thought of as a superposition of waves (*e.g.* Buerger, 1959), with wavevectors related to the interplanar spacings d_{hkl}, in the crystal lattice. Denoting the wavevector of a Fourier wave by $\mathbf{g}$ (a function of hkl), the phase of the Fourier wave at the point $\mathbf{r}$ in the crystal is given by $2\pi\mathbf{g}\cdot\mathbf{r}$, and the triple Fourier series corresponding to the expansion of the periodic function, say $G(\mathbf{r})$, can be written as

$$G(\mathbf{r}) = \sum_{\mathbf{g}} C(\mathbf{g}) \exp(-2\pi i \mathbf{g}\cdot\mathbf{r}), \tag{1.1.2.7}$$

where $C(\mathbf{g})$ are the amplitudes of the Fourier waves, or Fourier coefficients, which are related to the experimental data. Numerous examples of such expansions appear throughout this volume.

The permissible wavevectors in the above expansion are restricted by the periodicity of the function $G(\mathbf{r})$. Since, by definition, $G(\mathbf{r}) = G(\mathbf{r}+\mathbf{r}_{\rm L})$, where $\mathbf{r}_{\rm L}$ is a direct-lattice vector, the right-hand side of (1.1.2.7) must remain unchanged when $\mathbf{r}$ is replaced by $\mathbf{r}+\mathbf{r}_{\rm L}$. This, however, can be true only if the scalar product $\mathbf{g}\cdot\mathbf{r}_{\rm L}$ is an integer.

Each of the above three aspects of crystallography may lead, independently, to a useful introduction of the reciprocal vectors, and there are many examples of this in the literature. It is interesting, however, to consider the representation of the equation

$$\mathbf{v}\cdot\mathbf{r}_{\rm L} = n, \tag{1.1.2.8}$$

which is common to all three, in its most convenient form. Obviously, the vector $\mathbf{v}$ which stands for the plane normal, the diffraction vector, and the wavevector in a Fourier expansion, may still be referred to any permissible basis and so may $\mathbf{r}_{\rm L}$, by an appropriate transformation.

Let $\mathbf{v} = U\mathbf{A} + V\mathbf{B} + W\mathbf{C}$, where $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ are linearly independent vectors. Equation (1.1.2.8) can then be written as

$$(U\mathbf{A} + V\mathbf{B} + W\mathbf{C})\cdot(u\mathbf{a} + v\mathbf{b} + w\mathbf{c}) = n, \tag{1.1.2.9}$$

or, in matrix notation,

$$(UVW)\begin{pmatrix}\mathbf{A}\\ \mathbf{B}\\ \mathbf{C}\end{pmatrix}\cdot(\mathbf{abc})\begin{pmatrix}u\\ v\\ w\end{pmatrix} = n, \tag{1.1.2.10}$$

or

$$(UVW)\begin{pmatrix}\mathbf{A}\cdot\mathbf{a} & \mathbf{A}\cdot\mathbf{b} & \mathbf{A}\cdot\mathbf{c}\\ \mathbf{B}\cdot\mathbf{a} & \mathbf{B}\cdot\mathbf{b} & \mathbf{B}\cdot\mathbf{c}\\ \mathbf{C}\cdot\mathbf{a} & \mathbf{C}\cdot\mathbf{b} & \mathbf{C}\cdot\mathbf{c}\end{pmatrix}\begin{pmatrix}u\\ v\\ w\end{pmatrix} = n. \tag{1.1.2.11}$$

The simplest representation of equation (1.1.2.8) results when the matrix of scalar products in (1.1.2.11) reduces to a unit matrix. This can be achieved (i) by choosing the basis vectors **ABC** to be orthonormal to the basis vectors **abc**, while requiring that the components of $\mathbf{r}_{\rm L}$ be integers, or (ii) by requiring that the bases **ABC** and **abc** coincide with the same orthonormal basis, *i.e.* expressing both $\mathbf{v}$ and $\mathbf{r}_{\rm L}$, in (1.1.2.8), in the same Cartesian system. If we choose the first alternative, it is seen that:

(1) The components of the vector $\mathbf{v}$, and hence those of $\mathbf{N}$, $\mathbf{h}$ and $\mathbf{g}$, are of necessity integers, since u, v and w are already integral. The components of $\mathbf{v}$ include Miller indices in the case of the lattice plane, they coincide with the orders of diffraction from a three-dimensional lattice of scatterers, and correspond to the summation indices in the triple Fourier series (1.1.2.7).

