# Crystal structure, X-ray diffraction and Oblique geometry

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The main mathematical difficulty in crystal geometry and X-ray diffraction stems from oblique system of coordinates as soon as we move on from the simple cubic to the body-centered cubic case without mentioning the non-cubic systems. We show in this work that there exists a simple way for dealing with oblique geometry for all crystal systems by combining direct and reciprocal space geometrical elements with the help of a small set of vector identities that are not usually taught in a general physics curriculum. This allows us to derive for all crystalline systems compact formulae describing directions, planes, moduli, angles and scalar products of vectors belonging to either direct or reciprocal lattices. Interplanar distances and angles are derived as well with this approach.

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## I. INTRODUCTION

Solid State Physics at the graduate/undergraduate level usually starts à la Kittel (1), like many other books, with crystallography (2) concepts and its geometry with a first emphasis on local symmetry (fixed point symmetry) and afterwards on translational or space symmetry elements. Next, X-ray diffraction (3) is introduced as a tool for crystal structure determination with the introduction of reciprocal lattice concepts. Ashcroft and Mermin book represents an exception to this general scheme since it starts with the structureless electron gas (4).

While crystal structure requires knowledge of angles, distances, surfaces and volumes, directions and planes as well as other geometrical notions, the calculations are lengthy and tedious (5) since they should be based on oblique geometry as soon as we start dealing with the body-centered cubic lattice.

Traditionally, the Bravais conventional lattice approach is helpful in the sense it serves to visualize the different non-simple-cubic as close as possible to the simple cubic. Nevertheless it might induce student errors during the evaluation of geometrical quantities since it provides a false impression of orthogonality and normality.

While several books such as Cullity (3), Tilley (6), Phillips (7), Kittel (1), Ashcroft and Mermin (4), Busch *et al.* (8), Patterson *et al.* (9) and many other authors such as Donnay (10) and Blake *et al.* (11) contributors to the International Tables for X-ray crystallography series, present sets of tables containing formulas of cell volumes, interplanar angles and distances for some or all systems, they fail however to indicate a general, powerful yet easy method to obtain the desired results.

In this work, we show that by combining the original oblique lattice and its corresponding reciprocal version along with a small set of simple vector identities (not usually taught in the general physics curriculum), a student will be able to perform easily, quickly and flawlessly estimations of geometrical quantities that are generally required in crystallography and X-ray diffraction. A word of caution is needed at this level since we use geometrical formulas

involving explicitly the $2\pi$ scattering phase factor (3) originating from the scalar products between direct and reciprocal basis vectors whereas this factor is taken as unity in many crystallography books.

This work is organized as follows: In section 2, we introduce geometrical concepts based on standard Linear Algebra to describe crystallography in direct and reciprocal spaces. In section 3, we apply these notions to evaluate geometrical quantities such as unit cell volumes, interplanar distances and angles, crystallographic directions and planes and reticular density for all systems. The appendix covers derivations of cross and triple vector non-standard combination identities.

## II. DIRECT AND RECIPROCAL LATTICES

Crystal systems are classified according to the lengths $a, b, c$ of the unit cell and the angles $\alpha, \beta, \gamma$ the basis vectors $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$ make among themselves (see table I and fig.1).

| System | Lengths and angles |
|---|---|
| triclinic | $a \neq b \neq c$, $\alpha \neq \beta \neq \gamma \neq 90^\circ$ |
| monoclinic | $a \neq b \neq c$, $\alpha = 90^\circ$, $\beta \neq 90^\circ$, $\gamma = 90^\circ$ |
| orthorhombic | $a \neq b \neq c$, $\alpha = \beta = \gamma = 90^\circ$ |
| tetragonal | $a = b \neq c$, $\alpha = \beta = \gamma = 90^\circ$ |
| cubic | $a = b = c$, $\alpha = \beta = \gamma = 90^\circ$ |
| rhombohedral | $a = b = c$, $\alpha = \beta = \gamma < 120^\circ, \neq 90^\circ$ |
| hexagonal | $a = b \neq c$, $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$ |

TABLE I: Crystal systems characterized by the lengths and angles making the unit cell. We proceed from the most general structure (triclinic) to the most symmetric (cubic) followed by the rhombohedral and finally the hexagonal. The proximity of the cubic to the rhombohedral system highlights their similar characteristics.

The direct lattice is generated from nodes positioned at integer values $n_1, n_2, n_3$ in terms of three basis vectors $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$ such that $\boldsymbol{R}_n = n_1\boldsymbol{a} + n_2\boldsymbol{b} + n_3\boldsymbol{c}$.

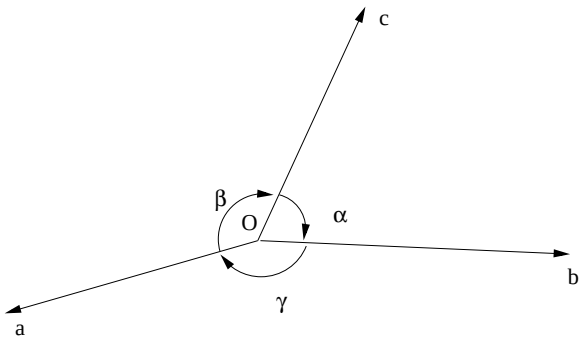


FIG. 1: Crystal axes defining the direct basis.

