## 1.1.4. Tensor-algebraic formulation

The present section summarizes the tensor-algebraic properties of mutually reciprocal sets of basis vectors, which are of importance in the various aspects of crystallography. This is not intended to be a systematic treatment of tensor algebra; for more thorough expositions of the subject the reader is referred to relevant crystallographic texts (*e.g.* Patterson, 1967; Sands, 1982), and other texts in the physical and mathematical literature that deal with tensor algebra and analysis.

Let us first recall that symbolic vector and matrix notations, in which basis vectors and coordinates do not appear explicitly, are often helpful in qualitative considerations. If, however, an expression has to be evaluated, the various quantities appearing in it must be presented in component form. One of the best ways to achieve a concise presentation of geometrical expressions in component form, while retaining much of their 'transparent' symbolic character, is their tensor-algebraic formulation.

### 1.1.4.1. *Conventions*

We shall adhere to the following conventions:

(i) Notation for direct and reciprocal basis vectors:

$$\mathbf{a} = \mathbf{a}_1, \mathbf{b} = \mathbf{a}_2, \mathbf{c} = \mathbf{a}_3$$
$$\mathbf{a}^* = \mathbf{a}^1, \mathbf{b}^* = \mathbf{a}^2, \mathbf{c}^* = \mathbf{a}^3.$$

Subscripted quantities are associated in tensor algebra with *covariant*, and superscripted with *contravariant* transformation properties. Thus the basis vectors of the direct lattice are represented as covariant quantities and those of the reciprocal lattice as contravariant ones.

(ii) Summation convention: if an index appears twice in an expression, once as subscript and once as superscript, a summation over this index is thereby implied and the summation sign is omitted. For example,

$$\sum_i \sum_j x^i T_{ij} x^j \text{ will be written } x^i T_{ij} x^j$$

since both $i$ and $j$ conform to the convention. Such repeating indices are often called *dummy* indices. The implied summation over repeating indices is also often used even when the indices are at the same level and the coordinate system is Cartesian; there is no distinction between contravariant and covariant quantities in Cartesian frames of reference (see Chapter 3.3).

(iii) Components (coordinates) of vectors referred to the covariant basis are written as contravariant quantities, and *vice versa.* For example,

$$\mathbf{r} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c} = x^1\mathbf{a}_1 + x^2\mathbf{a}_2 + x^3\mathbf{a}_3 = x^i\mathbf{a}_i$$
$$\mathbf{h} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* = h_1\mathbf{a}^1 + h_2\mathbf{a}^2 + h_3\mathbf{a}^3 = h_i\mathbf{a}^i.$$

### 1.1.4.2. *Transformations*

A familiar concept but a fundamental one in tensor algebra is the transformation of coordinates. For example, suppose that an atomic position vector is referred to two unit-cell settings as follows:

$$\mathbf{r} = x^k\mathbf{a}_k \tag{1.1.4.1}$$

and

$$\mathbf{r} = x'^k\mathbf{a}'_k. \tag{1.1.4.2}$$

Let us multiply both sides of (1.1.4.1) and (1.1.4.2), on the right, by the vectors $\mathbf{a}^m$, $m$ = 1, 2, or 3, *i.e.* by the reciprocal vectors to the basis $\mathbf{a}_1\mathbf{a}_2\mathbf{a}_3$. We obtain from (1.1.4.1)

$$x^k\mathbf{a}_k \cdot \mathbf{a}^m = x^k\delta^m_k = x^m,$$

where $\delta^m_k$ is the Kronecker symbol which equals 1 when $k = m$ and equals zero if $k \neq m$, and by comparison with (1.1.4.2) we have

$$x^m = x'^k T^m_k, \tag{1.1.4.3}$$

where $T^m_k = \mathbf{a}'_k \cdot \mathbf{a}^m$ is an element of the required transformation matrix. Of course, the same transformation could have been written as

$$x^m = T^m_k x'^k, \tag{1.1.4.4}$$

where $T^m_k = \mathbf{a}^m \cdot \mathbf{a}'_k$.

A *tensor* is a quantity that transforms as the product of coordinates, and the *rank* of a tensor is the number of transformations involved (Patterson, 1967; Sands, 1982). *E.g.* the product of two coordinates, as in the above example, transforms from the $\mathbf{a}'$ basis to the $\mathbf{a}$ basis as

$$x^m x^n = T^m_p T^n_q x'^p x'^q; \tag{1.1.4.5}$$

the same transformation law applies to the components of a contravariant tensor of rank two, the components of which are referred to the primed basis and are to be transformed to the unprimed one:

$$Q^{mn} = T^m_p T^n_q Q'^{pq}. \tag{1.1.4.6}$$

### 1.1.4.3. *Scalar products*

The expression for the scalar product of two vectors, say $\mathbf{u}$ and $\mathbf{v}$, depends on the bases to which the vectors are referred. If we admit only the covariant and contravariant bases defined above, we have four possible types of expression:

(I) $\mathbf{u} = u^i\mathbf{a}_i, \mathbf{v} = v^i\mathbf{a}_i$

$$\mathbf{u} \cdot \mathbf{v} = u^i v^j(\mathbf{a}_i \cdot \mathbf{a}_j) \equiv u^i v^j g_{ij}, \tag{1.1.4.7}$$

(II) $\mathbf{u} = \mathbf{u}_i\mathbf{a}^i, \mathbf{v} = v_i\mathbf{a}^i$

$$\mathbf{u} \cdot \mathbf{v} = u_i v_j(\mathbf{a}^i \cdot \mathbf{a}^j) \equiv u_i v_j g^{ij}, \tag{1.1.4.8}$$

(III) $\mathbf{u} = u^i\mathbf{a}_i, \mathbf{v} = v_i\mathbf{a}^i$

$$\mathbf{u} \cdot \mathbf{v} = u^i v_j(\mathbf{a}_i \cdot \mathbf{a}^j) \equiv u^i v_j \delta^j_i = u^i v_i, \tag{1.1.4.9}$$

(IV) $\mathbf{u} = u_i\mathbf{a}^i, \mathbf{v} = v^i\mathbf{a}_i$

$$\mathbf{u} \cdot \mathbf{v} = u_i v^j(\mathbf{a}^i \cdot \mathbf{a}_j) \equiv u_i v^j \delta^i_j = u_i v^i. \tag{1.1.4.10}$$

(i) The sets of scalar products $g_{ij} = \mathbf{a}_i \cdot \mathbf{a}_j$ (1.1.4.7) and $g^{ij} = \mathbf{a}^i \cdot \mathbf{a}^j$ (1.1.4.8) are known as the *metric* tensors of the covariant (direct) and contravariant (reciprocal) bases, respectively; the corresponding matrices are presented in conventional notation in equations (1.1.3.11) and (1.1.3.13). Numerous applications of these tensors to the computation of distances and angles in crystals are given in Chapter 3.1.

(ii) Equations (1.1.4.7) to (1.1.4.10) furnish the relationships between the covariant and contravariant *components* of the same vector. Thus, comparing (1.1.4.7) and (1.1.4.9), we have

$$v_i = v^j g_{ij}. \tag{1.1.4.11}$$

Similarly, using (1.1.4.8) and (1.1.4.10) we obtain the inverse relationship

$$v^i = v_j g^{ij}. \tag{1.1.4.12}$$

The corresponding relationships between covariant and contravariant *bases* can now be obtained if we refer a vector, say $\mathbf{v}$, to each of the bases

$$\mathbf{v} = v^i\mathbf{a}_i = v_k\mathbf{a}^k,$$

and make use of (1.1.4.11) and (1.1.4.12). Thus, *e.g.*,

$$v^i\mathbf{a}_i = (v_k g^{ik})\mathbf{a}_i = v_k\mathbf{a}^k.$$

Hence

$$\mathbf{a}^k = g^{ik}\mathbf{a}_i \qquad (1.1.4.13)$$

and, similarly,

$$\mathbf{a}_k = g_{ik}\mathbf{a}^i. \qquad (1.1.4.14)$$

(iii) The tensors $g_{ij}$ and $g^{ij}$ are symmetric, by definition.

(iv) It follows from (1.1.4.11) and (1.1.4.12) or (1.1.4.13) and (1.1.4.14) that the matrices of the direct and reciprocal metric tensors are mutually inverse, *i.e.*

$$\begin{pmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{pmatrix}^{-1} = \begin{pmatrix} g^{11} & g^{12} & g^{13} \\ g^{21} & g^{22} & g^{23} \\ g^{31} & g^{32} & g^{33} \end{pmatrix}, \qquad (1.1.4.15)$$

and their determinants are mutually reciprocal.

### 1.1.4.4. *Examples*

There are numerous applications of tensor notation in crystallographic calculations, and many of them appear in the various chapters of this volume. We shall therefore present only a few examples.

(i) The (squared) magnitude of the diffraction vector $\mathbf{h} = h_i\mathbf{a}^i$ is given by

$$|h|^2 = \frac{4\sin^2\theta}{\lambda^2} = h_i h_j g^{ij}. \qquad (1.1.4.16)$$

This concise relationship is a starting point in a derivation of unit-cell parameters from experimental data.

(ii) The structure factor, including explicitly anisotropic displacement tensors, can be written in symbolic matrix notation as

$$F(\boldsymbol{h}) = \sum_{j=1}^{N} f_{(i)} \exp(-\boldsymbol{h}^T\boldsymbol{\beta}_{(j)}\boldsymbol{h}) \exp(2\pi i\boldsymbol{h}^T\boldsymbol{r}_{(j)}), \qquad (1.1.4.17)$$

where $\boldsymbol{\beta}_{(j)}$ is the matrix of the anisotropic displacement tensor of the $j$th atom. In tensor notation, with the quantities referred to their natural bases, the structure factor can be written as

$$F(h_1h_2h_3) = \sum_{j=1}^{N} f_{(j)} \exp(-h_ih_k\beta^{ik}_{(j)}) \exp(2\pi i h_i x^i_{(j)}), \qquad (1.1.4.18)$$

and similarly concise expressions can be written for the derivatives of the structure factor with respect to the positional and displacement parameters. The summation convention applies only to indices denoting components of vectors and tensors; the atom subscript $j$ in (1.1.4.18) clearly does not qualify, and to indicate this it has been surrounded by parentheses.

