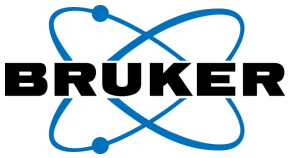
Coordinate System Transformations with application to the Bruker Esprit/DynamicS EBSD system

AIMO WINKELMANN
aimo.winkelmann@bruker.com
Bruker Nano GmbH, Berlin



2015
Bruker Nano

Chapter 1

Crystal Geometry & Coordinate Systems

1.1 Transformations between coordinate systems

It is a common problem in crystallographic computations to change from one coordinate system to another. The choice of coordinate system might be motivated by simplifications implied by the symmetry of the crystal structure or by practical considerations, like the need to describe crystallographic features in a suitable laboratory frame connected e.g. to the diffraction pattern of a crystal or to its external shape. In the following we will shortly outline the basic approach and compile the necessary formulas. The focus of the treatment here is on a systematic derivation which should make it possible for the reader to understand the general framework and to implement these relations into computer code.

1.1.1 Conventions

We name the basis vectors of the initial, untransformed, "old" system by $\vec{\mathbf{a}}_i$ and the basis vectors of the transformed "new" system by $\vec{\mathbf{B}}_i$. A basis is given as an ordered list of basis vectors $a = (\vec{\mathbf{a}}_1, \vec{\mathbf{a}}_2, \vec{\mathbf{a}}_3)$.

Demonstrating the Einstein sum convention, a vector $\vec{\mathbf{x}}$ can be written with coordinates x_i or X_i in the old and new system, respectively:

$$\vec{\mathbf{x}} = \sum_i x_i \vec{\mathbf{a}}_i = x_i \vec{\mathbf{a}}_i = X_i \vec{\mathbf{B}}_i \tag{1.1}$$

The column matrix of the vector components x_i (coordinates) with respect to a basis $a = (\vec{\mathbf{a}}_1, \vec{\mathbf{a}}_2, \vec{\mathbf{a}}_3)$ can be written in different ways:

$$[\vec{\mathbf{x}}]_a = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = [x_1, x_2, x_3] = (x_1, x_2, x_3)^T \tag{1.2}$$

where $[x_1, x_2, x_3]$ is a (3×1) column matrix and (x_1, x_2, x_3) is a (1×3) row matrix with $(x_1, x_2, x_3)^T = [x_1, x_2, x_3]$ and the T superscript indicates transposition of a matrix.

Matrix components A_{ij} refer to row i and column j. The notation (A_{ij}) represents a complete scheme of matrix components, instead of just to the matrix element

A_{ij}. The action of a matrix on coordinate vectors can be realized via matrix multiplication using column vectors:

$$[\vec{\mathbf{b}}]_a = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = (A_{ij})[\vec{\mathbf{a}}]_a = (A_{ij}) \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = (A_{ij})[a_1, a_2, a_3] \rightarrow b_i = A_{ij}a_j \tag{1.3}$$

To get the same components b_i for row vectors by matrix multiplication, we need to use the transposed matrix:

$$[\vec{\mathbf{b}}]_a^T = (b_1, b_2, b_3) = [\vec{\mathbf{a}}]_a^T (A_{ij})^T = [\vec{\mathbf{a}}]_a^T (A_{ji}) = (a_1, a_2, a_3)(A_{ji}) \rightarrow b_j = a_i A_{ji} \tag{1.4}$$

Note how the sum convention expressions in the last two equations result in exactly the same coordinates of $\vec{\mathbf{b}}$ irrespective of its column or row representation.

In the following, we will base our treatment on matrices acting on column vectors by default. The conversion to row vectors is easily achieved by transposing the relevant matrix for column vectors. While some relations can be more succinctly written by switching between column and row vectors, this can make the treatment of several subsequently combined transformations less clear. In the summary, section 1.2.3, we provide all relations in their simplest form using both column and row vectors.

1.1.2 Transformation Matrices

In order to describe transformations between two coordinate systems, we first have to define the mathematical relationship between both of them. To this end, we decompose the new basis vectors $\vec{\mathbf{B}}_i$ as weighted sums of the old basis vectors $\vec{\mathbf{a}}_j$:

Basis Vector Transformation:

$$\begin{aligned} \vec{\mathbf{B}}_1 &= p_1\vec{\mathbf{a}}_1 + q_1\vec{\mathbf{a}}_2 + r_1\vec{\mathbf{a}}_3 \\ \vec{\mathbf{B}}_2 &= p_2\vec{\mathbf{a}}_1 + q_2\vec{\mathbf{a}}_2 + r_2\vec{\mathbf{a}}_3 \\ \vec{\mathbf{B}}_3 &= p_3\vec{\mathbf{a}}_1 + q_3\vec{\mathbf{a}}_2 + r_3\vec{\mathbf{a}}_3 \end{aligned} \tag{1.5}$$

This is is the central relationship which is the key for the transformation of various entities between two coordinate systems.[1]

Equations (1.5) lead to the definition of the

Basis Transformation Matrix **U**:

$$\mathbf{U} = (u_{ij}) = \begin{pmatrix} u_{11} & u_{12} & u_{13} \\ u_{21} & u_{22} & u_{23} \\ u_{31} & u_{32} & u_{33} \end{pmatrix} = \begin{pmatrix} p_1 & q_1 & r_1 \\ p_2 & q_2 & r_2 \\ p_3 & q_3 & r_3 \end{pmatrix} \tag{1.6}$$

$$\vec{\mathbf{B}}_i = u_{ij}\vec{\mathbf{a}}_j \tag{1.7}$$

where we used the sum convention in (1.7).

In order to understand the meaning of the components of (u_{ij}), we can use column matrices to represent the vectors $\vec{\mathbf{a}}_j$ and $\vec{\mathbf{B}}_i$ in (1.5). We then simply have

[1] Note that equation (1.5) is a general relationship for *vectors* $\vec{\mathbf{a}}_j$ and $\vec{\mathbf{B}}_i$, which might or might not be represented by column or row matrices. For example, we can also interpret equation (1.5) purely geometrically in terms of vector addition.

to multiply all components of each vector by the respective p/q/r-coefficient, which makes equations (1.5) look like:

$$\begin{aligned}
\begin{pmatrix} B_{11} \\ B_{12} \\ B_{13} \end{pmatrix} &= p_1 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + q_1 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + r_1 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \\
\begin{pmatrix} B_{21} \\ B_{22} \\ B_{23} \end{pmatrix} &= p_2 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + q_2 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + r_2 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \qquad (1.8) \\
\begin{pmatrix} B_{31} \\ B_{32} \\ B_{33} \end{pmatrix} &= p_3 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + q_3 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + r_3 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}
\end{aligned}$$

(1.9)

The basis transformation matrix $\mathbf{U}$, which results in a single new basis vector $\vec{\mathbf{B}}_i$ for each corresponding old basis vector $\vec{\mathbf{a}}_i$, is a representation of a linear transformation known from linear algebra [1, 2]. A comparison of (1.8) with (1.6) shows that each ***row*** i of (u_{ij}) contains the ***coordinates*** of the basis vector $\vec{\mathbf{B}}_i$ in the basis of the $\vec{\mathbf{a}}_j$. Thus, the coordinates of an original basis vector $\vec{\mathbf{a}}_i$ are mapped to the coordinates of the corresponding image vector $\vec{\mathbf{B}}_i$ by a matrix $\mathbf{P}$ which in the ***column*** i contains the coordinates of $\vec{\mathbf{B}}_i$ with respect to the initial basis a:

Coordinate Transformation Matrix $\mathbf{P}$:

$$\mathbf{P} = (p_{ij}) = \mathbf{U}^T = (u_{ji}) = \begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ B_{31} & B_{32} & B_{33} \end{pmatrix} = \begin{pmatrix} p_1 & p_2 & p_3 \\ q_1 & q_2 & q_3 \\ r_1 & r_2 & r_3 \end{pmatrix} \qquad (1.10)$$

The matrix $\mathbf{P}$ is convenient for actual computations as it can be set up by directly writing down the coordinates of the new, transformed basis vectors in the fixed system of the untransformed basis.

