

3.1. DISTANCES, ANGLES, AND THEIR STANDARD UNCERTAINTIES

or

$$\mathbf{u} \cdot \mathbf{v} = u_i v^i. \quad (3.1.4.4)$$

With this notation, the angle calculation of (3.1.4.1) becomes

$$\varphi = \cos^{-1}[u^i v_i / (uv)] = \cos^{-1}[u_i v^i / (uv)]. \quad (3.1.4.5)$$

The summations in (3.1.4.3), (3.1.4.4) and (3.1.4.5) include only three terms, and are thus equivalent in numerical effort to the computation in a Cartesian system, in which the metric tensor is represented by the unit matrix and there is no numerical distinction between covariant components and contravariant components.

Appreciation of the elegance of tensor formulations may be enhanced by noting that corresponding to the metric tensor  $\mathbf{g}$  with components  $g_{ij}$  there is a contravariant metric tensor  $\mathbf{g}^*$  with components

$$g^{ij} = \mathbf{a}^i \cdot \mathbf{a}^j. \quad (3.1.4.6)$$

The  $\mathbf{a}^i$  are contravariant basis vectors, known to crystallographers as reciprocal axes. Expressions parallel to (3.1.4.2) may be written, in which  $\mathbf{g}^*$  plays the role of converting covariant components to contravariant components. These tensors thus express mathematically the crystallographic notions of crystal space and reciprocal space [see Chapter 1.1 and Sands (1982a)].

3.1.5. Vector product

The scalar product defined in Section 3.1.2 is one multiplicative operation of two vectors that may be defined; another is the vector product, which is denoted as  $\mathbf{u} \wedge \mathbf{v}$  (or  $\mathbf{u} \times \mathbf{v}$  or  $[\mathbf{u}\mathbf{v}]$ ). The vector product of vectors  $\mathbf{u}$  and  $\mathbf{v}$  is defined as a vector of length  $uv \sin \varphi$ , where  $\varphi$  is the angle between the vectors, and of direction perpendicular to both  $\mathbf{u}$  and  $\mathbf{v}$  in the sense that  $\mathbf{u}$ ,  $\mathbf{v}$  and  $\mathbf{u} \wedge \mathbf{v}$  form a right-handed system;  $\mathbf{u} \wedge \mathbf{v}$  is generated by rotating  $\mathbf{u}$  into  $\mathbf{v}$  and advancing in the direction of a right-handed screw. The magnitude of  $\mathbf{u} \wedge \mathbf{v}$ , given by

$$|\mathbf{u} \wedge \mathbf{v}| = uv \sin \varphi \quad (3.1.5.1)$$

is equal to the area of the parallelogram defined by  $\mathbf{u}$  and  $\mathbf{v}$ .

It follows from the definition that

$$\mathbf{u} \wedge \mathbf{v} = -\mathbf{v} \wedge \mathbf{u}. \quad (3.1.5.2)$$

3.1.6. Permutation tensors

Many relationships involving vector products may be expressed compactly and conveniently in terms of the permutation tensors, defined as

$$\varepsilon_{ijk} = \mathbf{a}_i \cdot \mathbf{a}_j \wedge \mathbf{a}_k \quad (3.1.6.1)$$

$$\varepsilon^{ijk} = \mathbf{a}^i \cdot \mathbf{a}^j \wedge \mathbf{a}^k. \quad (3.1.6.2)$$

Since  $\mathbf{a}_i \cdot \mathbf{a}_j \wedge \mathbf{a}_k$  represents the volume of the parallelepiped defined by vectors  $\mathbf{a}_i$ ,  $\mathbf{a}_j$ ,  $\mathbf{a}_k$ , it follows that  $\varepsilon_{ijk}$  vanishes if any two indices are equal to each other. The same argument applies, of course, to  $\varepsilon^{ijk}$ . That is,

$$\varepsilon_{ijk} = 0, \quad \varepsilon^{ijk} = 0, \quad \text{if } j = i \text{ or } k = i \text{ or } k = j. \quad (3.1.6.3)$$

If the indices are all different,

$$\varepsilon_{ijk} = PV, \quad \varepsilon^{ijk} = PV^* \quad (3.1.6.4)$$

for even permutations of  $ijk$  (123, 231, or 312), and

$$\varepsilon_{ijk} = -PV, \quad \varepsilon^{ijk} = -PV^* \quad (3.1.6.5)$$

for odd permutations (132, 213, or 321). Here,  $P = +1$  for right-handed axes,  $P = -1$  for left-handed axes,  $V$  is the unit-cell volume, and  $V^* = 1/V$  is the volume of the reciprocal cell defined by the reciprocal basis vectors  $\mathbf{a}^i$ ,  $\mathbf{a}^j$ ,  $\mathbf{a}^k$ .

A discussion of the properties of the permutation tensors may be found in Sands (1982a). In right-handed Cartesian systems, where  $P = 1$ , and  $V = V^* = 1$ , the permutation tensors are equivalent to the permutation symbols denoted by  $e_{ijk}$ .

3.1.7. Components of vector product

As is shown in Sands (1982a), the components of the vector product  $\mathbf{u} \wedge \mathbf{v}$  are given by

$$\mathbf{u} \wedge \mathbf{v} = \varepsilon_{ijk} u^i v^j \mathbf{a}^k, \quad (3.1.7.1)$$

where again  $\mathbf{a}^k$  is a reciprocal basis vector (some writers use  $\mathbf{a}^*$ ,  $\mathbf{b}^*$ ,  $\mathbf{c}^*$  to represent the reciprocal axes). A special case of (3.1.7.1) is

$$\mathbf{a}_i \wedge \mathbf{a}_j = \varepsilon_{ijk} \mathbf{a}^k, \quad (3.1.7.2)$$

which may be taken as a defining equation for the reciprocal basis vectors. Similarly,

$$\mathbf{a}^i \wedge \mathbf{a}^j = \varepsilon^{ijk} \mathbf{a}_k, \quad (3.1.7.3)$$

which completes the characterization of the dual vector system with basis vectors  $\mathbf{a}_i$  and  $\mathbf{a}^j$  obeying

$$\mathbf{a}_i \cdot \mathbf{a}^j = \delta_i^j. \quad (3.1.7.4)$$

In (3.1.7.4),  $\delta_i^j$  is the Kronecker delta, which equals 1 if  $i = j$ , 0 if  $i \neq j$ . The relationships between these quantities are explored at some length in Sands (1982a).

3.1.8. Some vector relationships

The results developed above lead to several useful relationships between vectors; for derivations, see Sands (1982a).

3.1.8.1. Triple vector product

$$\mathbf{u} \wedge (\mathbf{v} \wedge \mathbf{w}) = (\mathbf{u} \cdot \mathbf{w})\mathbf{v} - (\mathbf{u} \cdot \mathbf{v})\mathbf{w} \quad (3.1.8.1)$$

$$(\mathbf{u} \wedge \mathbf{v}) \wedge \mathbf{w} = -(\mathbf{v} \cdot \mathbf{w})\mathbf{u} + (\mathbf{u} \cdot \mathbf{w})\mathbf{v}. \quad (3.1.8.2)$$