(2) The basis vectors $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ are reciprocal to $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$, as can be seen by comparing the scalar products in (1.1.2.11) with those in (1.1.2.1) and (1.1.2.2). In fact, the bases **ABC** and **abc** are mutually reciprocal. Since there are no restrictions on the integers U, V and W, the vector $\mathbf{v}$ belongs to a lattice which, on account of its basis, is called the reciprocal lattice.

It follows that, at least in the present case, algebraic simplicity goes together with ease of interpretation, which certainly accounts for much of the importance of the reciprocal lattice in crystallography. The second alternative of reducing the matrix in (1.1.2.11) to a unit matrix, a transformation of (1.1.2.8) to a Cartesian system, leads to non-integral components of the vectors, which makes any interpretation of $\mathbf{v}$ or $\mathbf{r}_{\rm L}$ much less transparent. However, transformations to Cartesian systems are often very useful in crystallographic computing and will be discussed below (see also Chapters 2.3 and 3.3 in this volume).

We shall, in what follows, abandon all the temporary notation used above and write the reciprocal-lattice vector as

$$\mathbf{h} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \tag{1.1.2.12}$$

or

$$\mathbf{h} = h_1\mathbf{a}^1 + h_2\mathbf{a}^2 + h_3\mathbf{a}^3 = \sum_{i=1}^{3} h_i\mathbf{a}^i, \tag{1.1.2.13}$$

and denote the direct-lattice vectors by $\mathbf{r}_{\rm L} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$, as above, or by

$$\mathbf{r}_{\rm L} = u^1\mathbf{a}_1 + u^2\mathbf{a}_2 + u^3\mathbf{a}_3 = \sum_{i=1}^{3} u^i\mathbf{a}_i. \tag{1.1.2.14}$$

The representations (1.1.2.13) and (1.1.2.14) are used in the tensor-algebraic formulation of the relationships between mutually reciprocal bases (see Section 1.1.4 below).

1.1.3. Fundamental relationships

We now present a brief derivation and a summary of the most important relationships between the direct and the reciprocal bases. The usual conventions of vector algebra are observed and the results are presented in the conventional crystallographic notation. Equations (1.1.2.1) and (1.1.2.2) now become

$$\mathbf{a}\cdot\mathbf{b}^* = \mathbf{a}\cdot\mathbf{c}^* = \mathbf{b}\cdot\mathbf{a}^* = \mathbf{b}\cdot\mathbf{c}^* = \mathbf{c}\cdot\mathbf{a}^* = \mathbf{c}\cdot\mathbf{b}^* = 0 \tag{1.1.3.1}$$

and

$$\mathbf{a}\cdot\mathbf{a}^* = \mathbf{b}\cdot\mathbf{b}^* = \mathbf{c}\cdot\mathbf{c}^* = 1, \tag{1.1.3.2}$$

respectively, and the relationships are obtained as follows.

1.1.3.1. Basis vectors

It is seen from (1.1.3.1) that $\mathbf{a}^*$ must be proportional to the vector product of $\mathbf{b}$ and $\mathbf{c}$,

$$\mathbf{a}^* = K(\mathbf{b}\times\mathbf{c}),$$

and, since $\mathbf{a}\cdot\mathbf{a}^* = 1$, the proportionality constant K equals $1/[\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c})]$. The mixed product $\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c})$ can be interpreted as the positive volume of the unit cell in the direct lattice only if $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ form a *right-handed* set. If the above condition is fulfilled, we obtain

$$\mathbf{a}^* = \frac{\mathbf{b}\times\mathbf{c}}{V}, \quad \mathbf{b}^* = \frac{\mathbf{c}\times\mathbf{a}}{V}, \quad \mathbf{c}^* = \frac{\mathbf{a}\times\mathbf{b}}{V} \tag{1.1.3.3}$$

and analogously

$$\mathbf{a} = \frac{\mathbf{b}^*\times\mathbf{c}^*}{V^*}, \quad \mathbf{b} = \frac{\mathbf{c}^*\times\mathbf{a}^*}{V^*}, \quad \mathbf{c} = \frac{\mathbf{a}^*\times\mathbf{b}^*}{V^*}, \tag{1.1.3.4}$$

where V and V^* are the volumes of the unit cells in the associated direct and reciprocal lattices, respectively. Use has been made of the fact that the mixed product, say $\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c})$, remains unchanged under cyclic rearrangement of the vectors that appear in it.