An arbitrary position in the lattice is written as $\boldsymbol{r} = x\boldsymbol{a} + y\boldsymbol{b} + z\boldsymbol{c}$ with $x, y, z \in \mathcal{R}$. The scalar product between two arbitrary position vectors can be written in the form:

$$\boldsymbol{r}_1 \cdot \boldsymbol{r}_2 = (x_1\boldsymbol{a} + y_1\boldsymbol{b} + z_1\boldsymbol{c}) \cdot (x_2\boldsymbol{a} + y_2\boldsymbol{b} + z_2\boldsymbol{c}) = \begin{pmatrix} x_1, & y_1, & z_1 \end{pmatrix} G \begin{pmatrix} x_2, & y_2, & z_2 \end{pmatrix}^t \tag{1}$$

where $\begin{pmatrix} x_2, & y_2, & z_2 \end{pmatrix}^t$ is the transpose (column form) of the (line form) vector $\begin{pmatrix} x_2, & y_2, & z_2 \end{pmatrix}$ and

$$G = \begin{pmatrix} \boldsymbol{a}\cdot\boldsymbol{a} & \boldsymbol{a}\cdot\boldsymbol{b} & \boldsymbol{a}\cdot\boldsymbol{c} \\ \boldsymbol{b}\cdot\boldsymbol{a} & \boldsymbol{b}\cdot\boldsymbol{b} & \boldsymbol{b}\cdot\boldsymbol{c} \\ \boldsymbol{c}\cdot\boldsymbol{a} & \boldsymbol{c}\cdot\boldsymbol{b} & \boldsymbol{c}\cdot\boldsymbol{c} \end{pmatrix} = \begin{pmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ab\cos\gamma & b^2 & bc\cos\alpha \\ ac\cos\beta & bc\cos\alpha & c^2 \end{pmatrix} \tag{2}$$

is the metric matrix of the direct basis.
The modulus of any vector $\boldsymbol{r}$ is written as:

$$||r|| = \sqrt{\boldsymbol{r}\cdot\boldsymbol{r}} = \sqrt{\Big(x,\ y,\ z\Big)\, G\Big(x,\ y,\ z\Big)^{t}} \tag{3}$$

Applying this to any crystalline direction $[u,v,w]$ or $u\boldsymbol{a}+v\boldsymbol{b}+w\boldsymbol{c}$, we define a unit vector $\boldsymbol{n} = \frac{u\boldsymbol{a}+v\boldsymbol{b}+w\boldsymbol{c}}{||u\boldsymbol{a}+v\boldsymbol{b}+w\boldsymbol{c}||}$ where:

$$||u\boldsymbol{a}+v\boldsymbol{b}+w\boldsymbol{c}|| = \sqrt{\Big(u,\ v,\ w\Big)\, G\Big(u,\ v,\ w\Big)^{t}} \tag{4}$$

### A. Reciprocal lattice

The reciprocal lattice is generated from $\boldsymbol{a}^*, \boldsymbol{b}^*, \boldsymbol{c}^*$ chosen in a way such that:

$$\begin{array}{lll} \boldsymbol{a}^*\cdot\boldsymbol{a} = 2\pi, & \boldsymbol{a}^*\cdot\boldsymbol{b} = 0, & \boldsymbol{a}^*\cdot\boldsymbol{c} = 0, \\ \boldsymbol{b}^*\cdot\boldsymbol{a} = 0, & \boldsymbol{b}^*\cdot\boldsymbol{b} = 2\pi, & \boldsymbol{b}^*\cdot\boldsymbol{c} = 0, \\ \boldsymbol{c}^*\cdot\boldsymbol{a} = 0, & \boldsymbol{c}^*\cdot\boldsymbol{c} = 0, & \boldsymbol{c}^*\cdot\boldsymbol{c} = 2\pi \end{array} \tag{5}$$

This leads to the definitions:

$$\boldsymbol{a}^* = \left(\frac{2\pi}{\Omega}\right)\boldsymbol{b}\times\boldsymbol{c}, \quad \boldsymbol{b}^* = \left(\frac{2\pi}{\Omega}\right)\boldsymbol{c}\times\boldsymbol{a}, \quad \boldsymbol{c}^* = \left(\frac{2\pi}{\Omega}\right)\boldsymbol{a}\times\boldsymbol{b} \tag{6}$$

where $\Omega$ is the unit cell volume given by the triple product $\Omega = (\boldsymbol{a},\boldsymbol{b},\boldsymbol{c})$. The above definitions are easily verified by simply taking the dot products as in the Appendix (eq. A2).
From the above definitions we get the moduli of $\boldsymbol{a}^*, \boldsymbol{b}^*, \boldsymbol{c}^*$ as:

$$||\boldsymbol{a}^*|| = \left(\frac{2\pi}{\Omega}\right) bc\sin\alpha, \quad ||\boldsymbol{b}^*|| = \left(\frac{2\pi}{\Omega}\right) ca\sin\beta, \quad ||\boldsymbol{c}^*|| = \left(\frac{2\pi}{\Omega}\right) ab\sin\gamma \tag{7}$$

Reciprocal lattice basis vectors $\boldsymbol{a}^*, \boldsymbol{b}^*, \boldsymbol{c}^*$ make the angles $\alpha^*, \beta^*, \gamma^*$ such that: $\alpha^* = (\boldsymbol{b}^*, \boldsymbol{c}^*)$, $\beta^* = (\boldsymbol{c}^*, \boldsymbol{a}^*)$, and $\gamma^* = (\boldsymbol{a}^*, \boldsymbol{b}^*)$.
Angles $\alpha^*, \beta^*, \gamma^*$ can be obtained in terms of $\alpha, \beta, \gamma$ by deriving several interesting relations concerning dot and cross products of reciprocal vectors. For instance, if we want to evaluate the angle $\gamma^* = (\boldsymbol{a}^*, \boldsymbol{b}^*)$, we start from the dot product:

$$\boldsymbol{a}^*\cdot\boldsymbol{b}^* = ||\boldsymbol{a}^*||\,||\boldsymbol{b}^*||\cos\gamma^* \tag{8}$$

and use the Appendix for the dot product (eq. A2) as:

$$\boldsymbol{a}^*\cdot\boldsymbol{b}^* = \left(\frac{2\pi}{\Omega}\right)^2 (\boldsymbol{b}\times\boldsymbol{c})\cdot(\boldsymbol{c}\times\boldsymbol{a}) = \left(\frac{2\pi}{\Omega}\right)^2 [(\boldsymbol{b}\cdot\boldsymbol{c})(\boldsymbol{a}\cdot\boldsymbol{c}) - c^2(\boldsymbol{a}\cdot\boldsymbol{b})] \tag{9}$$