Since $\mathbf{P}$ represents a linear transformation, it can be used to transform the coordinates of any combination of basis vectors $\vec{\mathbf{a}}_i$. In the fixed basis a, this assigns a new vector $[\vec{\mathbf{y}}]_a$ to each vector $[\vec{\mathbf{x}}]_a$ via $[\vec{\mathbf{y}}]_a = \mathbf{P}\,[\vec{\mathbf{x}}]_a$. Alternatively, the transformation of the bases from $a = (\vec{\mathbf{a}}_1, \vec{\mathbf{a}}_2, \vec{\mathbf{a}}_3)$ to $B = (\vec{\mathbf{B}}_1, \vec{\mathbf{B}}_2, \vec{\mathbf{B}}_3)$ can be seen as a homogeneous deformation of space (with respect to the space spanned by the basis a) if we note that the two points $\vec{\mathbf{x}} = x_i\vec{\mathbf{a}}_i$ and $\vec{\mathbf{y}} = X_i\vec{\mathbf{B}}_i$ retain the same coordinates $x_i = X_i$. This means that the coordinates of the new vector in the new basis are the same as the coordinates of the old vector in the old basis (!). We can thus obtain the coordinates $[\vec{\mathbf{y}}]_a$ in the old, undeformed space by back-transforming the "conserved" coordinates $[\vec{\mathbf{y}}]_B = [x_1, x_2, x_3]_B = [\vec{\mathbf{x}}]_a$ from the new system to the old (note the small x_i). This back-transformation will be shown below to occur via $\mathbf{U}^T$ in equation (1.26). We see that $\mathbf{U}^T$ and $\mathbf{P}$ simply represent two equivalent views on the transformation of $[\vec{\mathbf{x}}]_a$:

Coordinates of transformed vectors in the old system:

$$[\vec{\mathbf{x}}]_a \stackrel{!}{=} [\vec{\mathbf{y}}]_B \qquad \rightarrow \qquad [\vec{\mathbf{y}}]_a = \mathbf{U}^T[\vec{\mathbf{x}}]_a = \mathbf{P}\,[\vec{\mathbf{x}}]_a \qquad (1.11)$$

The deformation of the initial basis vector coordinates (which are simply unit column vectors) into the coordinates of the new basis vectors can be compactly

written as:

$$\mathbf{B} = ([\vec{\mathbf{B}}_1]_a, [\vec{\mathbf{B}}_2]_a, [\vec{\mathbf{B}}_3]_a) = \begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ B_{31} & B_{32} & B_{33} \end{pmatrix} = \mathbf{P} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \mathbf{P}\,\mathbf{E} \tag{1.12}$$

where we define the coordinate representations of the old basis $\mathbf{E} = ([\vec{\mathbf{a}}_1]_a, [\vec{\mathbf{a}}_2]_a, [\vec{\mathbf{a}}_3]_a)$ and the new basis $\mathbf{B}$.

1.1.3 Eight Questions

$\vec{\mathbf{B}}_i(\vec{\mathbf{a}}_j)$: How are the *new* basis vectors determined by the *old* basis vectors?

New basis vectors in terms of old basis vectors:

$$\vec{\mathbf{B}}_i = u_{ij}\vec{\mathbf{a}}_j \qquad \text{or} \qquad \begin{pmatrix} \vec{\mathbf{B}}_1 \\ \vec{\mathbf{B}}_2 \\ \vec{\mathbf{B}}_3 \end{pmatrix} = \mathbf{U} \begin{pmatrix} \vec{\mathbf{a}}_1 \\ \vec{\mathbf{a}}_2 \\ \vec{\mathbf{a}}_3 \end{pmatrix} \tag{1.13}$$

The old basis is transformed into the new basis by the transformation matrix $\mathbf{U}$.

$\vec{\mathbf{a}}_i(\vec{\mathbf{B}}_j)$: How are the *old* basis vectors determined by the *new* basis vectors?

We look for a matrix (U_{ij}) which provides the back-transformation[2] from the new basis vectors $\vec{\mathbf{B}}_j$ to the old basis vectors $\vec{\mathbf{a}}_i$:

$$\vec{\mathbf{a}}_i = U_{ij}\vec{\mathbf{B}}_j = U_{ij}u_{jk}\vec{\mathbf{a}}_k \tag{1.14}$$

which requires

$$U_{ij}u_{jk} = \begin{cases} 1 & \text{if} \quad i = k \\ 0 & \text{if} \quad i \neq k \end{cases} \tag{1.15}$$

We compare this with the definition for the inverse $\mathbf{U}^{-1}$ of the transformation matrix $\mathbf{U}$:

$$(\mathbf{U}^{-1})_{ij}u_{jk} = \mathbb{1}_{ik} = \begin{cases} 1 & \text{if} \quad i = k \\ 0 & \text{if} \quad i \neq k \end{cases} \tag{1.16}$$

and we see that the U_{ij} are the components of $\mathbf{U}^{-1}$ for which we can write

$$(U_{ij}) = \mathbf{U}^{-1} = (u_{ij})^{-1} \tag{1.17}$$

The elements of (U_{ij}) can be determined by one of the standard methods of matrix inversion which are available in numerical libraries for linear algebra.

[2]Note the capital U to distinguish this matrix from (u_{ij})

Old basis vectors in terms of new basis vectors:

$$\vec{\mathbf{a}}_i = U_{ij}\vec{\mathbf{B}}_j \qquad \text{or} \qquad \begin{pmatrix}\vec{\mathbf{a}}_1\\ \vec{\mathbf{a}}_2\\ \vec{\mathbf{a}}_3\end{pmatrix} = \mathbf{U^{-1}} \begin{pmatrix}\vec{\mathbf{B}}_1\\ \vec{\mathbf{B}}_2\\ \vec{\mathbf{B}}_3\end{pmatrix} \tag{1.18}$$

The new basis is transformed into the old basis by the inverse $\mathbf{U^{-1}}$ *of the transformation matrix* $\mathbf{U}$.

$X_i(x_j)$: How are the *new* coordinates of a *fixed* vector determined from its *old* coordinates?

We are looking for the coordinates $[\vec{\mathbf{x}}]_B$ of a fixed vector $\vec{\mathbf{x}} = X_j\vec{\mathbf{B}}_j$ in the new system when the coordinates $[\vec{\mathbf{x}}]_a$ are given in the old system as:

$$\vec{\mathbf{x}} = x_i\vec{\mathbf{a}}_i \quad \text{with} \quad \vec{\mathbf{a}}_i = U_{ij}\vec{\mathbf{B}}_j \tag{1.19}$$

This leads to

$$\vec{\mathbf{x}} = x_iU_{ij}\vec{\mathbf{B}}_j = X_j\vec{\mathbf{B}}_j \tag{1.20}$$

which requires

$$x_iU_{ij} = X_j \tag{1.21}$$

Renaming of the indices gives for column vectors $[\vec{\mathbf{x}}]_a = [x_1, x_2, x_3]$ and $[\vec{\mathbf{x}}]_B = [X_1, X_2, X_3]$:

$$X_i = U_{ji}x_j \quad \rightarrow \quad [\vec{\mathbf{x}}]_B = (\mathbf{U^{-1}})^T\,[\vec{\mathbf{x}}]_a \tag{1.22}$$

The coordinates of a vector in the old system are transformed into the coordinates of the new system by the transposed inverse $(\mathbf{U^{-1}})^T$ *of the transformation matrix* $\mathbf{U}$.

$x_i(X_j)$: How are the *old* coordinates of a *fixed* vector obtained from its *new* coordinates?

We are looking for the coordinates $[\vec{\mathbf{x}}]_a$ of a fixed vector $\vec{\mathbf{x}} = x_j\vec{\mathbf{a}}_j$ in the old system when the coordinates $[\vec{\mathbf{x}}]_B$ are given in the new system by:

$$\vec{\mathbf{x}} = X_i\vec{\mathbf{B}}_i \quad \text{with} \quad \vec{\mathbf{B}}_i = u_{ij}\vec{\mathbf{a}}_j \tag{1.23}$$

This leads to

$$\vec{\mathbf{x}} = X_iu_{ij}\vec{\mathbf{a}}_j = x_j\vec{\mathbf{a}}_j \tag{1.24}$$

requiring

$$x_j = X_iu_{ij} \tag{1.25}$$

After renaming the indices, we obtain for column vectors $[\vec{\mathbf{x}}]_a = [x_1, x_2, x_3]$ and $[\vec{\mathbf{x}}]_B = [X_1, X_2, X_3]$:

$$x_i = u_{ji} X_j \quad \text{or} \quad [\vec{\mathbf{x}}]_a = \mathbf{U}^T [\vec{\mathbf{x}}]_B \tag{1.26}$$

The coordinates of a vector in the new system are transformed into the coordinates of the old system by the transposed $\mathbf{U}^T$ *of the transformation matrix* $\mathbf{U}$*.*

$H_i(h_j)$: How are the *new* coordinates of a *fixed* reciprocal space vector determined by its *old* reciprocal space coordinates?

