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Parameterization of rotations in reference frames with redundant crystallographic axes

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Abstract. Parameterizations of rotations in three-dimensional space are fundamental for description of crystallographic textures. Such parameterizations (e.g., Rodrigues parameters) are usually specified using orthonormal coordinate systems, whereas bases of crystal lattices are generally non-orthogonal. In the case of crystals with hexagonal or rhombohedral lattices, the reference frames involve redundant crystallographic axes, and hence a question arises about feasibility of the generalization of the rotation parameterizations to such frames. The definition of Rodrigues parameters can be extended so they are directly linked to non-Cartesian bases of crystal lattices. The new Rodrigues parameters are contra- or covariant components of vectors specified with respect to exactly the same lattice basis as atomic positions in a unit cell. The generalized formalism allows for using redundant crystallographic axes. Also the orientation matrices can be represented in such frames. The Rodrigues parameterization in non-Cartesian coordinate frames is convenient for crystallographic applications because the generalized parameters are directly related to indices of rotation-invariant lattice directions and to Miller indices of rotation-invariant lattice planes. In the case of the hexagonal and rhombohedral lattices, the frames with redundant axes are used to account for lattice symmetry, but one may apply such frames for other reasons. They can be convenient for handling arbitrary symmetries, in particular symmetries arising in description of some phenomena or symmetries of physical processes. The practicality of frames is illustrated by an alternative description of body-centered lattices, a formula for lattice rotation in deformation by slip, and a new interpretation of indexing of single crystal diffraction patterns.

1. Introduction

Texture analysis relies heavily on the notions of reference frames and rotations in three-dimensional space [1, 2]. The usual approach is to represent proper rotations by special orthogonal matrices. Also rotation vectors are a commonly used representation. In particular, the so-called Rodrigues vector is convenient in analysis of crystal misorientations.

Special orthogonal matrices and Rodrigues vectors are defined in reference to Cartesian systems [1, 3]. On the other hand, bases of crystalline lattices are often non-orthogonal. Rotation matrix formalism in non-orthogonal bases has been used in crystallography for a long time; cf. [4]. The issue of referring Rodrigues vectors directly to oblique frames was considered only recently in [5]. The latter paper describes a more general formalism which allows to deal with rotations not only in arbitrary lattice bases comprised of linearly independent vectors but also in frames with redundant crystallographic axes. This formalism encompasses the description of rotations in the hexagonal and rhombohedral cases with four axes of the frame. It can be

applied to any finite number (≥ 3) of axes, and it can be seen as a generalization of the classic schemes of indexing of lattice planes and directions. The concept of indexing in systems with redundant crystallographic axes has been considered before [6, 7, 8]. For complete understanding of indexing in systems with redundant axes, one needs to establish a link between the frame and its dual on one side, and the lattice and its reciprocal on the other, and this issue has been clarified in [5]. The formalism relies on the equivalence between the indices of nodes of direct and reciprocal lattices and contra- and co-variant vector coordinates [4, 9]. In particular, the generalized Rodrigues parameters are defined as contra- or co-variant components of vectors in the physical space of the crystal.

The paper illustrates some simple but quite different applications of the frames: these are a symmetric description of body-centered lattices, a new formula for lattice rotation in deformation by slip, and an original interpretation of ab initio indexing of single crystal diffraction patterns. The nomenclature and notation of the paper are close to those of [5] and some chapters of the International Tables for Crystallography [4, 9]. The summation convention is assumed, i.e., there is a summation over each index which appears in a term twice, as a subscript and a superscript. At the outset, the concepts of [5] are briefly reformulated so one can easily grasp the essence of the formalism.

