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An Easier Way to Calculate the Crystallographic Interplanar Angles

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Abstract

The equations for the calculation of the crystallographic interplanar angles for the seven crystal systems are described using only the real crystal unit cell parameters.

1. Introduction

The interplanar angles, which are needed in crystallography from time to time, have been mentioned only in three books to the best of my knowledge.

J. D. H. Donnay and Gabrielle Donnay[1)] expressed the crystallographic interplanar angles in terms of only reciprocal lattice constants: a^*, b^*, c^*, α^*, β^*, γ^* and B. D. Cullity[2)] in terms of real lattice constants a, b, c, α, β, γ together with interplanar spacing $d(hkl)$ and unit cell volume V, and E. Koch[3)] showed only how to calculate the angle between crystal faces $(h_1k_1l_1)$ and $(h_2k_2l_2)$ using reciprocal lattice parameters without giving any explicit expression for each of the seven crystal systems. In order to get an interplanar angle using the above-mentioned formula, therefore, either the reciprocal lattice parameters or the interplanar distance $d(hkl)$ and the unit cell volume V must be calculated first at least for triclinic, monoclinic and trigonal systems.

In this paper, the interplanar angles between crystal faces $(h_1k_1l_1)$ and $(h_2k_2l_2)$ are described only with real cell constants a, b, c, α, β, γ and so it is much easier to calculate them.

2. Theory

If $\vec{a}^*$, $\vec{b}^*$, $\vec{c}^*$ are defined as unit reciprocal lattice vectors of arbitrary crystal cells, the vector $\vec{d}^*(hkl) = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$ is parallel to the direction of plane (hkl) and its absolute value is $1/d(hkl)$, where h, k, l are Miller indices being integer and $d(hkl)$ is an interplanar distance. Therefore interplanar angle between two planes $(h_1k_1l_1)$ and $(h_2k_2l_2)$ for arbitrary crystal systems can be obtained from the scalar product of the reciprocal lattice vectors $\vec{d}_1^*(h_1k_1l_1)$ and $\vec{d}_2^*(h_2k_2l_2)$: $\vec{d}_1^* \bullet \vec{d}_2^* = d_1^* d_2^* \cos\phi$, where $\vec{d}_1^*(h_1k_1l_1) = h_1\vec{a}^* + k_1\vec{b}^* + l_1\vec{c}^*$ and $\vec{d}_2^*(h_2k_2l_2) = h_2\vec{a}^* + k_2\vec{b}^* + l_2\vec{c}^*$.

The value of $\vec{d}_1^* \bullet \vec{d}_2^*$ and the absolute values of $\vec{d}_1^*(h_1k_1l_1)$, $\vec{d}_2^*(h_2k_2l_2)$ are calculated as follows:

$$\vec{d}_1^*(h_1k_1l_1) \bullet \vec{d}_2^*(h_2k_2l_2) = (h_1\vec{a}^* + k_1\vec{b}^* + l_1\vec{c}^*) \bullet (h_2\vec{a}^* + k_2\vec{b}^* + l_2\vec{c}^*) = h_1h_2a^{*2} + k_1k_2b^{*2} + l_1l_2c^{*2} + (h_1k_2 + h_2k_1)\vec{a}^* \bullet \vec{b}^* + (h_1l_2 + h_2l_1)\vec{a}^* \bullet \vec{c}^* + (k_1l_2 + k_2l_1)\vec{b}^* \bullet \vec{c}^*$$

Substituting $\vec{a}^* = \frac{\vec{b} \times \vec{c}}{V}$, $\vec{b}^* = \frac{\vec{c} \times \vec{a}}{V}$, $\vec{c}^* = \frac{\vec{a} \times \vec{b}}{V}$ into the above equation,

$$\vec{d}_1^*(h_1k_1l_1) \bullet \vec{d}_2^*(h_2k_2l_2) = \frac{1}{V^2}\{h_1h_2(\vec{b} \times \vec{c})^2 + k_1k_2(\vec{c} \times \vec{a})^2 + l_1l_2(\vec{a} \times \vec{b})^2 + (h_1k_2 + h_2k_1)(\vec{b} \times \vec{c}) \bullet (\vec{c} \times \vec{a}) + (h_1l_2 + h_2l_1)(\vec{b} \times \vec{c}) \bullet (\vec{a} \times \vec{b}) + (k_1l_2 + k_2l_1)(\vec{c} \times \vec{a}) \bullet (\vec{a} \times \vec{b})\}$$