Since we know from above, the moduli $||\boldsymbol{a}^*||, ||\boldsymbol{b}^*||$, we are able to extract the value of $\cos\gamma^*$ and cyclically for all other angles, obtaining:

$$\cos\alpha^* = \frac{\cos\beta\cos\gamma - \cos\alpha}{\sin\beta\sin\gamma}, \quad \cos\beta^* = \frac{\cos\alpha\cos\gamma - \cos\beta}{\sin\alpha\sin\gamma}, \quad \cos\gamma^* = \frac{\cos\alpha\cos\beta - \cos\gamma}{\sin\alpha\sin\beta} \tag{10}$$

In reciprocal space, an arbitrary wavevector $\boldsymbol{q}$ is given by:

$$\boldsymbol{q} = u\boldsymbol{a}^* + v\boldsymbol{b}^* + w\boldsymbol{c}^* \tag{11}$$

Its modulus is:

$$||\boldsymbol{q}|| = \sqrt{\Big(u,\ v,\ w\Big)\, G^*\Big(u,\ v,\ w\Big)^t} \tag{12}$$

where the reciprocal metric matrix $G^*$ is:

$$G^* = \begin{pmatrix} \boldsymbol{a}^* \cdot \boldsymbol{a}^* & \boldsymbol{a}^* \cdot \boldsymbol{b}^* & \boldsymbol{a}^* \cdot \boldsymbol{c}^* \\ \boldsymbol{b}^* \cdot \boldsymbol{a}^* & \boldsymbol{b}^* \cdot \boldsymbol{b}^* & \boldsymbol{b}^* \cdot \boldsymbol{c}^* \\ \boldsymbol{c}^* \cdot \boldsymbol{a}^* & \boldsymbol{c}^* \cdot \boldsymbol{b}^* & \boldsymbol{c}^* \cdot \boldsymbol{c}^* \end{pmatrix} \tag{13}$$

In order to express $G^*$ in terms of $a, b, c$ and the angles $\alpha, \beta, \gamma$, we use eq. 7 for the moduli and eq. 10 for the angles, obtaining, for instance, the expression:

$$\boldsymbol{a}^* \cdot \boldsymbol{b}^* = ||\boldsymbol{a}^*||\, ||\boldsymbol{b}^*|| \cos\gamma^* = \left(\frac{2\pi}{\Omega}\right) bc \sin\alpha \left(\frac{2\pi}{\Omega}\right) ca \sin\beta \frac{(\cos\alpha\cos\beta - \cos\gamma)}{\sin\alpha\sin\beta} = \left(\frac{2\pi}{\Omega}\right)^2 abc^2(\cos\alpha\cos\beta - \cos\gamma) \tag{14}$$

Using cyclic symmetry, the rest of the $G^*$ elements are found, yielding:

$$G^* = \left(\frac{2\pi}{\Omega}\right)^2 \begin{pmatrix} b^2c^2\sin^2\alpha & abc^2(\cos\alpha\cos\beta - \cos\gamma) & ab^2c(\cos\alpha\cos\gamma - \cos\beta) \\ abc^2(\cos\alpha\cos\beta - \cos\gamma) & c^2a^2\sin^2\beta & a^2bc(\cos\beta\cos\gamma - \cos\alpha) \\ ab^2c(\cos\alpha\cos\gamma - \cos\beta) & a^2bc(\cos\beta\cos\gamma - \cos\alpha) & a^2b^2\sin^2\gamma \end{pmatrix} \tag{15}$$

Using standard crystallographic definitions (3; 6): $S_{11} = b^2c^2\sin^2\alpha$, $S_{22} = a^2c^2\sin^2\beta, S_{33} = a^2b^2\sin^2\gamma$, $S_{12} = abc^2(\cos\alpha\cos\beta - \cos\gamma)$, $S_{23} = a^2bc(\cos\beta\cos\gamma - \cos\alpha)$, $S_{13} = ab^2c(\cos\alpha\cos\gamma - \cos\beta)$, the reciprocal metric matrix is written more compactly in terms of the $S$ matrix elements as:

$$G^* = \left(\frac{2\pi}{\Omega}\right)^2 \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{12} & S_{22} & S_{23} \\ S_{13} & S_{23} & S_{33} \end{pmatrix} \equiv \left(\frac{2\pi}{\Omega}\right)^2 S \tag{16}$$

### B. Reticular planes and Miller indices

A reticular plane goes through crystal nodes. Macroscopically it is noticeable as a shiny facet observable in table salt, sugar grains or jewels made from properly cut (1) gem stones like diamond, emerald, ruby...

Let us suppose the plane cuts the crystal axes $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$ respectively at $p_1a, p_2b, p_3c$ where $p_1, p_2, p_3 \in \mathcal{N}$. The plane equation is obtained by taking $x_{i+1} = x_{i+2} = 0$ and verifying that the plane indeed intersects the $x_i$ axis at $x_i = p_ia$, checking in a circular fashion (i.e. $i = 1, 2, 3$):

$$\frac{x_1}{p_1a} + \frac{x_2}{p_2b} + \frac{x_3}{p_3c} = 1 \tag{17}$$

Multiplying by $p_1p_2p_3$ leads to the plane Miller indices $(h, k, l)$ defined as $h = p_2p_3, k = p_2p_3, l = p_2p_3$, leading to the plane equation:

$$h\frac{x_1}{a} + k\frac{x_2}{b} + l\frac{x_3}{c} = p_1p_2p_3 \tag{18}$$

where $x_1, x_2, x_3$ are the coordinates along the crystal basis set $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$ directions respectively.

Any vector $\boldsymbol{r}$ with its tip lying in that plane is written as:

$$\boldsymbol{r} = \frac{x_1}{a}\boldsymbol{a} + \frac{x_2}{b}\boldsymbol{b} + \frac{x_3}{c}\boldsymbol{c} \tag{19}$$

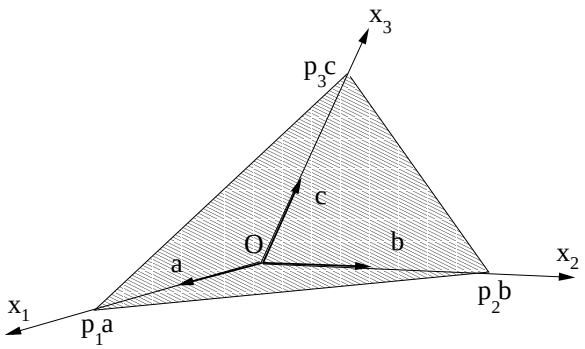


FIG. 2: Miller plane cutting at $p_1a, p_2b, p_3c$ crystal axes $(x_1, x_2, x_3)$ defined from the $(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c})$ basis set.

