parallel \circ \mathbf{r}_\parallel = \mathbf{r}$ and $\mathbf{r}_\perp$ is an arbitrary vector perpendicular to $\mathbf{r}$.

A2. Local metric

With high-order terms omitted, the squared distance between $\mathbf{r}$ and $\mathbf{r}+\mathrm{d}\mathbf{r}$ when expressed in contravariant components r^i is $\mathrm{d}\omega^2 = 4|(-\mathbf{r})\circ(\mathbf{r}+\mathrm{d}\mathbf{r})|^2 = 4G_{ij}\mathrm{d}r^i\mathrm{d}r^j$, where $G_{ij} = \beta^{-2}(\beta g_{ij} - g_{ik}r^k g_{jl}r^l)$ and $\beta = \beta(r^i) = 1 + g_{ij}r^i r^j$. The square root of the determinant of the metric tensor G_{ij} is proportional to the invariant measure $\mathrm{d}\Omega$ in the manifold of rotations. It is given by $\mathrm{d}\Omega = (\pi\beta)^{-2}|V|\,\mathrm{d}r^1\,\mathrm{d}r^2\,\mathrm{d}r^3$, where the normalization is such that the integration over the whole manifold leads to $\int \mathrm{d}\Omega = 1$. These general formulas for $\mathrm{d}\omega^2$ and $\mathrm{d}\Omega$ comprise corresponding expressions applicable in the Cartesian case with $g_{ij} = \delta_{ij}$ (see, *e.g.*, Morawiec, 2004). [The distance $|(-\mathbf{r})\circ(\mathbf{r}+\mathrm{d}\mathbf{r})|$ can also be expressed using the changes of the covariant components r_i as independent variables, and the procedure and results are analogous to those used for the contravariant components. In this case, however, the increments $\mathrm{d}r_i$ covariant in the physical space are contravariant as increments in the manifold of rotations parameterized by r_i.]

APPENDIX *B*
Data for a 'symmetric basis' of a hexagonal lattice

Let $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$, $\mathbf{c}$, $a = |\mathbf{a}_i|$ and $c = |\mathbf{c}|$ be conventional vectors and parameters of a hexagonal lattice. With the lattice scaled by $1/a$, the vectors $\mathbf{a}_4$ and $\mathbf{e}_3$ along the principal axis $\mathbf{c}$, $\mathbf{a}_1 = \mathbf{e}_1$, and $\mathbf{e}_2 \cdot \mathbf{a}_2 > 0$, one has

$$[T_\mu^{\ J}] = \begin{bmatrix} A/2 & 0 \\ 0 & c/a \end{bmatrix},\quad [T^\mu_{\ J}] = \begin{bmatrix} A/3 & 0 \\ 0 & a/c \end{bmatrix},$$

$$[g_{\mu\nu}] = \begin{bmatrix} B/2 & 0 \\ 0 & (c/a)^2 \end{bmatrix},\quad [g_\mu^{\ \nu}] = \begin{bmatrix} B/3 & 0 \\ 0 & 1 \end{bmatrix},$$

$$[g^{\mu\nu}] = \begin{bmatrix} 2B/9 & 0 \\ 0 & (a/c)^2 \end{bmatrix},$$

$$\text{where } A = \begin{bmatrix} 2 & 0 \\ -1 & 3^{1/2} \\ -1 & -3^{1/2} \end{bmatrix} \text{ and } B = \begin{bmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{bmatrix}$$

(*cf.* Mackay, 1977). With the above $g_\mu^{\ \nu}$, the conditions (21) take the explicit form $v^1 + v^2 + v^3 = 0 = v_1 + v_2 + v_3$. The entries of $\epsilon_{\kappa\mu\nu}$ divided by $V = 3^{1/2}c/(2a)$ are equal to 0 or ± 1. Similarly, $\epsilon^{\kappa\mu\nu}$ multiplied by $3V$ are 0 or ± 1. The entries of $\epsilon_{\kappa\mu\nu}$ and $\epsilon^{\kappa\mu\nu}$ are zero if two indices are equal or if $(\kappa\mu\nu)$ is a permutation of (123). If all indices are different and $(\kappa\mu\nu)$ is a permutation of $(ij4)$, then $\epsilon_{\kappa\mu\nu}/V$ and $3V\epsilon^{\kappa\mu\nu}$ are equal to ε_{kmn}, where (kmn) is the same permutation of (ijl) with $l \le 3$ such that $i \ne l \ne j$.