We take $\vec{\mathbf{h}}$ as a fixed vector with coordinates relative to the old (h_j) and new (H_j) reciprocal space basis vectors:

$$\vec{\mathbf{h}} = H_i \vec{\mathbf{B}}_i^\star = h_k \vec{\mathbf{a}}_k^\star \tag{1.27}$$

Scalar multiplication with $\vec{\mathbf{B}}_i = u_{ij} \vec{\mathbf{a}}_j$ results in:

$$\vec{\mathbf{B}}_i \cdot \vec{\mathbf{h}} = H_i = u_{ij} \vec{\mathbf{a}}_j (h_k \vec{\mathbf{a}}_k^\star) = u_{ij} h_j \tag{1.28}$$

where we take into account

$$\vec{\mathbf{a}}_j \cdot \vec{\mathbf{a}}_k^\star = \begin{cases} 1 & \text{if} \quad j = k \\ 0 & \text{if} \quad j \neq k \end{cases} \tag{1.29}$$

$$H_i = u_{ij} h_j \quad \text{or} \quad [\vec{\mathbf{h}}]_{B^\star} = \mathbf{U} [\vec{\mathbf{h}}]_{a^\star} \tag{1.30}$$

A column vector of reciprocal space coordinates is transformed into the new system by the direct space basis transformation matrix $\mathbf{U}$*.*

$h_i(H_j)$: How are the *old* coordinates of a reciprocal space vector determined by its *new* reciprocal space coordinates?

Again, we take $\vec{\mathbf{h}}$ as a fixed vector with coordinates relative to the old (h_j) and new (H_j) reciprocal space basis vectors:

$$\vec{\mathbf{h}} = h_j \vec{\mathbf{a}}_j^\star = H_k \vec{\mathbf{B}}_k^\star \tag{1.31}$$

Scalar multiplication with $\vec{\mathbf{a}}_i = U_{ij} \vec{\mathbf{B}}_j$ results in:

$$\vec{\mathbf{a}}_i \cdot \vec{\mathbf{h}} = h_i = U_{ij} \vec{\mathbf{B}}_j (H_k \vec{\mathbf{B}}_k^\star) = U_{ij} H_j \tag{1.32}$$

where we have used again the conditions (1.29).

$$h_i = U_{ij} H_j \quad \text{or} \quad [\vec{\mathbf{h}}]_{a^\star} = \mathbf{U^{-1}} [\vec{\mathbf{h}}]_{B^\star} \tag{1.33}$$

A column vector of new reciprocal space coordinates is transformed into the old system by the inverse $\mathbf{U^{-1}}$ *of the basis transformation matrix* $\mathbf{U}$.

$B_i^\star(a_j^\star)$: How are the *new* basis vectors of the reciprocal space determined from the *old* ones??

From

$$\vec{\mathbf{h}} = H_j\vec{\mathbf{B}}_j^\star = h_i\vec{\mathbf{a}}_i^\star = (U_{ij}H_j)\vec{\mathbf{a}}_i^\star \tag{1.34}$$

we see that:

$$\vec{\mathbf{B}}_j^\star = U_{ij}\vec{\mathbf{a}}_i^\star \tag{1.35}$$

and after renaming the indices:

$$\vec{\mathbf{B}}_i^\star = U_{ji}\vec{\mathbf{a}}_j^\star \tag{1.36}$$

The new reciprocal space basis is obtained from the old reciprocal space basis by the transposed inverse $(\mathbf{U^{-1}})^\mathbf{T}$ *of the direct space basis transformation matrix* $\mathbf{U}$.

$a_i^\star(B_j^\star)$: How are the *old* reciprocal space basis vectors determined from the *new* ones?

From

$$\vec{\mathbf{h}} = h_j\vec{\mathbf{a}}_j^\star = H_i\vec{\mathbf{B}}_i^\star = (u_{ij}h_j)\vec{\mathbf{a}}_i^\star \tag{1.37}$$

we see that:

$$\vec{\mathbf{a}}_j^\star = U_{ij}\vec{\mathbf{B}}_i^\star \tag{1.38}$$

and after renaming the indices:

$$\vec{\mathbf{a}}_i^\star = u_{ji}\vec{\mathbf{B}}_j^\star \tag{1.39}$$

The old reciprocal space basis is obtained from the new reciprocal space basis by the transposed $\mathbf{U}^T$ *of the direct space basis transformation matrix* $\mathbf{U}$.

Remarks on different conventions used in the literature

In equation (1.6), we explicitly note the relation of the u_{ij} to the scheme of p/q/r-coefficients which is equivalent to the treatments in [3, 4, 5, 6]. Different texts, however, use different conventions for translating these p/q/r-coefficients into matrices. As we have seen, the various quantities relevant in a coordinate system are transformed, respectively, by the matrix (u_{ij}), its inverse matrix, its transpose or the combination of these. This is why different authors use the p/q/r-coefficients to define their respective equivalent of the (u_{ij})-matrix directly like $\mathbf{U}$ in equation (1.6) [3, 4, 5, 6, 7], or implicitly via its transpose $\mathbf{P}$ like in [8, 9, 10, 11], or via the transpose of the inverse [12, 13, 10], written there as $(B\mathbf{J}A)$. Some authors also define individual symbols for the different matrices to obtain simple transformation matrices for specific, often used quantities (instead of having to write down by some notation e.g. the transpose of the inverse of

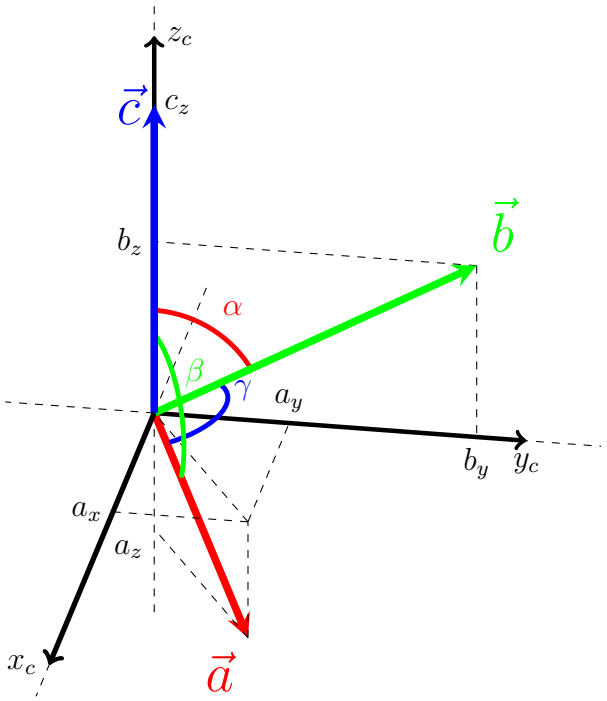


Figure 1.1: Geometrical relationship between crystal lattice vectors and a Cartesian reference system. Both systems are related by the structure matrix $\mathbf{A}_0$ as described in the text.

(u_{ij})). The issue is further compounded by switching from column to row vectors when indicated, which conveniently circumvents matrix transposition. Moreover, in dealing with transformations caused by rotated coordinate systems (see below), another twist in the plot is contributed by the property of rotation matrices that their inverse equals their transpose, which can somewhat disguise the details of the derivation of a transformation. A possible way to reduce problems which can occur while working with coordinate system transformations is the consistent use of a special notation due to Bowles&Mackenzie [14, 15] which is applied e.g. in [10, 12, 13].
Despite the various conventions for defining transformation matrices, we like to stress here that these conventions for the use of the p/q/r-coefficients of 1.5 cannot change the internal relation that the transformation properties of some quantities are similar to the transformation properties of the basis vectors $\vec{\mathbf{a}}_j$ ("covariant") while other transformation properties are similar to the transformation of vector coordinates x_j ("contravariant"). We do not use a special tensor notation in this text to distinguish between covariant and contravariant quantities, for which we can refer the reader e.g. to [16].