## III. APPLICATIONS TO CRYSTALLOGRAPHY AND X-RAY DIFFRACTION

### A. Unit cell volumes

The unit cell volume is given by the triple product $\Omega = (\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c})$, whereas the reciprocal unit cell volume is rather $\Omega^* = (\boldsymbol{a}^*, \boldsymbol{b}^*, \boldsymbol{c}^*)$

Let us start by evaluating the unit cell volume $\Omega$ by taking its square:

$$\Omega^2 = (\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c})(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}) = \begin{vmatrix} \boldsymbol{a}\cdot\boldsymbol{a} & \boldsymbol{a}\cdot\boldsymbol{b} & \boldsymbol{a}\cdot\boldsymbol{c} \\ \boldsymbol{b}\cdot\boldsymbol{a} & \boldsymbol{b}\cdot\boldsymbol{b} & \boldsymbol{b}\cdot\boldsymbol{c} \\ \boldsymbol{c}\cdot\boldsymbol{a} & \boldsymbol{c}\cdot\boldsymbol{b} & \boldsymbol{c}\cdot\boldsymbol{c} \end{vmatrix} = \begin{vmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ab\cos\gamma & b^2 & bc\cos\alpha \\ ac\cos\beta & bc\cos\alpha & c^2 \end{vmatrix} \tag{20}$$

The evaluation of the above determinant yields $\Omega = abc\sqrt{1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma}$ in the most general case (triclinic). In the rhombohedral case, we have $a = b = c$, $\alpha = \beta = \gamma$, hence $\Omega = a^3\sqrt{1-3\cos^2\alpha+2\cos^3\alpha}$ as in table II.

Unit cell volumes for all crystal systems are displayed in table II.

Incidentally, another way to evaluate $\Omega$ is through a combination of direct and reciprocal angles. Using the cross product $\boldsymbol{a}^* \times \boldsymbol{b}^*$ given by:

$$\boldsymbol{a}^* \times \boldsymbol{b}^* = \left(\frac{2\pi}{\Omega}\right)^2 (\boldsymbol{b}\times\boldsymbol{c}) \times (\boldsymbol{c}\times\boldsymbol{a}) \tag{21}$$

From the Appendix (eq. A3), we have:

$$(\boldsymbol{b}\times\boldsymbol{c}) \times (\boldsymbol{c}\times\boldsymbol{a}) = (\boldsymbol{b}, \boldsymbol{c}, \boldsymbol{a}) \quad \boldsymbol{c} \tag{22}$$

Taking the modulus:

$$\Omega = (\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}) = \frac{||(\boldsymbol{b}\times\boldsymbol{c}) \times (\boldsymbol{c}\times\boldsymbol{a})||}{c} \tag{23}$$

This can be rewritten as:

$$||(\boldsymbol{b}\times\boldsymbol{c}) \times (\boldsymbol{c}\times\boldsymbol{a})|| = (bc\sin\alpha)(ca\sin\beta)\sin\gamma^* = abc^2\sin\alpha\sin\beta\sin\gamma^* \tag{24}$$

since $\gamma^*$ is the angle $(\boldsymbol{a}^*, \boldsymbol{b}^*)$ and $\boldsymbol{a}^* \propto (\boldsymbol{b}\times\boldsymbol{c})$, $\boldsymbol{b}^* \propto (\boldsymbol{c}\times\boldsymbol{a})$.

Thus the result:

$$\Omega = (\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}) = abc\sin\alpha\sin\beta\sin\gamma^* \tag{25}$$

This might be viewed as a way to express the value of $\sin\gamma^*$ as:

$$\sin\gamma^* = \frac{\Omega}{abc\sin\alpha\sin\beta} \tag{26}$$

and cyclically:

$$\sin\alpha^* = \frac{\Omega}{abc\sin\gamma\sin\beta}, \quad \sin\beta^* = \frac{\Omega}{abc\sin\alpha\sin\gamma} \tag{27}$$

For instance, in the triclinic system we have $\Omega = abc\sqrt{1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma}$ and consequently:

$$\begin{aligned}
\sin\alpha^* &= \frac{\sqrt{1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma}}{\sin\gamma\sin\beta}, \\
\sin\beta^* &= \frac{\sqrt{1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma}}{\sin\alpha\sin\gamma}, \\
\sin\gamma^* &= \frac{\sqrt{1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma}}{\sin\alpha\sin\beta}
\end{aligned} \tag{28}$$

(29)

Moving on to the evaluation of the reciprocal unit cell volume $\Omega^* = (\boldsymbol{a}^*, \boldsymbol{b}^*, \boldsymbol{c}^*)$, we exploit scalar product properties between $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$ and $\boldsymbol{a}^*, \boldsymbol{b}^*, \boldsymbol{c}^*$ bases. We infer that $\Omega\Omega^* = (\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c})(\boldsymbol{a}^*, \boldsymbol{b}^*, \boldsymbol{c}^*)$. Product of triple products (see Appendix eq. A7) yields $\Omega\Omega^* = (2\pi)^3$. Thus it suffices to calculate $\Omega$ since $\Omega^* = (2\pi)^3/\Omega$.