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1.1.3.2. Volumes

The reciprocal relationship of V and V^* follows readily. We have from equations (1.1.3.2), (1.1.3.3) and (1.1.3.4)

$$\mathbf{c}\cdot\mathbf{c}^* = \frac{(\mathbf{a}\times\mathbf{b})\cdot(\mathbf{a}^*\times\mathbf{b}^*)}{VV^*} = 1.$$

If we make use of the vector identity

$$(\mathbf{A}\times\mathbf{B})\cdot(\mathbf{C}\times\mathbf{D}) = (\mathbf{A}\cdot\mathbf{C})(\mathbf{B}\cdot\mathbf{D}) - (\mathbf{A}\cdot\mathbf{D})(\mathbf{B}\cdot\mathbf{C}), \quad (1.1.3.5)$$

and equations (1.1.3.1) and (1.1.3.2), it is seen that $V^* = 1/V$.

1.1.3.3. Angular relationships

The relationships of the angles α, β, γ between the pairs of vectors (**b**, **c**), (**c**, **a**) and (**a**, **b**), respectively, and the angles $\alpha^*, \beta^*, \gamma^*$ between the corresponding pairs of reciprocal basis vectors, can be obtained by simple vector algebra. For example, we have from (1.1.3.3):

(i) $\mathbf{b}^*\cdot\mathbf{c}^* = b^*c^*\cos\alpha^*$, with

$$b^* = \frac{ca\sin\beta}{V} \quad \text{and} \quad c^* = \frac{ab\sin\gamma}{V}$$

and (ii)

$$\mathbf{b}^*\cdot\mathbf{c}^* = \frac{(\mathbf{c}\times\mathbf{a})\cdot(\mathbf{a}\times\mathbf{b})}{V^2}.$$

If we make use of the identity (1.1.3.5), and compare the two expressions for $\mathbf{b}^*\cdot\mathbf{c}^*$, we readily obtain

$$\cos\alpha^* = \frac{\cos\beta\cos\gamma - \cos\alpha}{\sin\beta\sin\gamma}. \quad (1.1.3.6)$$

Similarly,

$$\cos\beta^* = \frac{\cos\gamma\cos\alpha - \cos\beta}{\sin\gamma\sin\alpha} \quad (1.1.3.7)$$

and

$$\cos\gamma^* = \frac{\cos\alpha\cos\beta - \cos\gamma}{\sin\alpha\sin\beta}. \quad (1.1.3.8)$$

The expressions for the cosines of the direct angles in terms of those of the reciprocal ones are analogous to (1.1.3.6)–(1.1.3.8). For example,

$$\cos\alpha = \frac{\cos\beta^*\cos\gamma^* - \cos\alpha^*}{\sin\beta^*\sin\gamma^*}.$$

1.1.3.4. Matrices of metric tensors

Various computational and algebraic aspects of mutually reciprocal bases are most conveniently expressed in terms of the metric tensors of these bases. The tensors will be treated in some detail in the next section, and only the definitions of their matrices are given and interpreted below.