2. Rotations in three dimensions and frames

Rotation about $\mathbf{n}$ by the angle θ is frequently represented by the matrix

$$\mathbf{R} = \mathbf{g}\,\cos\theta + \mathbf{n}\otimes\mathbf{n}\,(1-\cos\theta) + \boldsymbol{\epsilon}\cdot\mathbf{n}\,\sin\theta \tag{1}$$

or Rodrigues vector $\mathbf{r} = \mathbf{n}\tan(\theta/2)$. Composition of rotations represented by matrices $\mathbf{S}$ and $\mathbf{P}$ is represented by matrix product of $\mathbf{P}$ and $\mathbf{S}$. Composition of rotations parametrized by Rodrigues vectors $\mathbf{p}$ and $\mathbf{s}$ is given by $\mathbf{p}\circ\mathbf{s} = (\mathbf{p}+\mathbf{s}+\mathbf{p}\times\mathbf{s})/(1-\mathbf{p}\cdot\mathbf{s})$. The vector $\mathbf{w}$ resulting form the rotation of $\mathbf{v}$ by a rotation represented by matrix $\mathbf{R}$ and Rodrigues vector $\mathbf{r}$ is $\mathbf{w} = \mathbf{R}\cdot\mathbf{v} = (-\mathbf{r})\circ\mathbf{v}\circ\mathbf{r}$. These two representations are linked by

$$\mathbf{R} = \frac{1}{1+\mathbf{r}\cdot\mathbf{r}}\,(\mathbf{g}\,(1-\mathbf{r}\cdot\mathbf{r}) + 2\,\mathbf{r}\otimes\mathbf{r} + 2\,\boldsymbol{\epsilon}\cdot\mathbf{r}) \quad \text{and} \quad \mathbf{r} = \boldsymbol{\epsilon} : \mathbf{R}/(1+\operatorname{tr}\mathbf{R})\ .$$

For small angle rotations $\mathbf{R}\approx\mathbf{g}+\boldsymbol{\Omega}$, where $\boldsymbol{\Omega}$ is linked to Rodrigues vector via $\boldsymbol{\Omega} = 2\,\boldsymbol{\epsilon}\cdot\mathbf{r}$ and $\mathbf{r} = \boldsymbol{\epsilon} : \boldsymbol{\Omega}/4$. The formulas listed above are well known. They are usually interpreted in Cartesian reference systems with $\mathbf{g}$ being the identity matrix and $\boldsymbol{\epsilon}$ representing the permutation symbol. It is interesting, however, that they can also be considered in more general terms. First, the vectors and tensors can be given in rectilinear non-orthonormal systems, in particular, in a basis of a trigonal crystal lattice. Second, the above expressions can be applied using frames with redundant axes. In particular, they are valid in the conventional four-axis frames used for describing hexagonal and rhombohedral crystals. Clearly, this general approach requires a proper interpretation of $\mathbf{g}$ and $\boldsymbol{\epsilon}$.

2.1. Overcomplete basis sets

For our purpose, a frame is a set of $M \geq 3$ non-coplanar vectors $\mathbf{a}_\mu$, where $\mu = 1, 2, ..., M$, and no two vectors are collinear. The metric tensor is defined as

$$g_{\mu\nu} = \mathbf{a}_\mu \cdot \mathbf{a}_\nu\ .$$

The rank of the corresponding matrix is 3. Let $g^{\mu\nu}$ be the components of the Moore-Penrose pseudoinverse [10] of the matrix $[g_{\mu\nu}]$. The vectors

$$\mathbf{a}^\mu = g^{\mu\nu}\mathbf{a}_\nu$$

constitute the frame canonically dual to $\mathbf{a}_\mu$. They satisfy the relationships $\mathbf{a}^\mu \cdot \mathbf{a}^\nu = g^{\mu\nu}$ and $g_{\mu\nu}\mathbf{a}^\nu = \mathbf{a}_\mu$. With $g_\mu{}^\nu = \mathbf{a}_\mu \cdot \mathbf{a}^\nu = g_{\mu\rho}\, g^{\rho\nu}$, one has $g_\mu{}^\nu = g^\nu{}_\mu$. The idempotent matrix corresponding to $g_\mu{}^\nu$ is equal to its pseudoinverse, its trace $g_\mu{}^\mu$ equals 3, and there occurs $g_{\mu\kappa}g^\kappa{}_\nu = g_{\mu\nu}$ and $g^{\mu\kappa}g_\kappa{}^\nu = g^{\mu\nu}$. Moreover, one has

$$g^\mu{}_\nu \mathbf{a}^\nu = \mathbf{a}^\mu \ , \quad g_\mu{}^\nu \mathbf{a}_\nu = \mathbf{a}_\mu \ . \tag{2}$$

