SHORT COMMUNICATIONS

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Vector algebra and crystallography

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Abstract

The volumes of a crystal unit cell and of its reciprocal cell, the relationships between direct and reciprocal interaxial angles and the coordinates of the reciprocal vectors in the direct basis are rederived in a concise way by means of an elementary formula in vector algebra. The product of two rotations is also considered.

The volumes of the direct and reciprocal cells of a crystal and the relationships between direct- and reciprocal-lattice quantities are classically derived using the algebra of determinants and spherical crystallography or advanced vector methods such as Lagrange formulas for products of four vectors. We present here a simple vector formula from which all these quantities are then rederived. Finally, the relationships between direct- and reciprocal-lattice quantities are applied to spherical trigonometry and the product of two rotations.

Consider three linearly independent vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ and introduce the coordinates x, y, z of $\mathbf{c}$ in the $\mathbf{a}, \mathbf{b}, \mathbf{a}\times\mathbf{b}$ basis:

$$\mathbf{c} = x\mathbf{a} + y\mathbf{b} + z\mathbf{a}\times\mathbf{b}.$$

Taking the scalar product of this relation successively by $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{a}\times\mathbf{b}$, we find:

$$\mathbf{a}\cdot\mathbf{c} = xa^2 + y\mathbf{a}\cdot\mathbf{b}$$
$$\mathbf{b}\cdot\mathbf{c} = x\mathbf{a}\cdot\mathbf{b} + yb^2$$
$$(\mathbf{a}, \mathbf{b}, \mathbf{c}) = z|\mathbf{a}\times\mathbf{b}|^2.$$

Using the Lagrange identity

$$|\mathbf{a}\times\mathbf{b}|^2 = a^2b^2 - (\mathbf{a}\cdot\mathbf{b})^2,$$

we get finally the 'basic' formula

$$|\mathbf{a}\times\mathbf{b}|^2\mathbf{c} = [b^2(\mathbf{a}\cdot\mathbf{c}) - (\mathbf{a}\cdot\mathbf{b})(\mathbf{b}\cdot\mathbf{c})]\mathbf{a} + [a^2(\mathbf{b}\cdot\mathbf{c}) - (\mathbf{a}\cdot\mathbf{b})(\mathbf{a}\cdot\mathbf{c})]\mathbf{b} + (\mathbf{a}, \mathbf{b}, \mathbf{c})\mathbf{a}\times\mathbf{b}. \quad (1)$$

(*a*) Suppose that the three vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ define a crystal unit cell: the cell edges are a, b, c and the interaxial angles are α, β, γ. The volume V of the cell is equal to the triple scalar product $(\mathbf{a}, \mathbf{b}, \mathbf{c}) = \mathbf{a}\times\mathbf{b}\cdot\mathbf{c} = \mathbf{a}\cdot\mathbf{b}\times\mathbf{c}$. Taking the scalar product of (1) by $\mathbf{c}$, we get the classical expression (Buerger, 1942; Carpenter, 1969; Neustadt & Cagle, 1968; Woolfson, 1970):

$$v^2 = a^2b^2c^2(1 + 2\cos\alpha\cos\beta\cos\gamma - \cos^2\alpha - \cos^2\beta - \cos^2\gamma), \quad (2)$$

which is generally derived using the theory of determinants. An interesting equivalent expression is (Donnay & Donnay, 1959)

$$v^2 = 4a^2b^2c^2[\sin s \sin(s-\alpha)\sin(s-\beta)\sin(s-\gamma)]$$

with $2s = \alpha + \beta + \gamma$.

(*b*) Consider now the reciprocal vectors $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$. We want to determine the reciprocal-cell edges a^*, b^*, c^*, the interaxial angles $\alpha^*, \beta^*, \gamma^*$ and the coordinates of the reciprocal vectors in the $\mathbf{a}, \mathbf{b}, \mathbf{c}$ basis. Since $v\mathbf{c}^* = \mathbf{a}\times\mathbf{b}$, we have $c^* = ab\sin\gamma/v$. Equation (1) gives immediately the expression for c^* in the direct basis:

$$v^2\mathbf{c}^* = [(\mathbf{a}\cdot\mathbf{b})(\mathbf{b}\cdot\mathbf{c}) - b^2(\mathbf{a}\cdot\mathbf{c})]\mathbf{a} + [(\mathbf{a}\cdot\mathbf{b})(\mathbf{a}\cdot\mathbf{c}) - a^2(\mathbf{b}\cdot\mathbf{c})]\mathbf{b} + |\mathbf{a}\times\mathbf{b}|^2\mathbf{c} \quad (3)$$

or

$$v^2\mathbf{c}^* = ab^2c(\cos\alpha\cos\gamma - \cos\beta)\mathbf{a} + a^2bc(\cos\beta\cos\gamma - \cos\alpha)\mathbf{b} + a^2b^2\sin^2\gamma\,\mathbf{c}. \quad (3')$$