1.2 Applications

1.2.1 Structure Matrix

The structure matrix $\mathbf{A}$ fixes the geometrical relationship between the crystal lattice base vectors $(\vec{\mathbf{a}}, \vec{\mathbf{b}}, \vec{\mathbf{c}})$ (the "new" system) and a Cartesian reference frame $(\vec{\mathbf{e_1}}, \vec{\mathbf{e_2}}, \vec{\mathbf{e_3}})$

(the "old" system) as a function of the lattice parameters $(a, b, c, \alpha, \beta, \gamma)$. Crystallographic computations are significantly simplified in the orthonormal Cartesian system. We use the following convention with $\mathbf{A} = \mathbf{A}_0$ according to McKie&McKie ([4], eq. (34) p.154), which places the $\vec{\mathbf{c}}$-basis vector of the lattice parallel to the z-axis of the Cartesian system:

$$\mathbf{A}_0 = \begin{pmatrix} a_x & 0 & 0 \\ a_y & b_y & 0 \\ a_z & b_z & c_z \end{pmatrix} = \begin{pmatrix} a\frac{\sqrt{1+2\cos\alpha\cos\beta\cos\gamma-(\cos\alpha^2+\cos\beta^2+\cos\gamma^2)}}{\sin\alpha} & 0 & 0 \\ a\frac{\cos\gamma-\cos\alpha\cos\beta}{\sin\alpha} & b\sin\alpha & 0 \\ a\cos\beta & b\cos\alpha & c \end{pmatrix} \quad (1.40)$$

In general, the structure matrix $\mathbf{A}$ contains as columns the Cartesian coordinates of the lattice basis vectors in the reference orientation of the respective convention:

$$\mathbf{A} = \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix} \quad (1.41)$$

We can thus view ${}_C\mathbf{A}_C$ as a deformation matrix which deforms the Cartesian basis coordinate vectors into the lattice basis coordinate vectors. The subscripts indicate that all coordinates are measured in the Cartesian system C:

$$[\vec{\mathbf{a}}]_C = {}_C\mathbf{A}_C \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}_C, \qquad [\vec{\mathbf{b}}]_C = {}_C\mathbf{A}_C \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}_C, \qquad [\vec{\mathbf{c}}]_C = {}_C\mathbf{A}_C \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}_C \quad (1.42)$$

Thus, a vector $[\vec{\mathbf{x}}]_C$ measured in the Cartesian system is transformed to a vector $[\vec{\mathbf{y}}]_C$ in the same system:

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}_C = {}_C\mathbf{A}_C \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}_C, \quad (1.43)$$

This is an example for a deformation of space with respect to the Cartesian system which was treated in equation (1.11). From there, we see that ${}_C\mathbf{A}_C$ is an equivalent of $\mathbf{U^T}$ and $\mathbf{P}$.

It may appear somewhat magical that exactly the same mathematical formulas can be repeated with a different interpretation when exactly the same matrix $\mathbf{A}$ is applied as a coordinate transformation matrix between different systems. Namely, the matrix ${}_C\mathbf{A}_K$ back-transforms the lattice system K basis vector coordinates into the Cartesian system C:

$$[\vec{\mathbf{a}}]_C = {}_C\mathbf{A}_K \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}_K, \qquad [\vec{\mathbf{b}}]_C = {}_C\mathbf{A}_K \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}_K, \qquad [\vec{\mathbf{c}}]_C = {}_C\mathbf{A}_K \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}_K \quad (1.44)$$

Thus, for a fixed vector $\vec{\mathbf{v}}$ with coordinates $(u, v, w)^T_K$ measured in terms of the real-space crystal lattice base vectors $(\vec{\mathbf{a}}, \vec{\mathbf{b}}, \vec{\mathbf{c}})$, we can obtain the coordinates $(x, y, z)^T_C$ of $\vec{\mathbf{v}}$ with respect to the Cartesian base vectors by the action of ${}_C\mathbf{A}_K$:

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix}_C = {}_C\mathbf{A}_K \begin{pmatrix} u \\ v \\ w \end{pmatrix}_K, \quad (1.45)$$

This is an example for the application of the general transformation of coordinates from the new (K) to the old (C) system treated in equation (1.26), from which we see, again, that ${}_C\mathbf{A}_K$ is an equivalent of $\mathbf{U^T}$ and $\mathbf{P}$.

It is important to realize the different meanings of the formulas above, because this illustrates that from a statement containing only a matrix, we can have different choices about the context in which the matrix is supposed to be applied.

The inverse transformations corresponding to equations (1.43) and (1.45) are of course determined by the inverse matrix $\mathbf{A^{-1}}$.

Finally, the basis transformation according to equation (1.13) is given by the corresponding $\mathbf{U} = \mathbf{A^T}$:

$$\begin{pmatrix} \vec{\mathbf{a}} \\ \vec{\mathbf{b}} \\ \vec{\mathbf{c}} \end{pmatrix} = \mathbf{A^T} \begin{pmatrix} \vec{\mathbf{e}}_1 \\ \vec{\mathbf{e}}_2 \\ \vec{\mathbf{e}}_3 \end{pmatrix}, \tag{1.46}$$

According to equation (1.30), the same matrix $\mathbf{A^T}$ also gives the indices $[H, K, L]_{K^\star}$ in the reciprocal space basis $K^\star$ of the crystal for a reciprocal space vector $[h, k, l]_{C^\star}$ in the Cartesian reciprocal system $C^\star$ (which coincides with C because C is orthonormal).

Reciprocal Structure Matrix The Reciprocal Structure Matrix $\mathbf{A}^+$ [10] deforms the Cartesian crystal system into the reciprocal lattice system instead of the direct lattice system:

$$\mathbf{A}^+ = (\mathbf{A}^{-1})^T \tag{1.47}$$

1.2.2 Rotations

The rotation of one coordinate system relative to another is a special case of a transformation. We deal first with rotations around the axes of a Cartesian system. A general rotation can be composed from these rotations.

Rotations around axes of a Cartesian frame

For a rotation by an angle φ around the $\vec{\mathbf{e}}_3$-axis of an orthornormal Cartesian system, we can write down the matrix $\mathbf{U}$ using the vectors of the unrotated system as shown in Figure 1.2:

$$\begin{aligned} \vec{\mathbf{e}'}_1 &= \cos\varphi\,\vec{\mathbf{e}}_1 + \sin\varphi\,\vec{\mathbf{e}}_2 + 0\,\vec{\mathbf{e}}_3 \\ \vec{\mathbf{e}'}_2 &= -\sin\varphi\,\vec{\mathbf{e}}_1 + \cos\varphi\,\vec{\mathbf{e}}_2 + 0\,\vec{\mathbf{e}}_3 \\ \vec{\mathbf{e}'}_3 &= 0\,\vec{\mathbf{e}}_1 + 0\,\vec{\mathbf{e}}_2 + 1\vec{\mathbf{e}}_3 \end{aligned} \tag{1.48}$$

$$\mathbf{U}_{R_z} = \begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{1.49}$$

For a *fixed* vector given with coordinates in the initially unrotated ("old") system, the transformation matrix $\mathbf{R}_Z(\varphi)$ to the new coordinates in the rotated system is given by $(\mathbf{U}_{R_z}^{-1})^T$, which coincides with $\mathbf{U}_{R_z}$ because rotation matrices are orthogonal, $\mathbf{U}_{R_z}^{-1} = \mathbf{U}_{R_z}^T$:

$$\mathbf{R}_Z(\varphi) =: (\mathbf{U}_{R_z}^{-1})^T = \mathbf{U}_{R_z} = \begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{1.50}$$

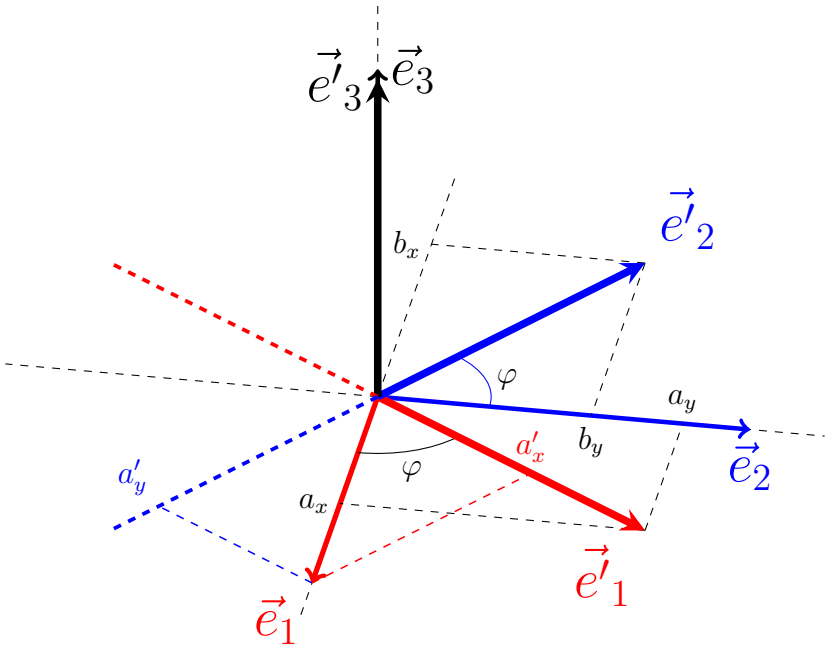


Figure 1.2: Rotation of the coordinate system by an angle φ about the $\vec{\mathbf{e}}_3$ - axis

For checking this relation for the fixed vector $\vec{\mathbf{e}}_1$, we can see from Figure 1.2, that $\vec{\mathbf{e}}_1$ seen in the new basis of $\vec{\mathbf{e}'}_1$ and $\vec{\mathbf{e}'}_2$ has components $(a'_x, a'_y, 0) = (\cos\varphi, -\sin\varphi, 0)$, which is the first row of U.