With $M > 3$, the decomposition of a given vector, say $\mathbf{v}$, into linear combinations

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

of $\mathbf{a}_\mu$ or $\mathbf{a}^\mu$ is ambiguous. It is made unique by imposing the constraints

$$g^\kappa{}_\nu v^\nu = v^\kappa \ , \quad g_\kappa{}^\nu v_\nu = v_\kappa \ \ . \tag{3}$$

With these conditions satisfied, one has

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

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

This formalism belongs to the well developed theory of frames; see, e.g., [11] and references therein. The principal applications of frames are in signal and image processing.

The frames of particular type described above (non-orthogonal overcomplete sets of vectors in finite-dimensional inner-product space) can also be applied in crystallography. The redundancy of frames has some advantages. First, frames improve computational robustness to random errors as information is spread over a larger number of vector components. More importantly, the redundancy of frames provides some flexibility; for instance, a frame can match a given symmetry, as it is in the case of hexagonal and rhombohedral lattices. Finally, from the crystallographic standpoint, the use of finite frames provides a panoramic view on indexing of lattice planes and directions.

Going back to expressions opening this section and the description of rotations in frames, the tensors $\mathbf{g}$ and $\boldsymbol{\epsilon}$ are shorthand symbols for the metric tensor and Levi–Civita tensor with components $\epsilon_{\kappa\mu\nu} = (\mathbf{a}_\kappa \times \mathbf{a}_\mu) \cdot \mathbf{a}_\nu$ and $\epsilon^{\kappa\mu\nu} = g^{\kappa\alpha}g^{\mu\beta}g^{\nu\gamma}\epsilon_{\alpha\beta\gamma} = (\mathbf{a}^\kappa \times \mathbf{a}^\mu) \cdot \mathbf{a}^\nu$. For instance, the explicit form of eq.(1) is $R^\mu{}_\nu = g^\mu{}_\nu \cos\theta + n^\mu n_\nu \,(1 - \cos\theta) + g^{\mu\kappa}\epsilon_{\kappa\nu\rho}n^\rho \sin\theta$. The entries $R^\mu{}_\nu$ satisfy the orthogonality conditions $g_{\kappa\rho}R^\kappa{}_\mu R^\rho{}_\nu = g_{\mu\nu}$ with the pseudodeterminant of $[R^\mu{}_\nu]$ equal to $+1$. Similarly, for small angle rotations, one can write

$$\Omega_{\mu\nu} = 2\epsilon_{\mu\nu\kappa}r^\kappa \quad \text{and} \quad r^\kappa = \epsilon^{\kappa\mu\nu}\Omega_{\mu\nu}/4 \ . \tag{4}$$

The explicit forms of other equations are available in [5]. They easily follow from the covariance principle and mechanical positioning of sub- and super-scripts.

3. Frames and crystallographic lattices

The representations of rotations in frames can be used in various fields, but our considerations are confined to the realm of classic crystallography in order to conform to the subject matter of ICOTOM. In crystallographic applications, the bases of reference systems are directly linked to crystal lattice bases. Also frames can be used for determining lattices. This has been unknowingly done for a long time in the case of symmetry-based four-index schemes of Miller-Bravais [12] and Weber [13].

The crucial point for using frames in description of a crystal lattice is to specify the link between the frame vectors $\mathbf{a}_\mu$ and the lattice nodes. Clearly, not every frame naturally induces

a lattice (as for some sets of vectors $\mathbf{a}_\mu$, integer combinations of these vectors can be arbitrarily close to each other), and it is easier to consider the link from the perspective of a given lattice. Two types of the relationship between the lattice nodes and the vectors $\mathbf{a}_\mu$ are more natural than other.