Comparing this with the general expression

$$\mathbf{c}^* = (\mathbf{a}^*\cdot\mathbf{c}^*)\mathbf{a} + (\mathbf{b}^*\cdot\mathbf{c}^*)\mathbf{b} + (\mathbf{c}^*\cdot\mathbf{c}^*)\mathbf{c} \quad (4)$$

and equating the coefficients of $\mathbf{b}$ in (3) and (4), we get the angle α^*:

$$\cos\alpha^* = (\cos\beta\cos\gamma - \cos\alpha)/\sin\beta\sin\gamma \quad (5)$$

Combining (3′) and (5) gives

$$v^2\mathbf{c}^* = a^2bc\sin\alpha\sin\gamma\cos\beta^*\,\mathbf{a} + ab^2c\sin\beta\sin\gamma\cos\alpha^*\,\mathbf{b} + a^2b^2\sin^2\gamma\,\mathbf{c}. \quad (6)$$

Calculating $\sin\alpha^*$ from (5) and (2) gives

$$v = abc\sin\beta\sin\gamma\sin\alpha^* \quad (7)$$

and the sine relation

$$\frac{\sin\alpha}{\sin\alpha^*} = \frac{\sin\beta}{\sin\beta^*} = \frac{\sin\gamma}{\sin\gamma^*}. \quad (8)$$

The volume v^* of the reciprocal cell is given by an expression similar to (7) and, from (8), one gets $vv^* = 1$.

(*c*) We translate now some of the preceding results into the language of spherical trigonometry. $\cos\gamma^*$ is given by a relation similar to (5) and the reciprocal relation is

$$\cos\gamma^* = \cos\alpha^*\cos\beta^* - \sin\alpha^*\sin\beta^*\cos\gamma. \quad (9)$$

Using (7) in the form $v = abc\sin\alpha\sin\beta\sin\gamma^*$ and (8), we may write (6) as

$$abc\sin\alpha^*\sin\beta^*\,\mathbf{a}\times\mathbf{b} = a^2bc\sin\alpha^*\cos\beta^*\,\mathbf{a} + ab^2c\sin\beta^*\cos\alpha^*\,\mathbf{b} + a^2b^2\sin\gamma^*\,\mathbf{c}. \quad (10)$$

Suppose that the extremities A, B and C of the three vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are on a unit sphere centered at the origin:

$a = b = c = 1$. The side lengths of the spherical triangle are equal to the interaxial angles α, β, γ and its dihedral angles are $\pi - \alpha^*, \pi - \beta^*, \pi - \gamma^*$. Using now the classical notations a, b, c for the side lengths and α, β, γ for the dihedral angles, we get from (9) and (10), respectively,

$$\cos\gamma = -\cos\alpha\cos\beta + \sin\alpha\sin\beta\cos c \qquad (11)$$

$$\sin\gamma\,\mathbf{c} = \sin\alpha\cos\beta\,\mathbf{a} + \cos\alpha\sin\beta\,\mathbf{b} + \sin\alpha\sin\beta\,\mathbf{a}\times\mathbf{b}. \qquad (12)$$

These formulas were found by Altmann by a more sophisticated procedure (Altmann, 1986). They can be used to derive the product of two rotations around intersecting axes from the Euler–Rodrigues–Hamilton theorem (Altmann, 1986; Sivardière, 1994, 1995). According to this theorem, a rotation of angle $\theta_1 = 2\alpha$ around $\mathbf{u}_1 = \mathbf{a}$ followed by a rotation of angle $\theta_2 = 2\beta$ around $\mathbf{u}_2 = \mathbf{b}$ is a rotation of angle $\theta_3 = 2(\pi - \gamma)$ around the unit vector $\mathbf{u}_3 = \mathbf{c}$. Introducing the Euler vectors $\mathbf{R}_i = \sin(\theta_i/2)\,\mathbf{u}_i$, we obtain

$$\cos(\theta_3/2) = \cos(\theta_1/2)\cos(\theta_2/2) - \mathbf{R}_1 \cdot \mathbf{R}_2$$

$$\mathbf{R}_3 = \cos(\theta_2/2)\,\mathbf{R}_1 + \cos(\theta_1/2)\,\mathbf{R}_2 - \mathbf{R}_1 \times \mathbf{R}_2.$$

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