Incidentally, note that using the Appendix double triple product formula A7, the determinant of $G^*$ can be written as: $\det(G^*)=(\Omega^*)^2$. The same can be written for $\det(G)=(\Omega)^2$. Consequently the relation $\Omega^* = (2\pi)^3/\Omega$ implies that $G^* = (2\pi)^6 G^{-1}$.

| System | Unit cell volume $\Omega$ |
|---|---|
| triclinic | $abc\sqrt{1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma}$ |
| monoclinic | $abc\sin\beta$ |
| orthorhombic | $abc$ |
| tetragonal | $a^2c$ |
| cubic | $a^3$ |
| rhombohedral | $a^3\sqrt{1-3\cos^2\alpha+2\cos^2\alpha}$ |
| hexagonal | $\frac{\sqrt{3}}{2}a^2c$ |

TABLE II: Unit cell volumes for all crystal systems. We proceed from the most general structure (triclinic) to the most symmetric (cubic) followed by the rhombohedral and finally the hexagonal.

### B. Interplanar distances

In X-ray diffraction, Bragg's law (1) $2d_{hkl}\sin\theta = n\lambda$ (with $n \in \mathcal{N}$) requires the knowledge of interplanar distances between $(hkl)$ Miller planes whereas $\theta$ and $\lambda$ are X-ray scattering angle and wavelength, respectively. Elastic X-ray diffraction is based on electromagnetic wave scattering by the crystal. It is described by the scattering vector (1):

$$\boldsymbol{q}_{hkl} = h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^* \tag{30}$$

Let us suppose the normal to the Miller $(hkl)$ plane is written as:

$$\boldsymbol{n}_{hkl} = \frac{d_{hkl}}{2\pi}\boldsymbol{q}_{hkl} \tag{31}$$

This can be verified by writing the Miller $(hkl)$ plane eq. 18 as (see fig. 3):

$$h\frac{x_1}{a} + k\frac{x_2}{b} + l\frac{x_3}{c} = p \tag{32}$$

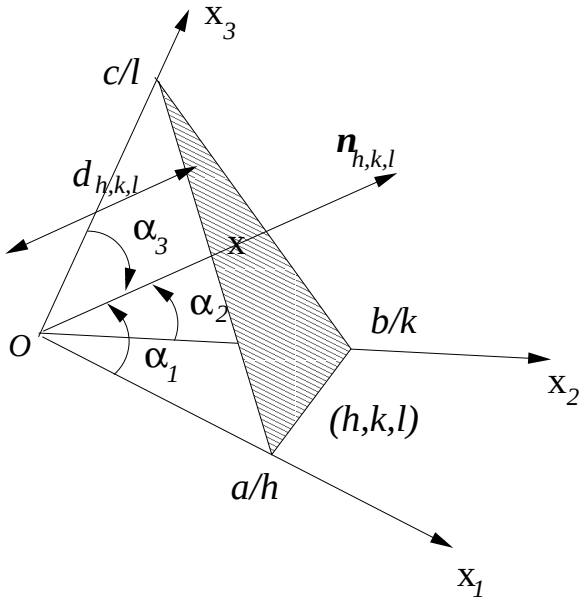


FIG. 3: Closest to origin $(hkl)$ Miller plane is displayed. Its equation $h\frac{x_1}{a} + k\frac{x_2}{b} + l\frac{x_3}{c} = 1$ confirms cutting the $(x_1, x_2, x_3)$ axes at $a/h, b/k, c/l$ respectively. The intersection between the normal $\boldsymbol{n}_{hkl}$ and the $(hkl)$ Miller plane yields $d_{hkl}$, the interplanar distance. Note the rotation of the axes with respect to those in the previous fig. 2 in order to reveal the normal $\boldsymbol{n}_{hkl}$ angles with respect to the crystal axes.

When $p = 1$ the minimal integer value, the distance between the origin and the intersection (8) of the normal $\boldsymbol{n}_{hkl}$ to the $(hkl)$ plane is $d_{hkl}$ (see fig. 3). Projecting $\boldsymbol{n}_{hkl}$ onto the $(x_1, x_2, x_3)$ axes, we get: $d_{hkl} = a\cos\alpha_1/h = b\cos\alpha_2/k = c\cos\alpha_3/l$ where $\alpha_1, \alpha_2, \alpha_3$ are the direction cosine angles (8) of $\boldsymbol{n}_{hkl}$.

This allows us to write: $\boldsymbol{n}_{hkl} = \frac{d_{hkl}}{2\pi}(h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*)$ that can be verified immediately by evaluating the scalar products $\boldsymbol{n}_{hkl}\cdot\boldsymbol{a}, \boldsymbol{n}_{hkl}\cdot\boldsymbol{b}, \boldsymbol{n}_{hkl}\cdot\boldsymbol{c}$. The values $d_{hkl}h = a\cos\alpha_1$ and circularly $d_{hkl}k = b\cos\alpha_2, d_{hkl}l = c\cos\alpha_3$ are obtained from the remarkable properties (see eq. 5) of the dot products between the $(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c})$ and $(\boldsymbol{a}^*, \boldsymbol{b}^*, \boldsymbol{c}^*)$ sets. Besides, they agree with the relations obtained previously from the $\boldsymbol{n}_{hkl}$ projections.

Since the modulus of the normal $\boldsymbol{n}_{hkl}$ is unity, $d_{hkl}$ can be evaluated from: $d_{hkl} = \frac{2\pi}{||\boldsymbol{q}_{hkl}||}$.

In order to evaluate the modulus of the elastic scattering vector we use:

$$||\boldsymbol{q}_{hkl}|| = \sqrt{\Big(h,\ k,\ l\Big)\, G^*\Big(h,\ k,\ l\Big)^t} \tag{33}$$

with $G^*$ the reciprocal metric matrix.

Finally the interplanar distance is given by:

$$d_{hkl} = \frac{2\pi}{\sqrt{\Big(h,\ k,\ l\Big)\, G^*\Big(h,\ k,\ l\Big)^t}} \tag{34}$$

In the following table III we give rather the values of $1/d^2_{hkl}$ for every system.