First, the standard or canonical case embodying the classic Miller-Bravais and Weber indexing is based on the following rule: $\mathbf{a}_\mu$ are direct lattice vectors, and *arbitrary* integer combinations of $\mathbf{a}_\mu$ constitute the lattice. The integer coefficients may fail to satisfy conditions (3). The lattice vectors, when expressed in the frame $\mathbf{a}_\mu$ as $q^\mu\mathbf{a}_\mu$ with $q^\mu = g^\mu{}_\nu q^\nu$, have rational (i.e., not necessarily integer) components q^μ. The above arrangement between the direct lattice nodes and $\mathbf{a}_\mu$ determines the relationship between the reciprocal lattice and the dual frame $\mathbf{a}^\mu$: the reciprocal lattice consists of linear combinations of $\mathbf{a}^\mu$ with integer coefficients satisfying conditions (3). One must be aware, however, that an arbitrary integer combination of $\mathbf{a}^\mu$ may not be a vector of the reciprocal lattice. In particular, the vector $\mathbf{a}^\mu$ of the dual frame may not be a vector of the reciprocal lattice.

Clearly, the above scheme is not the only possible. The other natural approach would be to exchange the roles of the direct and the reciprocal lattices. In such a 'dual-canonical' case, the direct lattice vectors would be linear combinations of $\mathbf{a}_\mu$ with integer coefficients satisfying eqs.(3), and the reciprocal lattice vectors would be linear combinations of $\mathbf{a}^\mu$ with arbitrary integer coefficients.

In what follows, the canonical scheme is assumed. Clearly, a frame determines a lattice, and the lattice can be based on numerous different frames. Classic lattice bases constitute particular types of frames. Having a given lattice frame $\mathbf{a}_\mu$, one can specify the lattice direction $q^\mu\mathbf{a}_\mu$ using the generalized Weber indices

$$[q^1\, q^2\, \ldots\, q^M] \propto [u\, v\, \ldots\, w]\ .$$

Similarily, the generalized Miller-Bravais indices

$$[k_1\, k_2\, \ldots\, k_M] \propto (h\, k\, \ldots\, l)$$

specify the plane normal to the vector $k_\mu\mathbf{a}^\mu$. Both q^μ and k_μ are expected to satisfy eqs.(3).

Now, assuming a crystal lattice is based on the frame $\mathbf{a}_\mu$, the Rodrigues parameters of a rotation have a simple crystallographic interpretation. Since covariant vector components are proportional to indices of a lattice plane, the covariant components r_μ are proportional to generalized Miller-Bravais indices $(h\, k\, \ldots\, l)$ of the rotation-invariant lattice plane. Similarly, the contravariant components r^μ are proportional to generalized Weber indices $[u\, v\, \ldots\, w]$ of the rotation-invariant lattice direction. Calculating the components of $\mathbf{r}$ in the reference system constituting the lattice frame is a natural way to get indices of the rotation-invariant lattice planes and directions in low-symmetry crystals.

4. Applications

With the use of frames, some old lattice-related issues can be viewed in a new light. Three example applications are presented below. We begin with a note on using the tetrahedral frame for describing body centered lattices.

4.1. Tetrahedral frame

Frames can be used to account for lattice centering in a 'symmetric' manner. Take the simplest case of the body-centered cubic (bcc) lattice. It is naturally described using the 'tetrahedral' frame. Let the vectors $\mathbf{a}_\mu$ ($\mu = 1, 2, 3, 4$) be related to the conventional orthonormal basis $\mathbf{e}_J$ by

$$\mathbf{a}_1 = a(\mathbf{e}_1+\mathbf{e}_2+\mathbf{e}_3)/2,\ \mathbf{a}_2 = a(\mathbf{e}_1-\mathbf{e}_2-\mathbf{e}_3)/2,\ \mathbf{a}_3 = a(-\mathbf{e}_1+\mathbf{e}_2-\mathbf{e}_3)/2,\ \mathbf{a}_4 = a(-\mathbf{e}_1-\mathbf{e}_2+\mathbf{e}_3)/2; \tag{5}$$