The hexagonal lattice is linked to the vectors $\mathbf{a}_\mu$ *via* the canonical scheme. Weber indices $[u\,v\,t\,w]$ of lattice directions (Weber, 1922) and Miller–Bravais indices $(h\,k\,i\,l)$ of lattice planes (Bravais, 1866) are, respectively, contra- and co-covariant components of vectors. The direct lattice based on three vectors $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_4$, *i.e.* the integer combinations $k\mathbf{a}_1 + l\mathbf{a}_2 + m\mathbf{a}_4$, is represented by the combinations $u^\mu\mathbf{a}_\mu$ of all four vectors $\mathbf{a}_\mu$ with the coefficients

$$\left[u^1\ u^2\ u^3\ u^4\right] = [u\,v\,t\,w] = [2k-l\ \ 2l-k\ \ -k-l\ \ 3m]/3$$

which satisfy $u^\mu = g^\mu_{\ \nu}u^\nu$, and not all u^μ are integers (Weber, 1922). To get the complete lattice reciprocal to that based on $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_4$ using four vectors $\mathbf{a}^\mu$ one needs all nodes $h_\mu\mathbf{a}^\mu$, where $(h_1\ h_2\ h_3\ h_4) = (h\,k\,i\,l)$ are integers and satisfy $h_\mu = g_\mu^{\ \nu}h_\nu$ (Bravais, 1866). The formula for rotating a vector gives directly the Weber indices of a rotated lattice direction if the calculation is carried out in contravariant vector components, and it gives Miller–Bravais indices of a rotated lattice plane if the calculation is carried out in covariant components. The rotation represented by $\mathbf{r} = r^\mu\mathbf{a}_\mu = r_\mu\mathbf{a}^\mu$ leaves the directions $[u\,v\,t\,w] \propto [r^1\,r^2\,r^3\,r^4]$ and the lattice planes $(h\,k\,i\,l) \propto (r_1\,r_2\,r_3\,r_4)$ invariant.

APPENDIX *C*
Quaternions

Instead of the M-component Rodrigues vector of §4, one can use $M+1$ finite numbers (q^0, q^μ) not all simultaneously zero such that the ratio q^μ/q^0 (or its limit, if $q^0 = 0$) is equal to the μth contravariant component r^μ of the Rodrigues vector. The extra parameter helps to account for half-turns. The multi-

[7] Such regions are used when some orientations are equivalent to others due to crystal point symmetries. They can be established as Voronoi cells around points representing symmetry operations. The cells are bounded by points (of the rotation manifold) equidistant to nearest points representing symmetry operations (see, *e.g.*, Morawiec, 1996, 1997).

plication rule for such $(M+1)$-component entities follows from equation (24) for composition of Rodrigues vectors:

$$q^0 = x^0 y^0 - g_{\mu\nu}\, x^\mu\, y^\nu, \quad q^\mu = x^\mu y^0 + y^\mu x^0 + g^{\mu\nu}\, \epsilon_{\nu\kappa\sigma}\, x^\kappa\, y^\sigma, \tag{25}$$

