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formula, and represent the components of the rotated vectors in coordinate systems that might be of interest.

Let us decompose the vector $\mathbf{r}$ and the (target) vector $\mathbf{r}'$ into their components which are parallel ($\|$) and perpendicular ($\perp$) to the axis of rotation:

$$\mathbf{r} = \mathbf{r}_{\|} + \mathbf{r}_{\perp} \qquad (1.1.4.22)$$

and

$$\mathbf{r}' = \mathbf{r}'_{\|} + \mathbf{r}'_{\perp}. \qquad (1.1.4.23)$$

It can be seen from Fig. 1.1.4.1 that the parallel components of $\mathbf{r}$ and $\mathbf{r}'$ are

$$\mathbf{r}_{\|} = \mathbf{r}'_{\|} = \mathbf{k}(\mathbf{k}\cdot\mathbf{r}) \qquad (1.1.4.24)$$

and thus

$$\mathbf{r}_{\perp} = \mathbf{r} - \mathbf{k}(\mathbf{k}\cdot\mathbf{r}). \qquad (1.1.4.25)$$

Only a suitable expression for $\mathbf{r}'_{\perp}$ is missing. We can find this by decomposing $\mathbf{r}'_{\perp}$ into its components (i) parallel to $\mathbf{r}_{\perp}$ and (ii) parallel to $\mathbf{k}\times\mathbf{r}_{\perp}$. We have, as in (1.1.4.24),

$$\mathbf{r}'_{\perp} = \frac{\mathbf{r}_{\perp}}{|\mathbf{r}_{\perp}|}\left(\frac{\mathbf{r}_{\perp}}{|\mathbf{r}_{\perp}|}\cdot\mathbf{r}'_{\perp}\right) + \frac{\mathbf{k}\times\mathbf{r}_{\perp}}{|\mathbf{k}\times\mathbf{r}_{\perp}|}\left(\frac{\mathbf{k}\times\mathbf{r}_{\perp}}{|\mathbf{k}\times\mathbf{r}_{\perp}|}\cdot\mathbf{r}'_{\perp}\right). \qquad (1.1.4.26)$$

We observe, using Fig. 1.1.4.1, that

$$|\mathbf{r}'_{\perp}| = |\mathbf{r}_{\perp}| = |\mathbf{k}\times\mathbf{r}_{\perp}|$$

and

$$\mathbf{k}\times\mathbf{r}_{\perp} = \mathbf{k}\times\mathbf{r},$$

and, further,

$$\mathbf{r}'_{\perp}\cdot\mathbf{r}_{\perp} = |\mathbf{r}_{\perp}|^2\cos\theta$$

and

$$\mathbf{r}'_{\perp}\cdot(\mathbf{k}\times\mathbf{r}_{\perp}) = \mathbf{k}\cdot(\mathbf{r}'_{\perp}\times\mathbf{r}_{\perp}) = |\mathbf{r}_{\perp}|^2\sin\theta,$$

since the unit vector $\mathbf{k}$ is perpendicular to the plane containing the vectors $\mathbf{r}_{\perp}$ and $\mathbf{r}'_{\perp}$. Equation (1.1.4.26) now reduces to

$$\mathbf{r}'_{\perp} = \mathbf{r}_{\perp}\cos\theta + (\mathbf{k}\times\mathbf{r})\sin\theta \qquad (1.1.4.27)$$

and equations (1.1.4.23), (1.1.4.25) and (1.1.4.27) lead to the required result

$$\mathbf{r}' = \mathbf{k}(\mathbf{k}\cdot\mathbf{r})(1-\cos\theta) + \mathbf{r}\cos\theta + (\mathbf{k}\times\mathbf{r})\sin\theta. \qquad (1.1.4.28)$$

The above general expression can be written as a linear transformation by referring the vectors to an appropriate basis or bases. We choose here $\mathbf{r} = x^j\mathbf{a}_j$, $\mathbf{r}' = x'^i\mathbf{a}_i$ and assume that the components of $\mathbf{k}$ are available in the direct and reciprocal bases.