The transformation matrix $\mathbf{P}_{R_z}$ for coordinates of a *fixed* vector given in the new, rotated system to the old,unrotated system can be written down by looking at Figure 1.2 and writing the components of the new, primed basis vectors as columns of $\mathbf{P}_{R_z}$:

$$\mathbf{P}_{R_z} = \mathbf{U}_{R_z}^T = \mathbf{R}_Z(\varphi)^T = \begin{pmatrix} a_x & b_x & 0 \\ a_y & b_y & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{1.51}$$

The matrices for the rotations around the other two Cartesian axes can be derived in a completely similar way from Figures 1.3 and 1.4, where we have drawn the relevant rotation axis along the vertical direction:

$$\mathbf{R}_X(\omega) =: (\mathbf{U}_{R_X}^{-1})^T = \mathbf{U}_{R_X} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\omega & \sin\omega \\ 0 & -\sin\omega & \cos\omega \end{pmatrix} \tag{1.52}$$

$$\mathbf{R}_Y(\vartheta) =: (\mathbf{U}_{R_Y}^{-1})^T = \mathbf{U}_{R_Y} = \begin{pmatrix} \cos\vartheta & 0 & \sin\vartheta \\ 0 & 1 & 0 \\ -\sin\vartheta & 0 & \cos\vartheta \end{pmatrix} \tag{1.53}$$

From the section on general coordinate system transformations, we know that the matrices $\mathbf{P} = \mathbf{U}^T$ applied to a coordinate vector in the rotated system provides the coordinates in the original unrotated system. Taking as an example a rotated cube, we can use $\mathbf{P}_{R_z}$ to plot in the fixed "old" laboratory frame a cube direction known in the internal cube coordinates [u,v,w]. In turn, to obtain the corresponding cube direction [u,v,w] from a direction in the Cartesian system, we have to use $\mathbf{P}^{-1} = \mathbf{R}_Z(\varphi)$. This is important for a subsequent transformation to crystal lattice coordinates via the structure matrix, as will be discussed below.

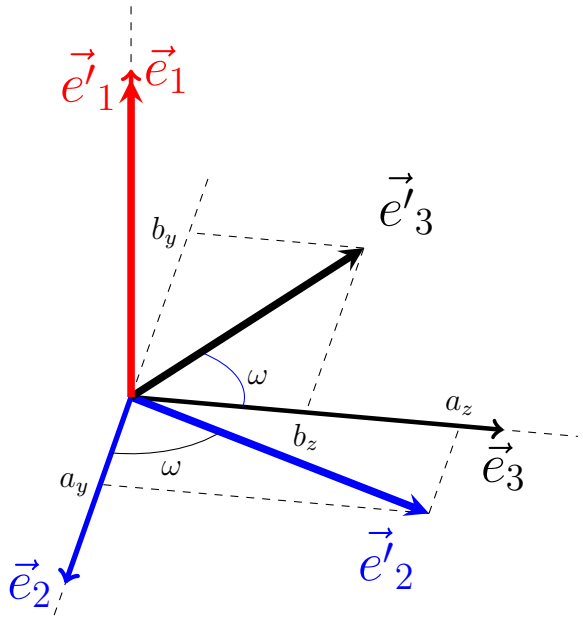


Figure 1.3: Rotation of the coordinate system by an angle ω about the $\vec{\mathbf{e}}_1$ - axis

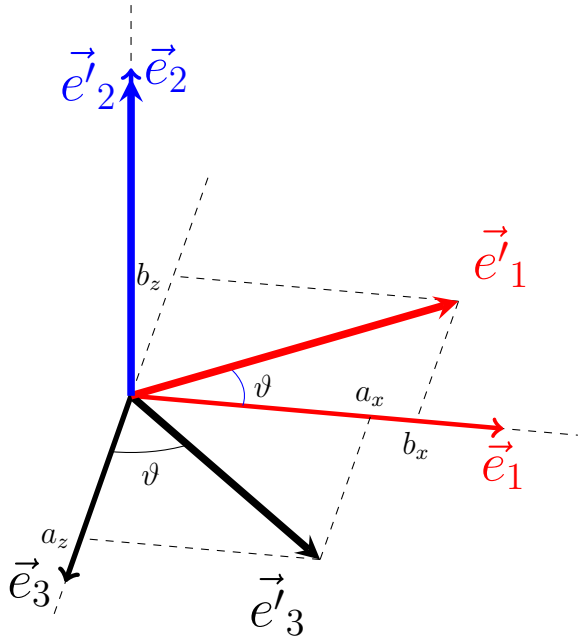


Figure 1.4: Rotation of the coordinate system by an angle ϑ about the $\vec{\mathbf{e}}_2$ - axis

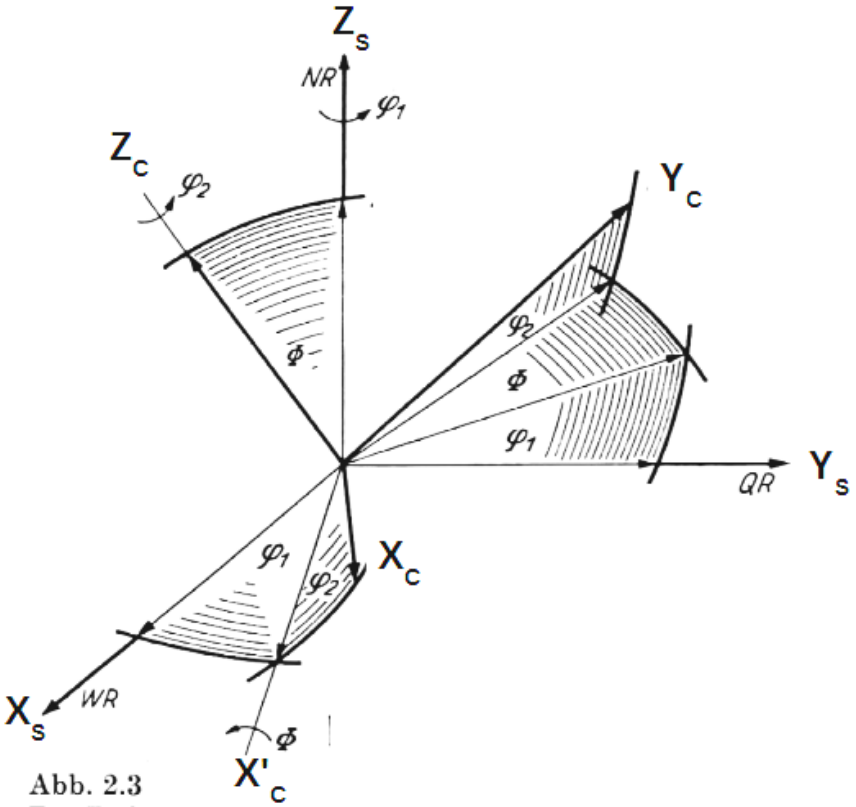


Abb. 2.3
Zur Definition der EULERschen Winkel φ_1, Φ, φ_2

Figure 1.5: Definition of the Euler angles by Bunge [18]. The sample point frame S is rotated to be parallel to the Cartesian crystal frame C by $\varphi_1, \Phi, \varphi_2$. Adapted from [18].

General Rotations: Euler Angles

A general rotation can be build up from three successive rotations around the axes of a Cartesian system [17]. The sets of rotation angles are called Euler angles, for which we will apply the Bunge convention [18, 11] which is used for the description of the orientation of crystallites in a sample.

Compositions of successive rotations are carried out via the respective matrices $\mathbf{R}$, i.e. a rotation $\mathbf{R}_z$ followed by a rotation $\mathbf{R}_x$ is represented by the matrix $\mathbf{R}_x\mathbf{R}_z$. This matrix transforms column coordinate vectors from the old system to the new system after the two successive rotations. The reversed task is achieved by $(\mathbf{R}_x\mathbf{R}_z)^{-1} = \mathbf{R}_z^T\mathbf{R}_x^T$ acting on column coordinate vectors from the new system and giving the old coordinates before the two rotations.

The orientation $\mathbf{O}$ of the crystallite at the origin of D is given by the rotation that takes the sample point system S to the Cartesian crystal frame C, as described by the basis vector transfromation matrix $\mathbf{U_O}$:

$$\mathbf{U_O} = \mathbf{R}_Z(\varphi_2)\mathbf{R}_X(\Phi)\mathbf{R}_Z(\varphi_1) \tag{1.54}$$

where the angles $\varphi_2, \Phi, \varphi_1$ are the Euler angles in the Bunge convention, see Figure 1.5 taken from [18].

