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, $G(\mathbf{r}) = G(\mathbf{r} + \mathbf{r}_L)$, where $\mathbf{r}_L$ is a direct-lattice vector, the right-hand side of (1.1.2.7) must remain unchanged when $\mathbf{r}$ is replaced by $\mathbf{r} + \mathbf{r}_L$. This, however, can be true only if the scalar product $\mathbf{g} \cdot \mathbf{r}_L$ 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

$$\mathbf{v} \cdot \mathbf{r}_L = n, \tag{1.1.2.8}$$

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 $\mathbf{r}_L$, 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 $\mathbf{r}_L$ 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 $\mathbf{r}_L$, 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 $\mathbf{r}_L$ 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 $\mathbf{r}_L = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$, as above, or by

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

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.

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

references