Since $G^* = \left(\frac{2\pi}{\Omega}\right)^2 S$ we have:

$$d_{hkl} = \frac{\Omega}{\sqrt{\Big(h,\ k,\ l\Big)\, S\Big(h,\ k,\ l\Big)^t}} \tag{35}$$

Consequently:

$$\frac{1}{d^2_{hkl}} = \frac{1}{\Omega^2}\Big(h,\ k,\ l\Big)\, S\Big(h,\ k,\ l\Big)^t \tag{36}$$

Lets us evaluate $\frac{1}{d^2_{hkl}}$ in the triclinic case from the above formula:

$$\frac{1}{d^2_{hkl}} = \frac{1}{\Omega^2}(S_{11}h^2 + S_{22}k^2 + S_{33}l^2 + 2S_{12}hk + 2S_{23}kl + 2S_{13}hl) \tag{37}$$

In the rhombohedral case, we have $a = b = c$, $\alpha = \beta = \gamma$, thus $S_{11} = S_{22} = S_{33} = a^4 \sin^2\alpha$, $S_{12} = S_{23} = S_{13} = a^4(\cos^2\alpha - \cos\alpha)$ and $\Omega = a^3\sqrt{1 - 3\cos^2\alpha + 2\cos^3\alpha}$ obtaining: $\frac{1}{d^2_{hkl}} = \frac{(h^2+k^2+l^2)\sin^2\alpha + 2(hk+kl+hl)(\cos^2\alpha - \cos\alpha)}{a^2(1-3\cos^2\alpha+2\cos^3\alpha)}$ as in table III.

For the remaining systems, it is possible to easily calculate $\frac{1}{d^2_{hkl}}$ as displayed in table III.

| System | $\frac{1}{d^2_{hkl}}$ |
|---|---|
| triclinic | $[1/\Omega^2]\{S_{11}h^2 + S_{22}k^2 + S_{33}l^2 + 2S_{12}hk + 2S_{23}kl + 2S_{13}hl\}$ |
| monoclinic | $\frac{1}{\sin^2\beta}\left([h^2]/a^2 + [k^2\sin^2\beta]/b^2 + [l^2]/c^2 - 2hl\cos\beta/ac\right)$ |
| orthorhombic | $[h^2]/a^2 + [k^2]/b^2 + [l^2]/c^2$ |
| tetragonal | $[h^2 + k^2]/a^2 + [l^2]/c^2$ |
| cubic | $[h^2 + k^2 + l^2]/a^2$ |
| rhombohedral | $[(h^2 + k^2 + l^2)\sin^2\alpha + 2(hk + kl + hl)(\cos^2\alpha - \cos\alpha)]/[a^2(1 - 3\cos^2\alpha + 2\cos^3\alpha)]$ |
| hexagonal | $\frac{4}{3}[h^2 + hk + k^2]/a^2 + [l^2]/c^2$ |

TABLE III: Interplanar spacing $d_{hkl}$ for all crystal systems.
$\Omega = abc\sqrt{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma}$

### C. Interplanar angles

The angle between two Miller planes $(h_1k_1l_1), (h_2k_2l_2)$ can be obtained from the dot product between normal vectors to the respective planes $\boldsymbol{n}_1 \cdot \boldsymbol{n}_2 = \cos\theta_{12}$.

The normal to each plane is written as:

$$\boldsymbol{n}_{1,2} = \frac{d^{(1,2)}_{hkl}}{2\pi}\boldsymbol{q}^{(1,2)}_{hkl} \tag{38}$$

where:

$$d^{(1,2)}_{hkl} = d_{h_{1,2}k_{1,2}l_{1,2}} \tag{39}$$

and

$$\boldsymbol{q}^{(1,2)}_{hkl} = h_{1,2}\boldsymbol{a}^* + k_{1,2}\boldsymbol{b}^* + l_{1,2}\boldsymbol{c}^* \tag{40}$$

Thus we have:

$$\cos\theta_{12} = \frac{d^{(1)}_{hkl}d^{(2)}_{hkl}}{4\pi^2}\boldsymbol{q}^{(1)}_{hkl} \cdot \boldsymbol{q}^{(2)}_{hkl} = \frac{\boldsymbol{q}^{(1)}_{hkl} \cdot \boldsymbol{q}^{(2)}_{hkl}}{||\boldsymbol{q}^{(1)}_{hkl}||\,||\boldsymbol{q}^{(2)}_{hkl}||} \tag{41}$$

with the scalar product of the scattering vectors evaluated with the reciprocal metric matrix $G^*$:

$$\boldsymbol{q}^{(1)}_{hkl} \cdot \boldsymbol{q}^{(2)}_{hkl} = \begin{pmatrix} h_1, & k_1, & l_1 \end{pmatrix} G^* \begin{pmatrix} h_2, & k_2, & l_2 \end{pmatrix}^t \tag{42}$$

Finally we have the compact result:

$$\cos\theta_{12} = \frac{\begin{pmatrix} h_1, & k_1, & l_1 \end{pmatrix} G^* \begin{pmatrix} h_2, & k_2, & l_2 \end{pmatrix}^t}{\sqrt{\begin{pmatrix} h_1, & k_1, & l_1 \end{pmatrix} G^* \begin{pmatrix} h_1, & k_1, & l_1 \end{pmatrix}^t}\sqrt{\begin{pmatrix} h_2, & k_2, & l_2 \end{pmatrix} G^* \begin{pmatrix} h_2, & k_2, & l_2 \end{pmatrix}^t}} \tag{43}$$

or in terms of the $S$ matrix:

$$\cos\theta_{12} = \frac{\Big(h_1,\ k_1,\ l_1\Big)\, S\Big(h_2,\ k_2,\ l_2\Big)^t}{\sqrt{\Big(h_1,\ k_1,\ l_1\Big)\, S\Big(h_1,\ k_1,\ l_1\Big)^t}\sqrt{\Big(h_2,\ k_2,\ l_2\Big)\, S\Big(h_2,\ k_2,\ l_2\Big)^t}} \tag{44}$$

It is possible to substitute the respective interplanar distances $d_{hkl}^{(1,2)} = d_{h_{1,2}k_{1,2}l_{1,2}}$ in the $\cos\theta_{12}$ formula through:

$$d_{hkl}^{(1,2)} = \frac{\Omega}{\sqrt{\Big(h_{1,2}, k_{1,2}, l_{1,2}\Big)\, S\Big(h_{1,2}, k_{1,2}, l_{1,2}\Big)^t}} \tag{45}$$

to obtain in a compact way:

$$\cos\theta_{12} = \frac{d_1 d_2}{\Omega^2}\Big(h_1,\ k_1,\ l_1\Big)\, S\Big(h_2,\ k_2,\ l_2\Big)^t \tag{46}$$