1.2.3 Summary: Coordinate System Transformations

Here we collect a number of relations which are useful when dealing with the transformation of coordinate systems. The coordinate transformations are written most shortly by using the matrices $\mathbf{P}$ and its inverse $\mathbf{P^{-1}}$ acting on column or row vectors as indicated.

Vectors in old bases:

$$\vec{\mathbf{x}} = x_i \vec{\mathbf{a}}_i \qquad \vec{\mathbf{h}}^\star = h_i \vec{\mathbf{a}}_i^\star \tag{1.55}$$

Vectors in new bases:

$$\vec{\mathbf{x}} = X_i \vec{\mathbf{B}}_i \qquad \vec{\mathbf{h}}^\star = H_i \vec{\mathbf{B}}_i^\star \tag{1.56}$$

New basis vectors from old basis vectors:

$$\begin{aligned} \vec{\mathbf{B}}_1 &= p_1\vec{\mathbf{a}}_1 + q_1\vec{\mathbf{a}}_2 + r_1\vec{\mathbf{a}}_3 \\ \vec{\mathbf{B}}_2 &= p_2\vec{\mathbf{a}}_1 + q_2\vec{\mathbf{a}}_2 + r_2\vec{\mathbf{a}}_3 \\ \vec{\mathbf{B}}_3 &= p_3\vec{\mathbf{a}}_1 + q_3\vec{\mathbf{a}}_2 + r_3\vec{\mathbf{a}}_3 \end{aligned} \tag{1.57}$$

$$\vec{\mathbf{B}}_i = u_{ij}\vec{\mathbf{a}}_j \qquad \text{or} \qquad \begin{pmatrix} \vec{\mathbf{B}}_1 \\ \vec{\mathbf{B}}_2 \\ \vec{\mathbf{B}}_3 \end{pmatrix} = \mathbf{U} \begin{pmatrix} \vec{\mathbf{a}}_1 \\ \vec{\mathbf{a}}_2 \\ \vec{\mathbf{a}}_3 \end{pmatrix} \tag{1.58}$$

Basis Transformation Matrix $\mathbf{U}$:

$$\mathbf{U} = (u_{ij}) = \begin{pmatrix} u_{11} & u_{12} & u_{13} \\ u_{21} & u_{22} & u_{23} \\ u_{31} & u_{32} & u_{33} \end{pmatrix} = \begin{pmatrix} p_1 & q_1 & r_1 \\ p_2 & q_2 & r_2 \\ p_3 & q_3 & r_3 \end{pmatrix} \tag{1.59}$$

Coordinate Transformation Matrix $\mathbf{P} = \mathbf{U}^T$:

$$\mathbf{P} = \mathbf{U}^T = (u_{ji}) = \begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ B_{31} & B_{32} & B_{33} \end{pmatrix} = \begin{pmatrix} p_1 & p_2 & p_3 \\ q_1 & q_2 & q_3 \\ r_1 & r_2 & r_3 \end{pmatrix} \tag{1.60}$$

Columns of $\mathbf{P}$ are the old-$\vec{\mathbf{a}}_i$-basis coordinates of the new basis vectors.

Old basis vectors in terms of new basis vectors:

$$\vec{\mathbf{a}}_i = U_{ij}\vec{\mathbf{B}}_j \qquad \text{or} \qquad \begin{pmatrix} \vec{\mathbf{a}}_1 \\ \vec{\mathbf{a}}_2 \\ \vec{\mathbf{a}}_3 \end{pmatrix} = \mathbf{U^{-1}} \begin{pmatrix} \vec{\mathbf{B}}_1 \\ \vec{\mathbf{B}}_2 \\ \vec{\mathbf{B}}_3 \end{pmatrix} \qquad (U_{ij}) = \mathbf{U^{-1}} = (\mathbf{P^{-1}})^T \tag{1.61}$$

Coordinates of transformed vectors, fixed old basis:

$$[\vec{\mathbf{x}}]_a \stackrel{!}{=} [\vec{\mathbf{y}}]_B \qquad \rightarrow \qquad [\vec{\mathbf{y}}]_a = \mathbf{U}^T[\vec{\mathbf{x}}]_a = \mathbf{P}\,[\vec{\mathbf{x}}]_a \qquad \mathbf{P} : \mathbf{A}, \mathbf{R}^T(\varphi) \tag{1.62}$$

Deformation of old to new basis vector coordinates:

$$\begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ B_{31} & B_{32} & B_{33} \end{pmatrix}_a = \mathbf{P} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}_a = \mathbf{P}\,\mathbf{E}_a \tag{1.63}$$

New from old coordinates, fixed vector:

$$X_i = U_{ji}x_j \quad [\vec{\mathbf{x}}]_B = (\mathbf{U^{-1}})^T\,[\vec{\mathbf{x}}]_a = \mathbf{P^{-1}}\,[\vec{\mathbf{x}}]_a \quad \begin{pmatrix} U \\ V \\ W \end{pmatrix} = \mathbf{P^{-1}} \begin{pmatrix} u \\ v \\ w \end{pmatrix} \quad \mathbf{P^{-1}} : \mathbf{R}(\varphi) \tag{1.64}$$

Old from new coordinates, fixed vector:

$$x_i = u_{ji}X_j \qquad [\vec{\mathbf{x}}]_a = \mathbf{U}^T\,[\vec{\mathbf{x}}]_B = \mathbf{P}\,[\vec{\mathbf{x}}]_a \quad \begin{pmatrix} u \\ v \\ w \end{pmatrix} = \mathbf{P} \begin{pmatrix} U \\ V \\ W \end{pmatrix} \tag{1.65}$$

New from old reciprocal space coordinates, fixed vector:

$$H_i = u_{ij}h_j \qquad [\vec{\mathbf{h}}]_{B^\star} = \mathbf{U}\,[\vec{\mathbf{h}}]_{a^\star} \qquad (HKL) = (hkl)\mathbf{P} \tag{1.66}$$

Old from new reciprocal space coordinates, fixed vector:

$$h_i = U_{ij}H_j \qquad [\vec{\mathbf{h}}]_{a^\star} = \mathbf{U^{-1}}\,[\vec{\mathbf{h}}]_{B^\star} \qquad (hkl) = (HKL)\mathbf{P^{-1}} \tag{1.67}$$

New from old reciprocal space basis :

$$\vec{\mathbf{B}}_i^\star = U_{ji}\vec{\mathbf{a}}_j^\star \qquad \begin{pmatrix} \vec{\mathbf{B}}_1^\star \\ \vec{\mathbf{B}}_2^\star \\ \vec{\mathbf{B}}_3^\star \end{pmatrix} = (\mathbf{U^{-1}})^T \begin{pmatrix} \vec{\mathbf{a}}_1^\star \\ \vec{\mathbf{a}}_2^\star \\ \vec{\mathbf{a}}_3^\star \end{pmatrix} = \mathbf{P^{-1}} \begin{pmatrix} \vec{\mathbf{a}}_1^\star \\ \vec{\mathbf{a}}_2^\star \\ \vec{\mathbf{a}}_3^\star \end{pmatrix} \tag{1.68}$$

Old from new reciprocal space basis:

$$\vec{\mathbf{a}}_i^\star = u_{ji}\vec{\mathbf{B}}_j^\star \qquad \begin{pmatrix} \vec{\mathbf{a}}_1^\star \\ \vec{\mathbf{a}}_2^\star \\ \vec{\mathbf{a}}_3^\star \end{pmatrix} = \mathbf{U}^T \begin{pmatrix} \vec{\mathbf{B}}_1^\star \\ \vec{\mathbf{B}}_2^\star \\ \vec{\mathbf{B}}_3^\star \end{pmatrix} = \mathbf{P} \begin{pmatrix} \vec{\mathbf{B}}_1^\star \\ \vec{\mathbf{B}}_2^\star \\ \vec{\mathbf{B}}_3^\star \end{pmatrix} \tag{1.69}$$

Chapter 2

EBSD coordinate systems

The transformation matrices defined in Chapter 1 enable us to systematically define the coordinate relationships which are relevant for EBSD measurements.

2.1 General Considerations

In an EBSD orientation map measurement, the electron beam scans a sequence of measurement points in the sample plane, which is assumed to be the XY-plane of the *Map Frame* M. The surface normal is parallel to the Z-direction of M, pointing outwards from the sample.

The electron beam is moved according to the specific scanning sequence in the SEM, characterized by position indices (IX, IY) for a two-dimensional grid of measurement points. For a perfectly plane sample surface, this is assumed to lead to a translation of the sampled map point by $(x_M(IX, IY), y_M(IX, IY), z_M = 0)$ measured from the origin of the map frame M in the sample plane with $z_M = 0$. For 3D-EBSD or for non-planar surfaces in general, the function $z_M(IX, IY)$ also has to be specified.