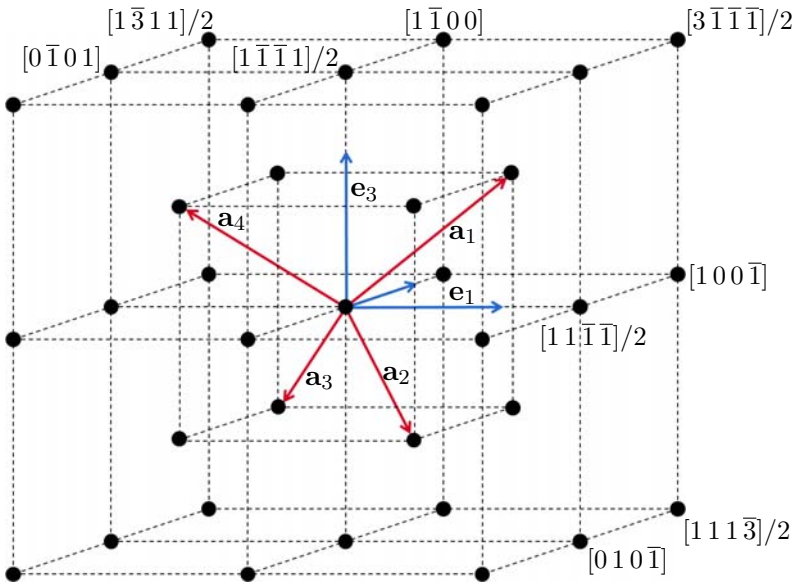

Figure 1. Schematic of body centered cubic lattice and the tetrahedral frame $\mathbf{a}_\mu$. The red and blue vectors constitute the tetrahedral frame and the basis of the Cartesian reference system, respectively. Indices of some lattice nodes in the tetrahedral frame are shown.

see Fig.1. Integer combinations of these vectors indicate nodes of a bcc lattice with the conventional lattice parameter a.[1] The metric corresponding to the above frame is

$$g_{\mu\nu}/a^2 = a^2 g^{\mu\nu} = g_\mu{}^\nu = \delta_\mu{}^\nu - 1/4 \ , \tag{6}$$

and eqs.(3) take the explicit form $v^1 + v^2 + v^3 + v^4 = 0 = v_1 + v_2 + v_3 + v_4$. With the canonical approach, the direct lattice is built of all integer combinations of $\mathbf{a}_\mu$, but the integer coefficients may violate conditions (3). For instance, the direct lattice node at $\mathbf{v} = a\,\mathbf{e}_1 + a\,\mathbf{e}_2 + a\,\mathbf{e}_3$ can be expressed as the integer combination $2\mathbf{a}_1 + 0\mathbf{a}_2 + 0\mathbf{a}_3 + 0\mathbf{a}_4$, but the integer coefficients do not satisfy eqs.(3). The coordinates of $\mathbf{v}$ satisfying (3) are rational: $\mathbf{v} = (3/2)\mathbf{a}_1 - (1/2)\mathbf{a}_2 - (1/2)\mathbf{a}_3 - (1/2)\mathbf{a}_4$.

The frame dual to (5) is given by $\mathbf{a}^\mu = \mathbf{a}_\mu/a^2$. The reciprocal lattice is built of combinations of vectors $\mathbf{a}^\mu$ with integer coefficients satisfying conditions (3). This lattice corresponds to linear combinations of vectors $\mathbf{e}^J/a$ with integer coefficients such that their sum is even. Thus, as expected, it is the face-centered cubic (fcc) lattice with the lattice parameter of $2/a$.[2] With the four-index labeling of the reciprocal lattice nodes, there are no diffraction selection rules (i.e., no centering-caused systematic extinctions); an arbitrary quadruple of integers summing up to zero corresponds to a diffraction reflection and vice versa. For illustration, here are some corresponding three- and four-index designations of reflecting planes:

Orthogonal basis	$(0\,0\,0)$	$(0\,0\,2)$	$(0\,1\,1)$	$(1\,1\,2)$	$(0\,2\,2)$	$(0\,1\,3)$	$(2\,2\,2)$
Tetrahedral frame	$(0\,0\,0\,0)$	$(1\,\bar{1}\,\bar{1}\,1)$	$(1\,\bar{1}\,0\,0)$	$(2\,\bar{1}\,\bar{1}\,0)$	$(2\,\bar{2}\,0\,0)$	$(2\,\bar{2}\,\bar{1}\,1)$	$(3\,\bar{1}\,\bar{1}\,\bar{1})$

The modification of the above considerations to body-centered tetragonal or body-centered orthorhombic lattices is straightforward, and the indexing scheme of all three body-centered cases is the same.

[1] Such reference system was discussed by Rogers and Klyne [14] in relation to tetrahedrally arranged bonds, i.e., a network of atoms, not a crystal lattice. Moreover, the coordinates v^μ are related to but different from tetrahedral coordinates used in applications of finite element method (e.g., [15], p.106).

[2] If $a = 1$, the frame $\mathbf{a}_\mu$ is self-dual ($\mathbf{a}^\mu = \mathbf{a}_\mu$), but obviously the lattice is not self-reciprocal.

4.2. Lattice rotation in deformation by slip

Frames can be applied to accommodate other symmetries. In particular, these can be symmetries arising in characterization of phenomena. For instance, in description of orientation changes during plastic deformation, convenient frames can be devised based on characteristic directions and/or planes of slip or twinning systems. The tetrahedral frame (5) spans the Thompson tetrahedron illustrating the fcc $\{111\}\langle 011\rangle$ slip systems [16], and these slip systems could be described using tetrahedral coordinates, but also other frames can be suitable.

Let us consider the general case without the limitation to the fcc lattice. Single slip results in a rotation of the lattice around certain axis, and this axis identifies the slip system. The unit vector along the axis will be taken as $\mathbf{a}_\mu$. The total rotation caused by slip on multiple systems is given in the Cartesian reference frame by the well known formula (see, e.g., [17])

$$\Omega_{IJ} = \textstyle\sum_\mu \gamma^\mu \left(n_I^\mu b_J^\mu - b_I^\mu n_J^\mu\right)/2 \ , \tag{7}$$

where b_I^μ and n_I^μ are Cartesian components of the unit vectors along the slip direction and slip plane normal, respectively, and γ^μ is the shear on the μ-th system. The (small) angle of rotation is $\gamma^\mu/2$. Based on eq.(4), the relationship (7) can be written in the form $\Omega_{IJ} = 2\varepsilon_{IJK} r^K$, where

$$r^K = \textstyle\sum_\mu (\varepsilon^{KIJ} n_I^\mu b_J^\mu)\,\gamma^\mu/4 = (\mathbf{a}_\mu \cdot \mathbf{e}^K)\,\gamma^\mu/4 = (\mathbf{a}_\mu\,\gamma^\mu/4)\cdot\mathbf{e}^K$$

are Cartesian components of the Rodrigues vector $\mathbf{r} = r^K\mathbf{e}_K$. The vector $\mathbf{r}$ can be expressed in the frame $\mathbf{a}_\mu$ as $\mathbf{r} = r^\mu\mathbf{a}_\mu$ with $r^\mu = \mathbf{r}\cdot\mathbf{a}^\mu$. Now, in this representation, equation (7) takes the simple form[3]