Consider the length of the vector $\mathbf{r} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c}$. This is given by

$$|\mathbf{r}| = [(x\mathbf{a} + y\mathbf{b} + z\mathbf{c})\cdot(x\mathbf{a} + y\mathbf{b} + z\mathbf{c})]^{1/2} \quad (1.1.3.9)$$

and can be written in matrix form as

$$|\mathbf{r}| = [\boldsymbol{x}^T\boldsymbol{G}\boldsymbol{x}]^{1/2}, \quad (1.1.3.10)$$

where

$$\boldsymbol{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \quad \boldsymbol{x}^T = (xyz)$$

and

$$\boldsymbol{G} = \begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} & \mathbf{a}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{b}\cdot\mathbf{c} \\ \mathbf{c}\cdot\mathbf{a} & \mathbf{c}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \end{pmatrix} \quad (1.1.3.11)$$

$$= \begin{pmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ba\cos\gamma & b^2 & bc\cos\alpha \\ ca\cos\beta & cb\cos\alpha & c^2 \end{pmatrix}. \quad (1.1.3.12)$$

This is the matrix of the metric tensor of the direct basis, or briefly the direct metric. The corresponding reciprocal metric is given by

$$\boldsymbol{G}^* = \begin{pmatrix} \mathbf{a}^*\cdot\mathbf{a}^* & \mathbf{a}^*\cdot\mathbf{b}^* & \mathbf{a}^*\cdot\mathbf{c}^* \\ \mathbf{b}^*\cdot\mathbf{a}^* & \mathbf{b}^*\cdot\mathbf{b}^* & \mathbf{b}^*\cdot\mathbf{c}^* \\ \mathbf{c}^*\cdot\mathbf{a}^* & \mathbf{c}^*\cdot\mathbf{b}^* & \mathbf{c}^*\cdot\mathbf{c}^* \end{pmatrix} \quad (1.1.3.13)$$

$$= \begin{pmatrix} a^{*2} & a^*b^*\cos\gamma^* & a^*c^*\cos\beta^* \\ b^*a^*\cos\gamma^* & b^{*2} & b^*c^*\cos\alpha^* \\ c^*a^*\cos\beta^* & c^*b^*\cos\alpha^* & c^{*2} \end{pmatrix}. \quad (1.1.3.14)$$

The matrices $\boldsymbol{G}$ and $\boldsymbol{G}^*$ are of fundamental importance in crystallographic computations and transformations of basis vectors and coordinates from direct to reciprocal space and *vice versa.* Examples of applications are presented in Part 3 of this volume and in the remaining sections of this chapter.

It can be shown (*e.g.* Buerger, 1941) that the determinants of $\boldsymbol{G}$ and $\boldsymbol{G}^*$ equal the squared volumes of the direct and reciprocal unit cells, respectively. Thus,

$$\det(\boldsymbol{G}) = [\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c})]^2 = V^2 \quad (1.1.3.15)$$

and

$$\det(\boldsymbol{G}^*) = [\mathbf{a}^*\cdot(\mathbf{b}^*\times\mathbf{c}^*)]^2 = V^{*2}, \quad (1.1.3.16)$$

and a direct expansion of the determinants, from (1.1.3.12) and (1.1.3.14), leads to

$$V = abc(1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma)^{1/2} \quad (1.1.3.17)$$

and

$$V^* = a^*b^*c^*(1 - \cos^2\alpha^* - \cos^2\beta^* - \cos^2\gamma^* + 2\cos\alpha^*\cos\beta^*\cos\gamma^*)^{1/2}. \quad (1.1.3.18)$$

The following algorithm has been found useful in computational applications of the above relationships to calculations in reciprocal space (*e.g.* data reduction) and in direct space (*e.g.* crystal geometry).

(1) Input the direct unit-cell parameters and construct the matrix of the metric tensor [*cf.* equation (1.1.3.12)].

(2) Compute the determinant of the matrix $\boldsymbol{G}$ and find the inverse matrix, $\boldsymbol{G}^{-1}$; this inverse matrix is just $\boldsymbol{G}^*$, the matrix of the metric tensor of the reciprocal basis (see also Section 1.1.4 below).

(3) Use the elements of $\boldsymbol{G}^*$, and equation (1.1.3.14), to obtain the parameters of the reciprocal unit cell.

The direct and reciprocal sets of unit-cell parameters, as well as the corresponding metric tensors, are now available for further calculations.

Explicit relations between direct- and reciprocal-lattice parameters, valid for the various crystal systems, are given in most

textbooks on crystallography [see also Chapters 1.1 and 1.2 of Volume C (Koch, 2004)].

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 δ^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

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