At each of the measured points in the map frame, we attach a *Sample Point Frame* S with its origin at the beam position (x_M, y_M, z_M). While this frame moves with each sampled point, the axes of S always stay parallel to the axes of M. This shift of the beam spot will change the relative position of the analyzed point on the sample with respect to the fixed Detector Frame D and thus leads to a corresponding shift of the Kikuchi pattern on the screen (see below). The relative angles, however, between the coordinate systems discussed here are not affected by the beam movement.

The actual Kikuchi pattern measurement is carried out in the *Detector Frame* D, which will take over the role of the "old" coordinate system discussed above. We first have to apply a general rotation $\mathbf{U_S}$ to align D with S. In the next step, a rotation $\mathbf{U_O}$ measured from the sample system S, leads to alignment of the rotated system with the *Cartesian crystal frame* C. This rotation from S (or M) to C defines the orientation $\mathbf{O}$ of the crystal at the measured point. Subsequently, the Cartesian crystal system C is transformed by $\mathbf{U_A}$ to the *crystal lattice frame* K. Within the crystal lattice frame K, we can further apply a suitable symmetry operation $\mathbf{U_\Sigma}$ of the crystal structure without changing the result. In a practical application, however, $\mathbf{U_\Sigma}$ could also be pseudo-symmetry operations when e.g. testing for small deviations from perfect symmetries in a Kikuchi pattern.

We write the resulting total transformation $\mathbf{U_K}$ as:

$$\mathbf{U_K} = \mathbf{U_\Sigma}\,\mathbf{U_A}\,\mathbf{U_O}\,\mathbf{U_S} \tag{2.1}$$

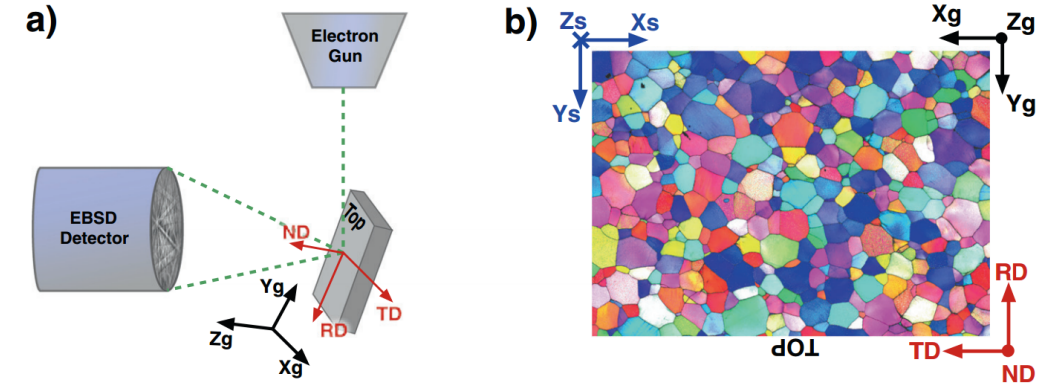


Figure 1 Schematic of EBSD data collection. (a) Schematic of typical EBSD data collection showing the orientation of the crystal reference frame, RD-TD-ND, as well as a user defined global reference frame, $X_g - Y_g - Z_g$. **(b)** Schematic of how the EBSD data appears within the data collection software with all relevant coordinate frames, including the scanning reference frame, $X_s - Y_s - Z_s$.

Figure 2.1: EBSD coordinate systems as shown in [19]. The Bruker Esprit/DynamicS Euler angle coordinate system is parallel to (x_g, y_g, z_g), the RD-TD-ND system is a choice in the EDAX system.

While the different manufacturers implement different conventions for the overall transformation from the Kikuchi pattern to the corresponding crystal lattice at the analyzed beam position, the general principle of transforming a crystal direction to a position in a Kikuchi pattern (and vice versa) needs to be treated in any EBSD analysis. The equation (2.1) merely represents a formal separation of different aspects of the problem, most importantly to single out the orientation $\mathbf{O}$ which is a main result of the EBSD orientation analysis.

2.2 Bruker Esprit & DynamicS

In the Bruker system, the detector frame D has the X-axis horizontally, and the origin of D coincides with the origin of S. The $\mathbf{U}_S$ detector-to-sample system transformation is specified as:

$$\mathbf{U}_S = \mathbf{R}_X(\tau) \tag{2.2}$$

which means that the sample system is assumed to be simply tilted around the detector X-axis by a total angle $\tau = (\tau_{Sample} - 90°) - \tau_{Detector}$. Here, τ_{Sample} is the sample tilt in the SEM and $\tau_{Detector}$ is a detector tilt which can be adjusted at the EBSD detector.

The orientation $\mathbf{O}$ of the crystallite at the origin of D is given by the rotation that takes the sample point system S to the Cartesian crystal frame C:

$$\mathbf{U_O} = \mathbf{R}_Z(\varphi_2)\mathbf{R}_X(\Phi)\mathbf{R}_Z(\varphi_1) \tag{2.3}$$

where the angles $\varphi_2, \Phi, \varphi_1$ are the Euler angles in the Bunge convention.

To transform to the crystal lattice, the Bruker system uses the structure matrix $\mathbf{A}_0$:

$$\mathbf{U_A} = (\mathbf{A}_0)^T \tag{2.4}$$

where we take into account that the structure matrix $\mathbf{A}$ was defined to give the new basis vector coordinates in the old system, which corresponds to $\mathbf{U}^T$.

Having defined the total coordinate system basis transformation $\mathbf{U_K}$, we can write down the matrix ${}_K(\mathbf{P_K^{-1}})_D$ which transforms *column coordinates* from the detector D ("old") to the lattice K ("new") frame in direct space:

$$ {}_K(\mathbf{P_K^{-1}})_D = (\mathbf{U_K}^{-1})^T = \mathbf{A}_0^{-1}\,\mathbf{R}_Z(\varphi_2)\mathbf{R}_X(\Phi)\mathbf{R}_Z(\varphi_1)\,\mathbf{R}_X(\tau) \tag{2.5} $$

where the subscripts on $\mathbf{P_K^{-1}}$ indicate the input and output coordinate frames involved, and we have used the property of rotation matrices that their inverse is their transpose.

Correspondingly, matrix ${}_D(\mathbf{P_K})_K$ transforms direct space lattice K ("new") to detector D ("old") coordinates:

$$ {}_D(\mathbf{P_K})_K = \mathbf{U_K}^T = \mathbf{R}_X^T(\tau)\mathbf{R}_Z^T(\varphi_1)\mathbf{R}_X^T(\Phi)\mathbf{R}_Z^T(\varphi_2)\,\mathbf{A}_0 \tag{2.6} $$

where the reversal of the order of matrices is due to the inversion of the combined matrix, consistent with the action of ${}_C\mathbf{A}_K$ on the "new" K-coordinates of a fixed vector as discussed above.

If we need the detector system coordinates of a fixed vector given with *reciprocal space* coordinates, we just need to adjust the transformation $\mathbf{U_A}$ in such a way that it transforms the Cartesian crystal system into the reciprocal lattice system instead of the direct lattice system. As stated in equation (1.47), this is achieved by the matrix $\mathbf{A}^+ = (\mathbf{A^{-1}})^T$:

$$ \mathbf{U_{A\star}} = (\mathbf{A_0^+})^T = \mathbf{A_0^{-1}} \tag{2.7} $$

The resulting total transformation $\mathbf{U_{K\star}}$ from the detector frame to the reciprocal lattice frame is:

$$ \mathbf{U_{K^\star}} = \mathbf{U_{A\star}}\,\mathbf{U_O}\,\mathbf{U_\Sigma} \tag{2.8} $$

where $\mathbf{U_{K^\star}}$ has to be replaced in the corresponding transformation matrices $\mathbf{P}$ above if we refer to the "new" coordinates in the crystal reciprocal space:

The matrix ${}_D(\mathbf{P_{K^\star}})_{K^\star}$ transforms reciprocal space $K^\star$ ("new") to detector D ("old") column coordinates:

$$ {}_D(\mathbf{P_{K^\star}})_{K^\star} = \mathbf{U_{K^\star}}^T \tag{2.9} $$

The matrix ${}_{K^\star}(\mathbf{P_{K^\star}^{-1}})_D$ transforms coordinates from the detector D ("old") to the reciprocal space $K^\star$ ("new"):

$$ {}_{K^\star}(\mathbf{P_{K^\star}^{-1}})_D = (\mathbf{U_{K^\star}}^{-1})^T \tag{2.10} $$

Gnomonic Projection In order to plot crystallographic features for comparison to a measured Kikuchi pattern, we place a gnomonic projection plane parallel to the detector system x-y-plane and assign 2D gnomonic coordinates (x_G, y_D) to a 3D point (x_D, y_D, z_D) in the detector frame as:

$$ x_G = \frac{x_D}{z_D} \qquad\qquad y_G = \frac{y_D}{z_D} \tag{2.11} $$

Points with $z_D = 0$ will accordingly appear at an infinite distance from the *Pattern Center* ***PC***, which is defined by the intersection of the detector frame Z-axis and the gnomonic projection plane at $(x_G = 0, y_G = 0)$.