Applying the scalar product, $(\vec{A} \times \vec{B}) \bullet (\vec{C} \times \vec{D}) = (\vec{A} \bullet \vec{C})(\vec{B} \bullet \vec{D}) - (\vec{A} \bullet \vec{D})(\vec{B} \bullet \vec{C})$

$$= \frac{1}{V^2}\{h_1h_2(\vec{b} \times \vec{c})^2 + k_1k_2(\vec{c} \times \vec{a})^2 + l_1l_2(\vec{a} \times \vec{b})^2$$

$$
\begin{aligned}
&+ (h_1k_2 + h_2k_1)[(\vec{b}\bullet\vec{c})(\vec{c}\bullet\vec{a}) - c^2(\vec{b}\bullet\vec{a})] \\
&+ (h_1l_2 + h_2l_1)[(\vec{b}\bullet\vec{a})(\vec{c}\bullet\vec{b}) - b^2(\vec{c}\bullet\vec{a})] \\
&+ (k_1l_2 + k_2l_1)[(\vec{c}\bullet\vec{a})(\vec{a}\bullet\vec{b}) - a^2(\vec{c}\bullet\vec{b})]\} \\
= &\frac{1}{V^2}\{h_1h_2b^2c^2\sin^2\alpha + k_1k_2c^2a^2\sin^2\beta \\
&+ l_1l_2a^2b^2\sin^2\gamma + (h_1k_2 + h_2k_1) \\
&\quad [(bc\cos\alpha)(ca\cos\beta) - c^2(ba\cos\gamma)] \\
&+ (h_1l_2 + h_2l_1)[(ba\cos\gamma)(cb\cos\alpha) \\
&-b^2(ca\cos\beta)] + (k_1l_2 + k_2l_1) \\
&\quad [(ca\cos\beta)(ab\cos\gamma) - a^2(cb\cos\alpha)]\}
\end{aligned}
$$

$$
\begin{aligned}
\therefore\ \vec{d}_1^*(h_1k_1l_1)\bullet\vec{d}_2^*(h_2k_2l_2) = &\frac{1}{V^2}\{h_1h_2b^2c^2\sin^2\alpha \\
&+ k_1k_2c^2a^2\sin^2\beta + l_1l_2a^2b^2\sin^2\gamma \\
&+ abc^2(h_1k_2 + h_2k_1)(\cos\alpha\cos\beta - \cos\gamma) \\
&+ ab^2c(h_1l_2 + h_2l_1)(\cos\gamma\cos\alpha - \cos\beta) \\
&+ a^2bc(k_1l_2 + k_2l_1)(\cos\beta\cos\gamma - \cos\alpha)\}
\end{aligned}
$$

Similarly

$$
\begin{aligned}
d_1^* = &\frac{1}{V}\{h_1^2b^2c^2\sin^2\alpha + k_1^2a^2c^2\sin^2\beta + l_1^2a^2b^2\sin^2\gamma \\
&+ 2h_1k_1abc^2(\cos\alpha\cos\beta - \cos\gamma) \\
&+ 2h_1l_1ab^2c(\cos\gamma\cos\alpha - \cos\beta) \\
&+ 2k_1l_1a^2bc(\cos\beta\cos\gamma - \cos\alpha)\}^{1/2}
\end{aligned}
$$

$$
\begin{aligned}
d_2^* = &\frac{1}{V}\{h_2^2b^2c^2\sin^2\alpha + k_2^2a^2c^2\sin^2\beta + l_2^2a^2b^2\sin^2\gamma \\
&+ 2h_2k_2abc^2(\cos\alpha\cos\beta - \cos\gamma) \\
&+ 2h_2l_2ab^2c(\cos\gamma\cos\alpha - \cos\beta) \\
&+ 2k_2l_2a^2bc(\cos\beta\cos\gamma - \cos\alpha)\}^{1/2}
\end{aligned}
$$

(2-1) The interplanar angle ϕ between $(h_1k_1l_1)$ and $(h_2k_2l_2)$ for triclinic system:

$$
\begin{aligned}
\cos\phi = \frac{\vec{d}_1^*\bullet\vec{d}_2^*}{d_1^*d_2^*} = &\{h_1h_2b^2c^2\sin^2\alpha \\
&+ k_1k_2c^2a^2\sin^2\beta + l_1l_2a^2b^2\sin^2\gamma \\
&+ abc^2(h_1k_2 + h_2k_1)(\cos\alpha\cos\beta - \cos\gamma) \\
&+ ab^2c(h_1l_2 + h_2l_1)(\cos\gamma\cos\alpha - \cos\beta) \\
&+ a^2bc(k_1l_2 + k_2l_1)(\cos\beta\cos\gamma - \cos\alpha)\} \\
&/[\{h_1^2b^2c^2\sin^2\alpha + k_1^2a^2c^2\sin^2\beta + l_1^2a^2b^2\sin^2\gamma \\
&+ 2h_1k_1abc^2(\cos\alpha\cos\beta - \cos\gamma) \\
&+ 2h_1l_1ab^2c(\cos\gamma\cos\alpha - \cos\beta) \\
&+ 2k_1l_1a^2bc(\cos\beta\cos\gamma - \cos\alpha)\}^{1/2} \\
&\times\{h_2^2b^2c^2\sin^2\alpha + k_2^2a^2c^2\sin^2\beta + l_2^2a^2b^2\sin^2\gamma \\
&+ 2h_2k_2abc^2(\cos\alpha\cos\beta - \cos\gamma) \\
&+ 2h_2l_2ab^2c(\cos\gamma\cos\alpha - \cos\beta) \\
&+ 2k_2l_2a^2bc(\cos\beta\cos\gamma - \cos\alpha)\}^{1/2}] \qquad (1)
\end{aligned}
$$