If we make use of equations (1.1.4.9) and (1.1.4.21), (1.1.4.28) can be written as

$$x'^i = k^i(k_jx^j)(1-\cos\theta) + \delta^i_jx^j\cos\theta + Vg^{im}e_{mpj}k^px^j\sin\theta, \qquad (1.1.4.29)$$

or briefly

$$x'^i = R^i_jx^j, \qquad (1.1.4.30)$$

where

$$R^i_j = k^ik_j(1-\cos\theta) + \delta^i_j\cos\theta + Vg^{im}e_{mpj}k^p\sin\theta \qquad (1.1.4.31)$$

is a matrix element of the rotation operator $\mathbf{R}$ which carries the vector $\mathbf{r}$ into the vector $\mathbf{r}'$. Of course, the representation (1.1.4.31) of $\mathbf{R}$ depends on our choice of reference bases.

If all the vectors are referred to a Cartesian basis, that is three orthogonal unit vectors, the direct and reciprocal metric tensors reduce to a unit tensor, there is no difference between covariant and contravariant quantities, and equation (1.1.4.31) reduces to

$$R_{ij} = k_ik_j(1-\cos\theta) + \delta_{ij}\cos\theta + e_{ipj}k_p\sin\theta, \qquad (1.1.4.32)$$

where all the indices have been taken as subscripts, but the summation convention is still observed. The relative simplicity of (1.1.4.32), as compared to (1.1.4.31), often justifies the transformation of all the vector quantities to a Cartesian basis. This is certainly the case for any extensive calculation in which covariances of the structural parameters are not considered.

1.1.5. Transformations

1.1.5.1. *Transformations of coordinates*

It happens rather frequently that a vector referred to a given basis has to be re-expressed in terms of another basis, and it is then required to find the relationship between the components (coordinates) of the vector in the two bases. Such situations have already been indicated in the previous section. The purpose of the present section is to give a general method of finding such relationships (transformations), and discuss some simplifications brought about by the use of mutually reciprocal and Cartesian bases. We do not assume anything about the bases, in the general treatment, and hence the tensor formulation of Section 1.1.4 is not appropriate at this stage.

Let

$$\mathbf{r} = \sum_{j=1}^{3}u_j(1)\mathbf{c}_j(1) \qquad (1.1.5.1)$$

and

$$\mathbf{r} = \sum_{j=1}^{3}u_j(2)\mathbf{c}_j(2) \qquad (1.1.5.2)$$

be the *given* and *required* representations of the vector $\mathbf{r}$, respectively. Upon the formation of scalar products of equations (1.1.5.1) and (1.1.5.2) with the vectors of the second basis, and employing again the summation convention, we obtain

$$u_k(1)[\mathbf{c}_k(1)\cdot\mathbf{c}_l(2)] = u_k(2)[\mathbf{c}_k(2)\cdot\mathbf{c}_l(2)], \quad l = 1,2,3 \qquad (1.1.5.3)$$

or

$$u_k(1)G_{kl}(12) = u_k(2)G_{kl}(22), \quad l = 1,2,3, \qquad (1.1.5.4)$$

where $G_{kl}(12) = \mathbf{c}_k(1)\cdot\mathbf{c}_l(2)$ and $G_{kl}(22) = \mathbf{c}_k(2)\cdot\mathbf{c}_l(2)$. Similarly, if we choose the basis vectors $\mathbf{c}_l(1)$, l = 1, 2, 3, as the multipliers of (1.1.5.1) and (1.1.5.2), we obtain

$$u_k(1)G_{kl}(11) = u_k(2)G_{kl}(21), \quad l = 1,2,3, \qquad (1.1.5.5)$$

where $G_{kl}(11) = \mathbf{c}_k(1)\cdot\mathbf{c}_l(1)$ and $G_{kl}(21) = \mathbf{c}_k(2)\cdot\mathbf{c}_l(1)$. Rewriting (1.1.5.4) and (1.1.5.5) in symbolic matrix notation, we have

$$\boldsymbol{u}^T(1)\boldsymbol{G}(12) = \boldsymbol{u}^T(2)\boldsymbol{G}(22), \qquad (1.1.5.6)$$

leading to

$$\boldsymbol{u}^T(1) = \boldsymbol{u}^T(2)\{\boldsymbol{G}(22)[\boldsymbol{G}(12)]^{-1}\}$$