The corners of the Kikuchi pattern in the gnomonic projection are then given by:

$$a_P = \quad w_P/h_P \tag{2.12}$$

$$y_G^{min} = -\frac{1-PCY}{DD} \qquad y_G^{max} = +\frac{PCY}{DD} \tag{2.13}$$

$$x_G^{min} = -\frac{PCX}{DD}a_P \qquad x_G^{max} = +\frac{1-PCX}{DD}a_P \tag{2.14}$$

where a_P is the aspect ratio defined by pattern width over pattern height. PCX, PCY, and DD are parameters of the pattern center given by the Bruker EBSD system as:

- PCX: horizontal position of the pattern center, normalized to w_P, measured from the left side of the Kikuchi pattern
- PCY: vertical position of the pattern center, normalized to h_P, measured from the top border of the Kikuchi pattern
- DD: position of the projection point perpendicular to the projection plane, normalized to h_P, measured from the beam position at the sample to the pattern center

The values of the pattern center parameters describe the electron beam position with respect to the borders of the fixed detector screen, and are thus functions of the position indices (IX, IY) of the electron beam in a measured map. The functions $PCX(IX, IY)$, $PCY(IX, IY)$, and $DD(IX, IY)$ are determined in the system calibration procedure.

In the gnomonic projection, the distance $r_G = \sqrt{(x_G^2 + y_G^2)}$ of a point measured from the pattern center is $r_G(x_g, y_G) = \tan\theta$ of the corresponding polar angle θ relative to the detector Z-axis. In this sense, the calibrated gnomonic projection enables us to directly read off the corresponding angle of a direction starting from the SEM beam spot on the sample and ending at the point (x_G, y_G) in the Kikuchi pattern.

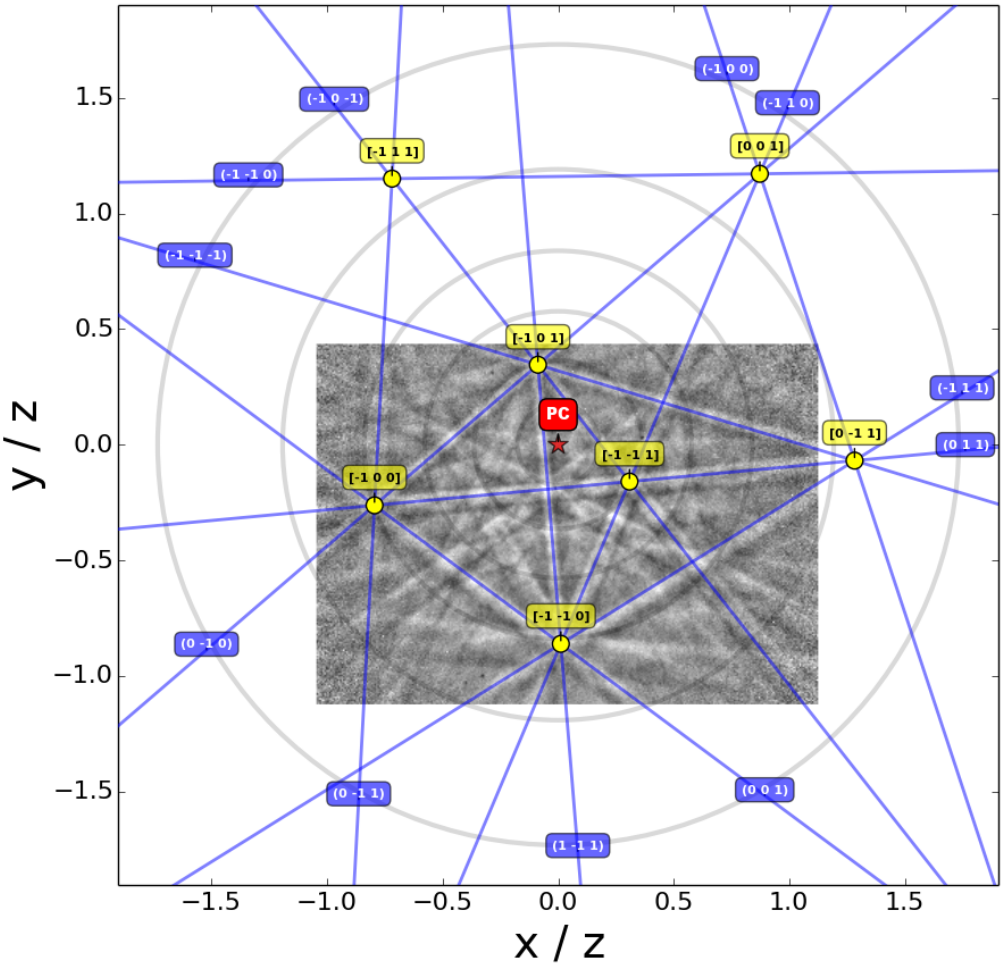


Figure 2.2: Nickel EBSD pattern in its "natural surrounding" of crystallographic features in gnomonic projection. Parameters: cubic lattice, $\varphi_1 = 126.7°, \Phi = 37.9°, \varphi_2 = 272.2°$, $\tau_{Sample} = 70°$, $\tau_{Detector} = 4.58°$, PCX= 0.483, PCY= 0.279, DD= 0.642, $a_P = 320/230$. The circles indicate the angular distance from the Pattern Center in steps of 10°.

Bibliography

[1] Smith, L., *Linear Algebra*, 3rd ed. (Springer, 1998)

[2] Fischer, G., *Lineare Algebra*, 18th ed. (Springer Spektrum, 2014)

[3] Buerger, M. J., *X-ray Crystallography* (John Wiley & Sons Inc, 1942)

[4] McKie, D. & McKie, C., *Essentials of Crystallography* (Blackwell Science Ltd, 1986)

[5] De Graef, M., *Introduction to Conventional Transmission Electron Microscopy* (Cambridge University Press, Cambridge, 2003)

[6] Haussühl, S., *Kristallographie. Kristallgeometrie* (Verlag Chemie, 1993)

[7] Giacovazzo, C., Monaco, H. L., Artioli, G., Viterbo, D., Milanesio, M., Gilli, G., Gilli, P., Zanotti, G., Ferraris, G. & Catti, M., *Fundamentals of Crystallography*, IUCr Texts on Crystallography, Vol. 7 (Oxford University Press, Oxford, 2011)

[8] Arnold, H., "Transformations of the coordinate system (unit-cell transformations)," in *International Tables for Crystallography* (John Wiley & Sons, Ltd, 2006)

[9] Boisen, M. B. & Gibbs, G. V., *Mathematical crystallography: an introduction to the mathematical foundations of crystallography*, Reviews in Mineralogy Vol. 15 (Mineralogical Society of America, 1985)

[10] Schumann, H., *Kristallgeometrie* (VEB Deutscher Verlag für Grundstoffindustrie, Leipzig, 1980)

[11] Morawiec, A., *Orientations and rotations* (Springer, 2003)

[12] Bhadeshia, H. K. D. H., *Worked examples in the Geometry of Crystals*, 2nd ed. (Institute of Materials, 2006) `http://www.msm.cam.ac.uk/phase-trans/2001/geometry2/Geometry.pdf`

[13] Christian, J. W., *The Theory of Transformations in Metals and Alloys* (Pergamon, 2002)

[14] Bowles, J. & Mackenzie, J., "The crystallography of martensite transformations I," Acta Metallurgica **2**, 129 – 137 (1954)

[15] Mackenzie, J. & Bowles, J., "The crystallography of martensite transformations II," Acta Metallurgica **2**, 138 – 147 (1954)

[16] Sands, D. E., *Vectors and tensors in crystallography* (Dover Publications, 1995)

[17] Kuipers, J. B., *Quaternions and Rotation Sequences* (Princeton University Press, Princeton, 1999)

[18] Bunge, H., *Mathematische Methoden der Texturanalyse* (Akademie-Verlag, Berlin, 1969)

[19] Jackson, M. A., Groeber, M. A., Uchic, M. D., Rowenhorst, D. J. & Graef, M., "h5ebsd: an archival data format for electron back-scatter diffraction data sets," Integrating Materials and Manufacturing Innovation **3**, 4 (2014)