where (x^0, x^μ) and (y^0, y^μ) are related to p^μ and s^μ, respectively, in the same way as (q^0, q^μ) to r^μ. If $M = 3$ and the reference system is Cartesian, equation (25) is the ordinary formula for quaternion multiplication and (q^0, q^μ) are standard quaternion components. Therefore, the designation 'quaternion' will be used below for (q^0, q^μ) even if the number $M+1$ exceeds 4. By analogy, one can define the covariant version of the quaternion (q_0, q_μ) with q_μ/q_0 equal to the μth covariant component of the Rodrigues vector. The co- and contravariant components are linked by $q_\mu = g_{\mu\nu} q^\nu$, $q^\mu = g^{\mu\nu} q_\nu$ and $q_0 = q^0$. Moreover, there occurs $q_\mu = g_\mu^{\ \nu}\, q_\nu$ and $q^\mu = g^\mu_{\ \nu}\, q^\nu$. For brevity, the entity with components (q^0, q^μ) and (q_0, q_μ) will be denoted by $\mathbf{q}$, and the product given by equation (25) and an analogous formula for covariant components will be jointly written as $\mathbf{q} = \mathbf{x} \circ \mathbf{y}$. The explicit component-based composition relationships (25) are specific to the considered case allowing for non-Cartesian reference frames and redundant crystallographic axes, but general aspects of quaternion algebra remain unchanged: there is a many-to-one morphism between non-zero quaternions and proper rotations. The neutral element $\mathbf{e} = (1, \mathbf{0})$ and other non-zero scalar (*i.e.* with $q^\mu = 0 = q_\mu$) quaternions represent the null rotation. The quaternion $\mathbf{q}^{-1}$ inverse to non-zero $\mathbf{q}$ (such that $\mathbf{q}^{-1} \circ \mathbf{q} = \mathbf{e} = \mathbf{q} \circ \mathbf{q}^{-1}$) can be calculated using $\mathbf{q}^{-1} = \mathbf{q}^*/|\mathbf{q}|^2$, where $|\mathbf{q}|^2 = q_0 q^0 + q_\mu q^\mu$ denotes the squared magnitude of $\mathbf{q}$, and $\mathbf{q}^* = (q^0, -q^\mu)$ is conjugate to $\mathbf{q} = (q^0, q^\mu)$. Inverse quaternions represent inverse rotations. As in the conventional case, the rotation $\mathbf{q}$ of a vector $\mathbf{v}$ is performed *via* $\mathbf{w}' = \mathbf{q}^{-1} \circ \mathbf{v}' \circ \mathbf{q}$, where $\mathbf{v}'$ and $\mathbf{w}'$ in this formula denote the quaternions obtained from $\mathbf{v}$ and $\mathbf{w}$ by adding a zero scalar component. The rotation matrix corresponding to $\mathbf{q}$ is given by

$$R^\mu_{\ \nu} = |\mathbf{q}|^{-2}\big[g^\mu_{\ \nu}\,(q^0\, q_0 - q^\kappa\, q_\kappa) + 2q^\mu\, q_\nu + 2g^{\mu\kappa}\, \epsilon_{\kappa\nu\sigma}\, q^\sigma q_0\big].$$

For the known rotation matrix $R^\mu_{\ \nu}$, the quaternion is

$$(q^0,\ q^\mu) \propto \pm\big(1 + R^\kappa_{\ \kappa},\ \epsilon^{\mu\nu\kappa}\, g_{\nu\sigma}\, R^\sigma_{\ \kappa}\big);$$

an analogous expression for covariant components follows directly from equation (23). It is easy to see that the same rotation is represented by each element of the family of quaternions $\xi\mathbf{q}$, where ξ is an arbitrary non-zero real number. As in the conventional case, the families can be constrained, and rotations can be represented by unimodular (unit) quaternions such that $|\mathbf{q}| = 1$. The product of two unit quaternions is a unit quaternion. Two unit quaternions $\mathbf{q}$ and $-\mathbf{q}$ represent the same rotation. It follows from $|\mathbf{q}| = q_0 q^0[1 + \tan^2(\theta/2)] = 1$ that $(q^0, q^\mu) = \pm[\cos(\theta/2),\ n^\mu \sin(\theta/2)]$.

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