and

$$\boldsymbol{u}^T(2) = \boldsymbol{u}^T(1)\{\boldsymbol{G}(12)[\boldsymbol{G}(22)]^{-1}\}, \qquad (1.1.5.7)$$

and

$$\boldsymbol{u}^T(1)\boldsymbol{G}(11) = \boldsymbol{u}^T(2)\boldsymbol{G}(21), \qquad (1.1.5.8)$$

leading to

$$\boldsymbol{u}^T(1) = \boldsymbol{u}^T(2)\{\boldsymbol{G}(21)[\boldsymbol{G}(11)]^{-1}\}$$

and

$$\boldsymbol{u}^T(2) = \boldsymbol{u}^T(1)\{\boldsymbol{G}(11)[\boldsymbol{G}(21)]^{-1}\}. \quad (1.1.5.9)$$

Equations (1.1.5.7) and (1.1.5.9) are symbolic general expressions for the transformation of the coordinates of $\mathbf{r}$ from one representation to the other.

In the general case, therefore, we require the matrices of scalar products of the basis vectors, $\boldsymbol{G}(12)$ and $\boldsymbol{G}(22)$ *or* $\boldsymbol{G}(11)$ and $\boldsymbol{G}(21)$ – depending on whether the basis $\mathbf{c}_k(2)$ or $\mathbf{c}_k(1)$, k = 1, 2, 3, was chosen to multiply scalarly equations (1.1.5.1) and (1.1.5.2). Note, however, the following simplifications.

(i) If the bases $\mathbf{c}_k(1)$ and $\mathbf{c}_k(2)$ are mutually reciprocal, each of the matrices of mixed scalar products, $\boldsymbol{G}(12)$ and $\boldsymbol{G}(21)$, reduces to a unit matrix. In this important special case, the transformation is effected by the matrices of the metric tensors of the bases in question. This can be readily seen from equations (1.1.5.7) and (1.1.5.9), which then reduce to the relationships between the covariant and contravariant components of the same vector [see equations (1.1.4.11) and (1.1.4.12) above].

(ii) If one of the bases, say $\mathbf{c}_k(2)$, is Cartesian, its metric tensor is by definition a unit tensor, and the transformations in (1.1.5.7) reduce to

$$\boldsymbol{u}^T(1) = \boldsymbol{u}^T(2)[\boldsymbol{G}(12)]^{-1}$$

and

$$\boldsymbol{u}^T(2) = \boldsymbol{u}^T(1)\boldsymbol{G}(12). \quad (1.1.5.10)$$

The transformation matrix is now the mixed matrix of the scalar products, whether or not the basis $\mathbf{c}_k(1)$, k = 1, 2, 3, is also Cartesian. If, however, both bases are Cartesian, the transformation can also be interpreted as a rigid rotation of the coordinate axes (see Chapter 3.3).

It should be noted that the above transformations do not involve any shift of the origin. Transformations involving such shifts, notably the symmetry transformations of the space group, are treated rather extensively in Volume A of *International Tables for Crystallography* (1995) [see *e.g.* Part 5 there (Arnold, 1983)].

1.1.5.2. *Example*

This example deals with the construction of a Cartesian system in a crystal with given basis vectors of its direct lattice. We shall also require that the Cartesian system bears a clear relationship to at least one direction in each of the direct and reciprocal lattices of the crystal; this may be useful in interpreting a physical property which has been measured along a given lattice vector or which is associated with a given lattice plane. For a better consistency of notation, the Cartesian components will be denoted as contravariant.

The appropriate version of equations (1.1.5.1) and (1.1.5.2) is now

$$\mathbf{r} = x^i\mathbf{a}_i \quad (1.1.5.11)$$

and

$$\mathbf{r} = X^k\mathbf{e}_k, \quad (1.1.5.12)$$

where the Cartesian basis vectors are: $\mathbf{e}_1 = \mathbf{r}_L/|\mathbf{r}_L|$, $\mathbf{e}_2 = \mathbf{r}^*/|\mathbf{r}^*|$ and $\mathbf{e}_3 = \mathbf{e}_1 \times \mathbf{e}_2$, and the vectors $\mathbf{r}_L$ and $\mathbf{r}^*$ are given by

$$\mathbf{r}_L = u^i\mathbf{a}_i \text{ and } \mathbf{r}^* = h_k\mathbf{a}^k,$$

where u^i and h_k, i, k = 1, 2, 3, are arbitrary integers. The vectors $\mathbf{r}_L$ and $\mathbf{r}^*$ must be mutually perpendicular, $\mathbf{r}_L \cdot \mathbf{r}^* = u^ih_i = 0$. The $X^1(X)$ axis of the Cartesian system thus coincides with a direct-lattice vector, and the $X^2(Y)$ axis is parallel to a vector in the reciprocal lattice.