This yields immediately for the triclinic system:

$$\cos\theta_{12} = \frac{d_1 d_2}{\Omega^2}\{S_{11}h_1h_2 + S_{22}k_1k_2 + S_{33}l_1l_2 + S_{23}(k_1l_2 + k_2l_1) + S_{13}(l_1h_2 + l_2h_1) + S_{12}(h_1k_2 + h_2k_1)\} \tag{47}$$

In the rhombohedral case, we have $S_{11} = S_{22} = S_{33} = a^4\sin^2\alpha$, $S_{12} = S_{23} = S_{13} = a^4(\cos^2\alpha - \cos\alpha)$ and $\Omega = a^3\sqrt{1 - 3\cos^2\alpha + 2\cos^3\alpha}$, thus:

$$\cos\theta_{12} = \frac{d_1 d_2[(h_1h_2 + k_1k_2 + l_1l_2)\sin^2\alpha + h_1(k_2 + l_2) + k_1(h_2 + l_2) + l_1(h_2 + k_2)(\cos^2\alpha - \cos\alpha)]}{a^2(1 - 3\cos^2\alpha + 2\cos^3\alpha)} \tag{48}$$

For the remaining systems, the interplanar angles are given in table IV.

| System | $\cos\theta_{12}$ |
|---|---|
| triclinic | $\frac{d_1d_2}{\Omega^2}\{S_{11}h_1h_2 + S_{22}k_1k_2 + S_{33}l_1l_2 + S_{23}(k_1l_2 + k_2l_1) + S_{13}(l_1h_2 + l_2h_1) + S_{12}(h_1k_2 + h_2k_1)\}$ |
| monoclinic | $d_1d_2\left(\frac{h_1h_2}{a^2\sin^2\beta} + \frac{k_1k_2}{b^2} + \frac{l_1l_2}{c^2\sin^2\beta} - \frac{(l_1h_2+l_2h_1)\cos\beta}{ac\sin^2\beta}\right)$ |
| orthorhombic | $[\frac{h_1h_2}{a^2} + \frac{k_1k_2}{b^2} + \frac{l_1l_2}{c^2}]/\sqrt{\left(\frac{h_1^2}{a^2} + \frac{k_1^2}{b^2} + \frac{l_1^2}{c^2}\right)\left(\frac{h_2^2}{a^2} + \frac{k_2^2}{b^2} + \frac{l_2^2}{c^2}\right)}$ |
| tetragonal | $[\frac{h_1h_2+k_1k_2}{a^2} + \frac{l_1l_2}{c^2}]/\sqrt{\left(\frac{h_1^2+k_1^2}{a^2} + \frac{l_1^2}{c^2}\right)\left(\frac{h_2^2+k_2^2}{a^2} + \frac{l_2^2}{c^2}\right)}$ |
| cubic | $[h_1h_2 + k_1k_2 + l_1l_2]/\sqrt{[h_1^2 + k_1^2 + l_1^2][h_2^2 + k_2^2 + l_2^2]}$ |
| rhombohedral | $\frac{a^4d_1d_2[(h_1h_2+k_1k_2+l_1l_2)\sin^2\alpha+(k_1l_2+k_2l_1+l_1h_2+l_2h_1+h_1k_2+h_2k_1)(\cos^2\alpha-\cos\alpha)]}{\Omega^2}$ |
| hexagonal | $[h_1h_2 + k_1k_2 + \frac{1}{2}(h_1k_2 + h_2k_1) + \frac{3a^2l_1l_2}{4c^2}]/\sqrt{\left(h_1^2 + k_1^2 + h_1k_1 + \frac{3a^2l_1^2}{4c^2}\right)\left(h_2^2 + k_2^2 + h_2k_2 + \frac{3a^2l_2^2}{4c^2}\right)}$ |

TABLE IV: Interplanar angle $\theta_{12}$ for all crystal systems. $d_1$ is the interplanar spacing for $(h_1, k_1, l_1)$ planes and $d_2$ is the interplanar spacing for $(h_2, k_2, l_2)$ ones. $\Omega = abc\sqrt{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma}$.

### D. Reticular density

Any reticular $(hkl)$ Miller plane is paved by cells whose surface is denoted $S(h,k,l)$. Since reticular planes are separated by the distance $d_{hkl}$, the volume comprised between two $S(h,k,l)$ cells on two neighbouring reticular $(hkl)$ Miller planes is given by $S(h,k,l) \times d_{hkl}$ and this volume is equal to the unit cell $\Omega$.

The reticular density (7) $\rho_{hkl}$ is the number of nodes per unit surface in any reticular $(hkl)$ Miller plane. Therefore we have $\rho_{hkl} = 1/S(h,k,l) = d_{hkl}/\Omega$, i.e.:

$$\rho_{hkl} = \frac{1}{\sqrt{\Big(h,\ k,\ l\Big)\, S\Big(h,\ k,\ l\Big)^{t}}} \tag{49}$$

## IV. CONCLUSION

The combined use of the geometrical properties of the direct and reciprocal lattices enables to derive a set of closed analytical formulas for several crystallographical and X-ray scattering properties. Directions, planes, interplanar distances and angles are derived in a straightforward manner without any mathematical difficulty and avoiding any traps set up by the awkwardness of oblique geometry.

Note that we have accounted for the $2\pi$ scattering phase factor (3) explicitly in all derived formulae in contrast to many crystallography books and papers since this work is aimed at Physics students.

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### APPENDIX A: Cross products and triple products

Below are given several cross product and triple product identities:

1. Double cross product:

$$\boldsymbol{A}\times(\boldsymbol{B}\times\boldsymbol{C}) = \begin{vmatrix} \boldsymbol{B} & \boldsymbol{C} \\ \boldsymbol{A}\cdot\boldsymbol{B} & \boldsymbol{A}\cdot\boldsymbol{C} \end{vmatrix} = (\boldsymbol{A}\cdot\boldsymbol{C})\boldsymbol{B} - (\boldsymbol{A}\cdot\boldsymbol{B})\boldsymbol{C} \tag{A1}$$

   This is obtained from the geometric assumption the result must belong to the $(\boldsymbol{B},\boldsymbol{C})$ plane and finding the components along axes $\boldsymbol{B}$ and $\boldsymbol{C}$ by inspection.