(iii) Geometrical calculations, such as those described in the chapters of Part 3, may be carried out in any convenient basis but there are often some definite advantages to computations that are referred to the natural, non-Cartesian bases (see Chapter 3.1). Usually, the output positional parameters from structure refinement are available as contravariant components of the atomic position vectors. If we transform them by (1.1.4.11) to their covariant form, and store these covariant components of the atomic position vectors, the computation of scalar products using equations (1.1.4.9) or (1.1.4.10) is *almost as efficient as it would be if the coordinates were referred to a Cartesian system.* For example, the right-hand side of the vector identity (1.1.3.5), which is employed in the computation of dihedral angles, can be written as

$$(A_iC^i)(B_kD^k) - (A_iD^i)(B_kC^k).$$

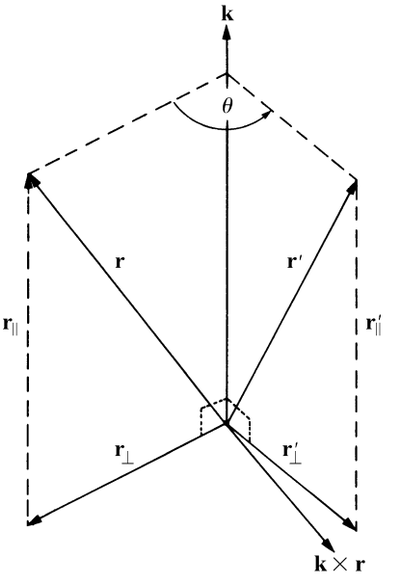


Fig. 1.1.4.1. Derivation of the general expression for the rotation operator. The figure illustrates schematically the decompositions and other simple geometrical considerations required for the derivation outlined in equations (1.1.4.22)–(1.1.4.28).

This is a typical application of reciprocal space to ordinary direct-space computations.

(iv) We wish to derive a tensor formulation of the vector product, along similar lines to those of Chapter 3.1. As with the scalar product, there are several such formulations and we choose that which has both vectors, say $\mathbf{u}$ and $\mathbf{v}$, and the resulting product, $\mathbf{u}\times\mathbf{v}$, referred to a covariant basis. We have

$$\begin{aligned}\mathbf{u}\times\mathbf{v} &= u^i\mathbf{a}_i \times v^j\mathbf{a}_j \\ &= u^iv^j(\mathbf{a}_i\times\mathbf{a}_j).\end{aligned} \qquad (1.1.4.19)$$

If we make use of the relationships (1.1.3.3) between the direct and reciprocal basis vectors, it can be verified that

$$\mathbf{a}_i\times\mathbf{a}_j = Ve_{kij}\mathbf{a}^k, \qquad (1.1.4.20)$$

where $V$ is the volume of the unit cell and the antisymmetric tensor $e_{kij}$ equals $+1$, $-1$, or 0 according as $kij$ is an even permutation of 123, an odd permutation of 123 or any two of the indices $kij$ have the same value, respectively. We thus have

$$\begin{aligned}\mathbf{u}\times\mathbf{v} &= Ve_{kij}u^iv^j\mathbf{a}^k \\ &= Vg^{lk}e_{kij}u^iv^j\mathbf{a}_l,\end{aligned} \qquad (1.1.4.21)$$

since by (1.1.4.13), $\mathbf{a}^k = g^{lk}\mathbf{a}_l$.

(v) *The rotation operator.* The general formulation of an expression for the rotation operator is of interest in crystal structure determination by Patterson techniques (see Chapter 2.3) and in molecular modelling (see Chapter 3.3), and another well known crystallographic application of this device is the derivation of the translation, libration and screw-motion tensors by the method of Schomaker & Trueblood (1968), discussed in Part 8 of Volume C (*IT* C, 1999) and in Chapter 1.2 of this volume. A digression on an elementary derivation of the above seems to be worthwhile.

Suppose we wish to rotate the vector $\mathbf{r}$, about an axis coinciding with the unit vector $\mathbf{k}$, through the angle $\theta$ and in the positive sense, *i.e.* an observer looking in the direction of $+\mathbf{k}$ will see $\mathbf{r}$ rotating in the clockwise sense. The vectors $\mathbf{r}$, $\mathbf{k}$ and the rotated (target) vector $\mathbf{r}'$ are referred to an origin on the axis of rotation (see Fig. 1.1.4.1). Our purpose is to express $\mathbf{r}'$ in terms of $\mathbf{r}$, $\mathbf{k}$ and $\theta$ by a general vector