(2-2) The interplanar angle ϕ between $(h_1k_1l_1)$ and $(h_2k_2l_2)$ for monoclinic system (b-axis unique):

$$
\begin{aligned}
\cos\phi = &[h_1h_2b^2c^2 + k_1k_2c^2a^2\sin^2\beta + l_1l_2a^2\mathrm{b}^2 \\
&-ab^2c(h_1l_2 + h_2l_1)\cos\beta]/[(h_1^2b^2c^2 \\
&+ k_1^2c^2a^2\sin^2\beta + l_1^2a^2b^2 - 2h_1l_1ab^2\cos\beta)^{1/2} \\
&\times(h_2^2b^2c^2 + k_2^2c^2a^2\sin^2\beta + l_2^2a^2b^2 \\
&-2h_2l_2ab^2c\cos\beta)^{1/2}]
\end{aligned}
$$

$$
\cos\phi = \frac{\dfrac{h_1h_2}{a^2} + \dfrac{k_1k_2\sin^2\beta}{b^2} + \dfrac{l_1l_2}{c^2} - \dfrac{(h_1l_2 + h_2l_1)\cos\beta}{ac}}{\sqrt{\left(\dfrac{h_1^2}{a^2} + \dfrac{k_1^2\sin^2\cos\beta}{b^2} + \dfrac{l_1^2}{c^2} - \dfrac{2h_1l_1\cos\beta}{ac}\right)\times \left(\dfrac{h_2^2}{a^2} + \dfrac{k_2^2\sin^2\cos\beta}{b^2} + \dfrac{l_2^2}{c^2} - \dfrac{2h_2l_2\cos\beta}{ac}\right)}} \qquad (2)
$$

(2-3) The interplanar angle ϕ between $(h_1k_1l_1)$ and $(h_2k_2l_2)$ for orthorhombic system:

$$
\begin{aligned}
\cos\phi = &(h_1h_2b^2c^2 + k_1k_2c^2a^2 + l_1l_2a^2b^2) \\
&/[(h_1^2b^2c^2 + k_1^2c^2a^2 + l_1^2a^2b^2)^{1/2} \\
&\times(h_2^2b^2c^2 + k_2^2c^2a^2 + l_2^2a^2b^2)^{1/2}]
\end{aligned}
$$

$$
\cos\phi = \frac{\dfrac{h_1h_2}{a^2} + \dfrac{k_1k_2}{b^2} + \dfrac{l_1l_2}{c^2}}{\sqrt{\left(\dfrac{h_1^2}{a^2} + \dfrac{k_1^2}{b^2} + \dfrac{l_1^2}{c^2}\right)\left(\dfrac{h_2^2}{a^2} + \dfrac{k_2^2}{b^2} + \dfrac{l_2^2}{c^2}\right)}} \qquad (3)
$$

(2-4) The interplanar angle ϕ between $(h_1k_1l_1)$ and $(h_2k_2l_2)$ for tetragonal system:

$$
\begin{aligned}
\cos\phi = &(h_1h_2b^2c^2 + k_1k_2c^2a^2 + l_1l_2a^2b^2) \\
&/[(h_2^2b^2c^2 + k_2^2c^2a^2 + l_2^2a^2b^2)^{1/2} \\
&\times(h_2^2b^2c^2 + k_2^2c^2a^2 + l_2^2a^2b^2)^{1/2}]
\end{aligned}
$$

$$\cos\phi = \frac{\dfrac{h_1h_2 + k_1k_2}{a^2} + \dfrac{l_1l_2}{c^2}}{\sqrt{\left(\dfrac{h_1^2 + k_1^2}{a^2} + \dfrac{l_1^2}{c^2}\right)\left(\dfrac{h_2^2 + k_2^2}{a^2} + \dfrac{l_2^2}{c^2}\right)}} \quad (4)$$