$$r^\mu = g^\mu{}_\nu \gamma^\nu/4 \ . \tag{8}$$

The components r^μ satisfy eqs.(3), whereas γ^μ are unconstrained. With given shears γ^μ, one can obtain the resultant rotation via $\mathbf{r} = r^\mu\mathbf{a}_\mu = (g^\mu{}_\nu\gamma^\nu/4)\mathbf{a}_\mu = \gamma^\nu(\mathbf{a}_\mu g^\mu{}_\nu)/4 = \gamma^\mu\mathbf{a}_\mu/4$. This relationship can be seen as a compact form of eq.(4) with $\mathbf{r} = \boldsymbol{\epsilon} : \boldsymbol{\Omega}/4 = \sum_\mu(\gamma^\mu/4)\boldsymbol{\epsilon} : (\mathbf{n}_\mu\times\mathbf{b}_\mu) = \gamma^\mu\mathbf{a}_\mu/4$ and $\mathbf{a}_\mu = \boldsymbol{\epsilon} : (\mathbf{n}_\mu\times\mathbf{b}_\mu)$; compare, e.g., eqs.(1–2) of [18]. The convenience of using frames lies in the presence of $g^\mu{}_\nu$ on the right hand side of eq.(8); by the properties of the pseudoinverse [10], if the resultant rotation vector $\mathbf{r}$ is known, the shears are given by

$$\gamma^\mu = 4\,\mathbf{r}\cdot\mathbf{a}^\mu + \xi^\mu \ ,$$

where the terms ξ^μ satisfy $g^\mu{}_\nu\xi^\nu = 0$, or $\xi^\mu = x^\mu - g^\mu{}_\nu x^\nu$ with x^μ being arbitrary numbers. In the case of $\xi^\mu = 0$, the shears $\gamma^\mu = 4\,\mathbf{r}\cdot\mathbf{a}^\mu$ are optimally distributed over the slip systems in the sense that $\sum_\mu(\gamma^\mu)^2$ is the smallest possible.

As a concrete example, let us consider the aforementioned case of fcc metals with slip on $\{111\}$ planes in $\langle 011\rangle$ directions leading to rotations about $\langle 112\rangle$ rotation axes. The frame consists of twelve vectors

$$\begin{array}{llllllllllll}
\mathbf{a}_1 &=& [2\,1\,1]a/2 & \mathbf{a}_4 &=& [2\,\bar1\,\bar1]a/2 & \mathbf{a}_7 &=& [\bar2\,1\,\bar1]a/2 & \mathbf{a}_{10} &=& [\bar2\,\bar1\,1]a/2 \\
\mathbf{a}_2 &=& [1\,2\,1]a/2 & \mathbf{a}_5 &=& [1\,\bar2\,\bar1]a/2 & \mathbf{a}_8 &=& [\bar1\,2\,\bar1]a/2 & \mathbf{a}_{11} &=& [\bar1\,\bar2\,1]a/2 \\
\mathbf{a}_3 &=& [1\,1\,2]a/2 & \mathbf{a}_6 &=& [1\,\bar1\,\bar2]a/2 & \mathbf{a}_9 &=& [\bar1\,1\,\bar2]a/2 & \mathbf{a}_{12} &=& [\bar1\,\bar1\,2]a/2
\end{array}$$

with $a = 2\times 6^{-1/2}$ so the vectors are of unit magnitude.[4] The tensors characterizing the frame have the form

$$\frac{1}{6\,a^2}\,[g_{\mu\nu}] = 6\,a^2\,[g^{\mu\nu}] = [g_\mu{}^\nu] = \frac{1}{24}\begin{bmatrix} l_0 & l_1 & l_2 & l_3 \\ & l_0 & l_3 & l_2 \\ & & l_0 & l_1 \\ \text{sym} & & & l_0 \end{bmatrix} \ ,$$

[3] This expression follows from $\mathbf{r}\cdot\mathbf{a}^\mu = (r^K\mathbf{e}_K)\cdot\mathbf{a}^\mu = (\mathbf{a}_\nu\cdot\mathbf{e}^K)(\mathbf{e}_K\cdot\mathbf{a}^\mu)(\gamma^\nu/4) = (\mathbf{a}^\mu\cdot\mathbf{a}_\nu)(\gamma^\nu/4)$ and the definition of $g^\mu{}_\nu$.

[4] This frame is linked to the fcc (direct) lattice with lattice parameter a.