Since the basis in (1.1.5.12) is a Cartesian one, the required transformations are given by equations (1.1.5.10) as

$$x^i = X^k(T^{-1})^i_k \text{ and } X^i = x^kT^i_k, \quad (1.1.5.13)$$

where $T^i_k = \mathbf{a}_k \cdot \mathbf{e}_i$, k, i = 1, 2, 3, form the matrix of the scalar products. If we make use of the relationships between covariant and contravariant basis vectors, and the tensor formulation of the vector product, given in Section 1.1.4 above (see also Chapter 3.1), we obtain

$$\begin{aligned} T^1_k &= \frac{1}{|\mathbf{r}_L|}g_{ki}u^i \\ T^2_k &= \frac{1}{|\mathbf{r}^*|}h_k \\ T^3_k &= \frac{V}{|\mathbf{r}_L||\mathbf{r}^*|}e_{kip}u^ig^{pl}h_l. \end{aligned} \quad (1.1.5.14)$$

Note that the other convenient choice, $\mathbf{e}_1 \propto \mathbf{r}^*$ and $\mathbf{e}_2 \propto \mathbf{r}_L$, interchanges the first two columns of the matrix $\boldsymbol{T}$ in (1.1.5.14) and leads to a change of the signs of the elements in the third column. This can be done by writing e_{kpi} instead of e_{kip}, while leaving the rest of T^3_k unchanged.

1.1.6. Some analytical aspects of the reciprocal space

1.1.6.1. *Continuous Fourier transform*

Of great interest in crystallographic analyses are Fourier transforms and these are closely associated with the dual bases examined in this chapter. Thus, *e.g.*, the inverse Fourier transform of the electron-density function of the crystal

$$F(\mathbf{h}) = \int_{\text{cell}} \rho(\mathbf{r})\exp(2\pi i\mathbf{h}\cdot\mathbf{r})\,\mathrm{d}^3\mathbf{r}, \quad (1.1.6.1)$$

where $\rho(\mathbf{r})$ is the electron-density function at the point $\mathbf{r}$ and the integration extends over the volume of a unit cell, is the fundamental model of the contribution of the distribution of crystalline matter to the intensity of the scattered radiation. For the conventional Bragg scattering, the function given by (1.1.6.1), and known as the *structure factor*, may assume nonzero values *only* if $\mathbf{h}$ can be represented as a reciprocal-lattice vector. Chapter 1.2 is devoted to a discussion of the structure factor of the Bragg reflection, while Chapters 4.1, 4.2 and 4.3 discuss circumstances under which the scattering need not be confined to the points of the reciprocal lattice only, and may be represented by reciprocal-space vectors with non-integral components.

1.1.6.2. *Discrete Fourier transform*

The electron density $\rho(\mathbf{r})$ in (1.1.6.1) is one of the most common examples of a function which has the periodicity of the crystal. Thus, for an ideal (infinite) crystal the electron density $\rho(\mathbf{r})$ can be written as

$$\rho(\mathbf{r}) = \rho(\mathbf{r} + u\mathbf{a} + v\mathbf{b} + w\mathbf{c}), \quad (1.1.6.2)$$

and, as such, it can be represented by a three-dimensional Fourier series of the form

$$\rho(\mathbf{r}) = \sum_{\mathbf{g}} C(\mathbf{g})\exp(-2\pi i\mathbf{g}\cdot\mathbf{r}), \quad (1.1.6.3)$$

where the periodicity requirement (1.1.6.2) enables one to represent all the $\mathbf{g}$ vectors in (1.1.6.3) as vectors in the reciprocal lattice (see also Section 1.1.2 above). If we insert the series (1.1.6.3) in the

references