2. Dot product of two cross products:

$$(\boldsymbol{A}\times\boldsymbol{B})\cdot(\boldsymbol{C}\times\boldsymbol{D}) = \begin{vmatrix} \boldsymbol{A}\cdot\boldsymbol{C} & \boldsymbol{A}\cdot\boldsymbol{D} \\ \boldsymbol{B}\cdot\boldsymbol{C} & \boldsymbol{B}\cdot\boldsymbol{D} \end{vmatrix} = (\boldsymbol{A}\cdot\boldsymbol{C})(\boldsymbol{B}\cdot\boldsymbol{D}) - (\boldsymbol{A}\cdot\boldsymbol{D})(\boldsymbol{B}\cdot\boldsymbol{C}) \tag{A2}$$

   The calculation of the vector quantity $(\boldsymbol{A}\times\boldsymbol{B})\cdot(\boldsymbol{C}\times\boldsymbol{D})$ is done by transforming it in a triple product and later exploiting double cross product expressions. Calling $\boldsymbol{E} = (\boldsymbol{A}\times\boldsymbol{B})$ the expression becomes the triple product: $(\boldsymbol{E},\boldsymbol{C},\boldsymbol{D})$. Exploiting circular symmetry of the triple product this becomes: $(\boldsymbol{C},\boldsymbol{D},\boldsymbol{E}) = \boldsymbol{C}\cdot(\boldsymbol{D}\times\boldsymbol{E}) = \boldsymbol{C}\cdot(\boldsymbol{D}\times[\boldsymbol{A}\times\boldsymbol{B}])$. Using the double cross product expression above, this becomes: $(\boldsymbol{A}\cdot\boldsymbol{C})(\boldsymbol{B}\cdot\boldsymbol{D}) - (\boldsymbol{A}\cdot\boldsymbol{D})(\boldsymbol{B}\cdot\boldsymbol{C})$.

3. Cross product of two cross products:

$$(\boldsymbol{A}\times\boldsymbol{B})\times(\boldsymbol{C}\times\boldsymbol{D}) = \begin{vmatrix} \boldsymbol{C} & \boldsymbol{D} \\ (\boldsymbol{A},\boldsymbol{B},\boldsymbol{C}) & (\boldsymbol{A},\boldsymbol{B},\boldsymbol{D}) \end{vmatrix} = (\boldsymbol{A},\boldsymbol{B},\boldsymbol{D})\boldsymbol{C} - (\boldsymbol{A},\boldsymbol{B},\boldsymbol{C})\boldsymbol{D} \tag{A3}$$

   This can be shown by writing $(\boldsymbol{A}\times\boldsymbol{B})\times(\boldsymbol{C}\times\boldsymbol{D})$ as $\boldsymbol{E}\times(\boldsymbol{C}\times\boldsymbol{D})$ with $\boldsymbol{E} = \boldsymbol{A}\times\boldsymbol{B}$ and using the previous double cross result.

4. Product of triple products:
   A volume based on three non-coplanar vectors $\boldsymbol{A},\boldsymbol{B},\boldsymbol{C}$ is given by the triple product $(\boldsymbol{A},\boldsymbol{B},\boldsymbol{C})$.

   Let us consider the matrix $M$ whose rows are given by the cartesian components of the vectors $\boldsymbol{A},\boldsymbol{B},\boldsymbol{C}$.

$$M = \begin{pmatrix} A_x & A_y & A_z \\ B_x & B_y & B_z \\ C_x & C_y & C_z \end{pmatrix} \tag{A4}$$

Consider another triplet of vectors $\boldsymbol{D}, \boldsymbol{E}, \boldsymbol{F}$ and its associated volume $(\boldsymbol{D}, \boldsymbol{E}, \boldsymbol{F})$ with the associated matrix $N$ whose columns are given by the Cartesian components of the vectors $\boldsymbol{D}, \boldsymbol{E}, \boldsymbol{F}$

$$N = \begin{pmatrix} D_x & E_x & F_x \\ D_y & E_y & F_y \\ D_z & E_z & F_z \end{pmatrix} \tag{A5}$$

The determinant of the product of two matrices is given by the product of the corresponding determinants $det(M)det(N) = det(MN)$, thus:

$$(\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C})(\boldsymbol{D}, \boldsymbol{E}, \boldsymbol{F}) = \begin{vmatrix} A_x & A_y & A_z \\ B_x & B_y & B_z \\ C_x & C_y & C_z \end{vmatrix} \begin{vmatrix} D_x & E_x & F_x \\ D_y & E_y & F_y \\ D_z & E_z & F_z \end{vmatrix} = \left| \begin{pmatrix} A_x & A_y & A_z \\ B_x & B_y & B_z \\ C_x & C_y & C_z \end{pmatrix} \cdot \begin{pmatrix} D_x & E_x & F_x \\ D_y & E_y & F_y \\ D_z & E_z & F_z \end{pmatrix} \right| \tag{A6}$$

Finally:

$$(\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C})(\boldsymbol{D}, \boldsymbol{E}, \boldsymbol{F}) = \begin{vmatrix} \boldsymbol{A} \cdot \boldsymbol{D} & \boldsymbol{A} \cdot \boldsymbol{E} & \boldsymbol{A} \cdot \boldsymbol{F} \\ \boldsymbol{B} \cdot \boldsymbol{D} & \boldsymbol{B} \cdot \boldsymbol{E} & \boldsymbol{B} \cdot \boldsymbol{F} \\ \boldsymbol{C} \cdot \boldsymbol{D} & \boldsymbol{C} \cdot \boldsymbol{E} & \boldsymbol{C} \cdot \boldsymbol{F} \end{vmatrix} \tag{A7}$$

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