$$\mathbf{e}_i \cdot \mathbf{e}'_j = A_i^j \mathbf{e}'_k \cdot e'_j = A_i^j g'_{kj} = A_i^j \delta_{kj} \quad \text{(written correctly)},$$

which can also be written, if one notes that variance is not apparent in an orthonormal frame of coordinates and that the position of indices is therefore not important, as

$$\mathbf{e}_i \cdot \mathbf{e}'_j = A_i^j \quad \text{(written incorrectly)}.$$

The matrix coefficients, A_i^j, are the direction cosines of $\mathbf{e}'_j$ with respect to the $\mathbf{e}_i$ basis vectors. Similarly, we have

$$B_j^i = \mathbf{e}_i \cdot \mathbf{e}'_j$$

so that

$$A_i^j = B_j^i \quad \text{or} \quad A = B^T,$$

where ^{T} indicates transpose. It follows that

$$A = B^T \text{ and } A = B^{-1}$$

so that

$$\left.\begin{aligned} A^T &= A^{-1} \quad \Rightarrow \quad A^T A = I \\ B^T &= B^{-1} \quad \Rightarrow \quad B^T B = I. \end{aligned}\right\} \qquad (1.1.2.7)$$

The matrices A and B are unitary matrices or matrices of rotation and

$$\Delta(A)^2 = \Delta(B)^2 = 1 \Rightarrow \Delta(A) = \pm 1. \qquad (1.1.2.8)$$

If $\Delta(A) = 1$ the senses of the axes are not changed – *proper* rotation.

If $\Delta(A) = -1$ the senses of the axes are changed – *improper* rotation. (The right hand is transformed into a left hand.)

One can write for the coefficients A_i^j

$$A_i^j B_j^k = \delta_i^k; \quad A_i^j A_j^k = \delta_i^k,$$

giving six relations between the nine coefficients A_i^j. There are thus *three* independent coefficients of the 3×3 matrix A.

1.1.2.4. *Covariant coordinates – dual or reciprocal space*

1.1.2.4.1. *Covariant coordinates*

Using the developments (1.1.2.1) and (1.1.2.5), the scalar products of a vector $\mathbf{x}$ and of the basis vectors $\mathbf{e}_i$ can be written

$$x_i = \mathbf{x} \cdot \mathbf{e}_i = x^j \mathbf{e}_j \cdot \mathbf{e}_i = x^j g_{ij}. \qquad (1.1.2.9)$$

The n quantities x_i are called *covariant* components, and we shall see the reason for this a little later. The relations (1.1.2.9) can be considered as a system of equations of which the components x^j are the unknowns. One can solve it since $\Delta(g_{ij}) \neq 0$ (see the end of Section 1.1.2.2). It follows that

$$x^j = x_i g^{ij} \qquad (1.1.2.10)$$

with

$$g^{ij} g_{jk} = \delta_k^i. \qquad (1.1.2.11)$$

The table of the g^{ij}'s is the inverse of the table of the g_{ij}'s. Let us now take up the development of $\mathbf{x}$ with respect to the basis $\mathbf{e}_i$:

$$\mathbf{x} = x^i \mathbf{e}_i.$$

Let us replace x^i by the expression (1.1.2.10):

$$\mathbf{x} = x_j g^{ij} \mathbf{e}_i, \qquad (1.1.2.12)$$

and let us introduce the set of n vectors

$$\mathbf{e}^j = g^{ij} \mathbf{e}_i \qquad (1.1.2.13)$$

which span the space E^n $(j = 1, \ldots, n)$. *This set of n vectors forms a basis* since (1.1.2.12) can be written with the aid of (1.1.2.13) as

$$\mathbf{x} = x_j \mathbf{e}^j. \qquad (1.1.2.14)$$

The x_j's are the components of $\mathbf{x}$ in the basis $\mathbf{e}^j$. This basis is called the *dual basis*. By using (1.1.2.11) and (1.1.2.13), one can show in the same way that

$$\mathbf{e}_j = g_{ij} \mathbf{e}^j. \qquad (1.1.2.15)$$

It can be shown that the basis vectors $\mathbf{e}^j$ transform in a change of basis like the components x^j of the physical space. They are therefore *contravariant*. In a similar way, the components x_j of a vector $\mathbf{x}$ with respect to the basis $\mathbf{e}^j$ transform in a change of basis like the basis vectors in direct space, $\mathbf{e}_j$; they are therefore *covariant*:

$$\left.\begin{aligned} \mathbf{e}^j = B_k^j \mathbf{e}'^k; \quad & \mathbf{e}'^k = A_j^k \mathbf{e}^j \\ x_i = A_i^j x'_j; \quad & x'_j = B_j^i x_i. \end{aligned}\right\} \qquad (1.1.2.16)$$

1.1.2.4.2. *Reciprocal space*

Let us take the scalar products of a covariant vector $\mathbf{e}_i$ and a contravariant vector $\mathbf{e}^j$:

$$\mathbf{e}_i \cdot \mathbf{e}^j = \mathbf{e}_i \cdot g^{jk} \mathbf{e}_k = \mathbf{e}_i \cdot \mathbf{e}_k g^{jk} = g_{ik} g^{jk} = \delta_i^j$$

[using expressions (1.1.2.5), (1.1.2.11) and (1.1.2.13)].

The relation we obtain, $\mathbf{e}_i \cdot \mathbf{e}^j = \delta_i^j$, is identical to the relations defining the reciprocal lattice in crystallography; *the reciprocal basis then is identical to the dual basis* $\mathbf{e}^i$.

1.1.2.4.3. *Properties of the metric tensor*

In a change of basis, following (1.1.2.3) and (1.1.2.5), the g_{ij}'s transform according to

$$\left.\begin{aligned} g_{ij} &= A_i^k A_j^m g'_{km} \\ g'_{ij} &= B_i^k B_j^m g_{km}. \end{aligned}\right\} \qquad (1.1.2.17)$$

Let us now consider the scalar products, $\mathbf{e}^i \cdot \mathbf{e}^j$, of two contravariant basis vectors. Using (1.1.2.11) and (1.1.2.13), it can be shown that

$$\mathbf{e}^i \cdot \mathbf{e}^j = g^{ij}. \qquad (1.1.2.18)$$

In a change of basis, following (1.1.2.16), the g^{ij}'s transform according to

$$\left.\begin{aligned} g^{ij} &= B_k^i B_m^j g'^{km} \\ g'^{ij} &= A_k^i A_m^j g^{km}. \end{aligned}\right\} \qquad (1.1.2.19)$$

The volumes V' and V of the cells built on the basis vectors $\mathbf{e}'_i$ and $\mathbf{e}_i$, respectively, are given by the triple scalar products of these two sets of basis vectors and are related by

$$\begin{aligned} V' &= (\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3) \\ &= \Delta(B_j^i)(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3) \\ &= \Delta(B_j^i) V, \end{aligned} \qquad (1.1.2.20)$$

where $\Delta(B_j^i)$ is the determinant associated with the transformation matrix between the two bases. From (1.1.2.17) and (1.1.2.20), we can write

$$\Delta(g'_{ij}) = \Delta(B_i^k)\Delta(B_j^m)\Delta(g_{km}).$$