

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 $[\mathbf{uv}]$). The vector product of vectors \mathbf{u} and \mathbf{v} is defined as a vector of length $uv \sin \varphi$, where φ 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 ε_{ijk} vanishes if any two indices are equal to each other. The same argument applies, of course, to ε^{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), δ_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

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

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

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3.1.8.2. Scalar product of vector products

$$(\mathbf{u} \wedge \mathbf{v}) \cdot (\mathbf{w} \wedge \mathbf{z}) = (\mathbf{u} \cdot \mathbf{w})(\mathbf{v} \cdot \mathbf{z}) - (\mathbf{u} \cdot \mathbf{z})(\mathbf{v} \cdot \mathbf{w}). \quad (3.1.8.3)$$

A derivation of this result may be found also in Shmueli (1974).

3.1.8.3. Vector product of vector products

$$(\mathbf{u} \wedge \mathbf{v}) \wedge (\mathbf{w} \wedge \mathbf{z}) = (\mathbf{u} \cdot \mathbf{w} \wedge \mathbf{z})\mathbf{v} - (\mathbf{v} \cdot \mathbf{w} \wedge \mathbf{z})\mathbf{u} \quad (3.1.8.4)$$

$$(\mathbf{u} \wedge \mathbf{v}) \wedge (\mathbf{w} \wedge \mathbf{z}) = (\mathbf{u} \cdot \mathbf{v} \wedge \mathbf{z})\mathbf{w} - (\mathbf{u} \cdot \mathbf{v} \wedge \mathbf{w})\mathbf{z}. \quad (3.1.8.5)$$

3.1.9. Planes

Among several ways of characterizing a plane in a general rectilinear coordinate system is a description in terms of the coordinates of three non-collinear points that lie in the plane. If the points are U , V and W , lying at the ends of vectors \mathbf{u} , \mathbf{v} and \mathbf{w} , the vectors $\mathbf{u} - \mathbf{v}$, $\mathbf{v} - \mathbf{w}$ and $\mathbf{w} - \mathbf{u}$ are in the plane. The vector

$$\mathbf{z} = (\mathbf{u} - \mathbf{v}) \wedge (\mathbf{v} - \mathbf{w}) \quad (3.1.9.1)$$

is normal to the plane. Expansion of (3.1.9.1) yields

$$\mathbf{z} = (\mathbf{u} \wedge \mathbf{v}) + (\mathbf{v} \wedge \mathbf{w}) + (\mathbf{w} \wedge \mathbf{u}). \quad (3.1.9.2)$$

Making use of (3.1.7.1),

$$\mathbf{z} = \varepsilon_{ijk}(u^j v^k + v^j w^k + w^j u^k)\mathbf{a}^i. \quad (3.1.9.3)$$

If now \mathbf{x} is any vector from the origin to the plane, $\mathbf{x} - \mathbf{u}$ is in the plane, and

$$(\mathbf{x} - \mathbf{u}) \cdot \mathbf{z} = 0. \quad (3.1.9.4)$$

From (3.1.9.2),

$$\mathbf{u} \cdot \mathbf{z} = \mathbf{u} \cdot \mathbf{v} \wedge \mathbf{w}. \quad (3.1.9.5)$$

Rearrangement of (3.1.9.4) with $\mathbf{x} \cdot \mathbf{z}$ on the left and $\mathbf{u} \cdot \mathbf{z}$ on the right, and using (3.1.9.3) for \mathbf{z} on the left leads to

$$\varepsilon_{ijk}x^i(u^j v^k + v^j w^k + w^j u^k) = \varepsilon_{ijk}u^i v^j w^k. \quad (3.1.9.6)$$

If, in particular, the points are on the coordinate axes, their designations are $[u^1, 0, 0]$, $[0, v^2, 0]$ and $[0, 0, w^3]$, and (3.1.9.6) becomes

$$x^1/u^1 + x^2/v^2 + x^3/w^3 = 1, \quad (3.1.9.7)$$

which may be written

$$x^i h_i = 1 \quad (3.1.9.8)$$

or

$$\mathbf{x} \cdot \mathbf{h} = 1 \quad (3.1.9.9)$$

in which the vector \mathbf{h} has coordinates

$$\mathbf{h} = (1/u^1, 1/v^2, 1/w^3). \quad (3.1.9.10)$$

That is, the covariant components of \mathbf{h} are given by the reciprocals of the intercepts of the plane on the axes. The vector \mathbf{h} is normal to the plane it describes (Sands, 1982a) and the length of \mathbf{h} is the reciprocal of the distance d of the plane from the origin; *i.e.*,

$$h = 1/d. \quad (3.1.9.11)$$

If the indices h_i are relatively prime integers, the theory of numbers tells us that the Diophantine equation (3.1.9.8) has solutions x^i that are integers. Points whose contravariant components are integers are lattice points, and such a plane passes through an infinite number of lattice points and is called a *lattice plane*. Thus, the h_i for lattice planes are the familiar Miller indices of crystallography.

Calculations involving planes become quite manageable when the normal vector \mathbf{h} is introduced. Thus, the distance l from a point P with coordinates p^i to a plane characterized by \mathbf{h} is

$$l = (1 - \mathbf{p} \cdot \mathbf{h})/h, \quad (3.1.9.12)$$

where a negative sign indicates that the point is on the opposite side of the plane from the origin.

The dihedral angle τ between planes with normals \mathbf{h} and \mathbf{h}' is

$$\tau = \cos^{-1}[-\mathbf{h} \cdot \mathbf{h}'/(hh')]. \quad (3.1.9.13)$$

A variation of (3.1.9.13) expresses τ in terms of vector \mathbf{u} in the first plane, vector \mathbf{w} in the second plane, and vector \mathbf{v} , the intersection of the planes, as (Shmueli, 1974)

$$\tau = \cos^{-1}[(\mathbf{u} \wedge \mathbf{v}) \cdot (\mathbf{v} \wedge \mathbf{w})/|\mathbf{u} \wedge \mathbf{v}||\mathbf{v} \wedge \mathbf{w}|]. \quad (3.1.9.14)$$

A similar calculation gives angles of torsion. Let \mathbf{t}_h and \mathbf{u}_h be, respectively, the projections of vectors \mathbf{t} and \mathbf{u} onto the plane with normal \mathbf{h} .

$$\mathbf{t}_h = \mathbf{t} - (\mathbf{t} \cdot \mathbf{h})\mathbf{h}/h^2 \quad (3.1.9.15)$$

$$\mathbf{u}_h = \mathbf{u} - (\mathbf{u} \cdot \mathbf{h})\mathbf{h}/h^2. \quad (3.1.9.16)$$

The angle between \mathbf{t}_h and \mathbf{u}_h represents a torsion about \mathbf{h} (Sands, 1982b). Another approach to the torsion angle, which gives equivalent results (Shmueli, 1974), is to compute the angle between $\mathbf{t} \wedge \mathbf{h}$ and $\mathbf{u} \wedge \mathbf{h}$ using (3.1.8.3).

3.1.10. Variance-covariance matrices

Refinement of a crystal structure yields both the parameters that describe the structure and estimates of the uncertainties of those parameters. Refinement by the method of least squares minimizes a weighted sum of squares of residuals. In the matrix notation of Hamilton's classic book (Hamilton, 1964), values of