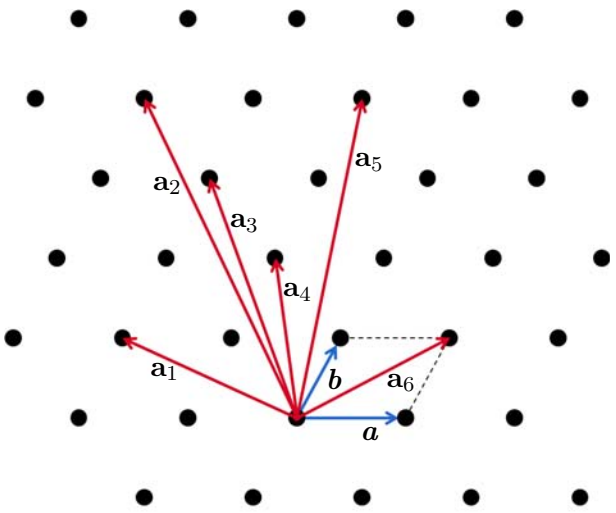

Figure 2. Schematic two-dimensional illustration of the indexing problem. Given positions of some (reciprocal) lattice nodes, determine the the parameters of the lattice, or given a frame (red vectors $\mathbf{a}_\mu$), get the (blue) vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ of the lattice basis.

where

$$l_0 = \begin{bmatrix} 6 & 5 & 5 \\ & 6 & 5 \\ \text{sym} & & 6 \end{bmatrix},\ l_1 = \begin{bmatrix} 2 & -1 & -1 \\ & -4 & -3 \\ \text{sym} & & -4 \end{bmatrix},\ l_2 = \begin{bmatrix} -4 & -1 & -3 \\ & 2 & -1 \\ \text{sym} & & -4 \end{bmatrix},\ l_3 = \begin{bmatrix} -4 & -3 & -1 \\ & -4 & -1 \\ \text{sym} & & 2 \end{bmatrix}.$$

With this $[g^{\mu\nu}]$, the dual frame is $\mathbf{a}^\mu = \mathbf{a}_\mu/(6a^2) = \mathbf{a}_\mu/4$. Thus, the principal part $(4\,\mathbf{r}\cdot\mathbf{a}^\mu)$ of the shear on the μ-th system is given simply by the scalar product of the rotation vector $\mathbf{r}$ and the unit vector $\mathbf{a}_\mu$ along the rotation axis of the system.

Clearly, other tensor quantities used for describing the slip-based deformation can also be expressed using frames, but such broader considerations are beyond the scope of this short communication.

4.3. Indexing of single crystal diffraction patterns

The ab initio indexing problem can be stated as follows: having measured positions of some diffraction reflections, get the parameters of the crystal lattice, and ascribe Miller indices to the reflections. One can formulate it more formally: having a number of vectors of the crystal reciprocal lattice, determine the basis of the crystal lattice; see, e.g., [19] and references therein. It is easy to notice that the input data (vectors of the reciprocal lattice) constitute a dual frame (an overcomplete set of basis vectors), and the problem is to reduce this frame to a conventional basis of the reciprocal lattice built of three linearly independent vectors; see Fig.2. This is similar to the (Pohst) problem of computer science: given some lattice vectors which exceed in number the space dimension, find a lattice basis made of short vectors, or in other words, given a frame, find a basis made of short vectors. This problem is solved by a modified version of LLL lattice reduction algorithm (sometimes referred to as MLLL) by Pohst [20]. With this solution, the center of the indexing problem is shifted to accounting for experimental inaccuracies in input data. This explicitely validates the frequently postulated property that indexing is simple for accurate data.

5. Final remarks

Summarizing, frames open an opportunity to take a new look at the subject of reference systems and rotation parameterizations. Since the restrictions on the vectors $\mathbf{a}_\mu$ are week, frames can match various geometries. They allow for general but also very concise formulation of problems. Therefore, one can expect numerous texture-related applications of frames. The most obvious use is in crystallographic software involving plane and direction indices. This includes software for analysis of orientation relationships, coincident lattices, slip systems, twinning systems et cetera. The most basic advantage of using frames is that the four-index (Miller-Bravais + Weber) system standardly used for crystals of the hexagonal family can be treated on an equal footing with the three-index system used for other crystal families.

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