(2-5) The interplanar angle ϕ between $(h_1k_1l_1)$ and $(h_2k_2l_2)$ for trigonal system (rhombohedral axes):

$$\begin{aligned}\cos\phi = [&a^4\sin^2(h_1h_2 + k_1k_2 + l_1l_2)\\ &+ a^4(h_1k_2 + h_2k_1)(\cos^2\alpha - \cos\alpha)\\ &+ a^4(h_1l_2 + h_2l_1)(\cos^2\alpha - \cos\alpha)\\ &+ a^4(k_1l_2 + k_2l_1)(\cos^2\alpha - \cos\alpha)]\\ &/[\{h_1^2a^4\sin^2\alpha + k_1^2a^4\sin^2\alpha\\ &+ l_1^2a^4\sin^2\alpha + 2h_1k_1a^4(\cos^2\alpha - \cos\alpha)\\ &+ 2h_1l_1a^4(\cos^2\alpha - \cos\alpha)\\ &+ 2k_1l_1a^4(\cos^2\alpha - \cos\alpha)\}^{1/2}\\ &\times\{h_2^2a^4\sin^2\alpha + k_2^2a^4\sin^2\alpha + l_2^2a^4\sin^2\alpha\\ &+ 2h_2k_2a^4(\cos^2\alpha - \cos\alpha)\\ &+ 2h_2l_2a^4(\cos^2\alpha - \cos\beta)\\ &+ 2k_2l_2a^4(\cos^2\alpha - \cos\alpha)\}^{1/2}]\end{aligned}$$

$$\cos\phi = \frac{\begin{aligned}&[\sin^2\alpha(h_1h_2 + k_1k_2 + l_1l_2)\\ &+ (\cos^2\alpha - \cos\alpha)(h_1k_2 + h_2k_1\\ &+ h_1l_2 + h_2l_1 + k_1l_2 + k_2l_1)]\end{aligned}}{\left[\sqrt{\begin{aligned}&\sin^2\alpha(h_1^2 + k_1^2 + l_1^2)\\ &+ 2(\cos^2\alpha - \cos\alpha)(h_1k_1 + h_1l_1 + k_1l_1)\end{aligned}} \times \sqrt{\begin{aligned}&\sin^2\alpha(h_2^2 + k_2^2 + l_2^2)\\ &+ 2(\cos^2\alpha - \cos\alpha)(h_2k_2 + h_2l_2 + k_1l_2)\end{aligned}}\right]} \quad (5)$$

(2-6) The interplanar angle ϕ between $(h_1k_1l_1)$ and $(h_2k_2l_2)$ for hexagonal system:

$$\begin{aligned}\cos\phi = &\left\{h_1h_2a^2c^2 + k_1k_2c^2a^2 + \frac{3}{4}l_1l_2a^4\right.\\ &\left.+ a^2c^2(h_1k_2 + h_2k_1)\left(\frac{1}{2}\right)\right\}\Big/\\ &\left[\left\{h_1^2a^2c^2 + k_1^2c^2a^2 + l_1^2a^4\left(\frac{3}{4}\right) + h_1k_1a^2c^2\right\}^{1/2}\right.\\ &\left.\times\left\{h_2^2a^2c^2 + k_2^2c^2a^2 + l_2^2a^4\left(\frac{3}{4}\right) + h_2k_2a^2c^2\right\}^{1/2}\right]\end{aligned}$$

$$\cos\phi = \frac{h_1h_2 + k_1k_2 + \dfrac{1}{2}(h_1k_2 + h_2k_1) + \dfrac{3}{4}\dfrac{a^2}{c^2}l_1l_2}{\sqrt{\left(h_1^2 + k_1^2 + h_1k_1 + \dfrac{3}{4}\dfrac{a^2}{c^2}l_1^2\right)\times\left(h_2^2 + k_2^2 + h_2k_2 + \dfrac{3}{4}\dfrac{a^2}{c^2}l_2^2\right)}} \quad (6)$$

(2-7) The interplanar angle ϕ between $(h_1k_1l_1)$ and $(h_2k_2l_2)$ for cubic system:

$$\begin{aligned}\cos\phi = &(h_1h_2b^2c^2 + k_1k_2c^2a^2 + l_1l_2a^2b^2)\\ &/[(h_1^2b^2c^2 + k_1^2c^2a^2 + l_1^2a^2b^2)^{1/2}\\ &\times(h_2^2b^2c^2 + k_2^2c^2a^2 + l_2^2a^2b^2)]^{1/2}\end{aligned}$$

$$\cos\phi = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{(h_1^2 + k_1^2 + l_1^2)(h_2^2 + k_2^2 + l_2^2)}} \quad (7)$$

3. Conclusion

The interplanar angle for each of the seven crystal systems can be calculated by substituting its real unit cell parameters a, b, c, α, β, γ into Eqs. (1), (2), (3), (4), (5), (6) and (7) shown above.

In trigonal system (rhombohedral axes), only an angle α between primitive crystallographic two basis vectors and Miller indices are needed as shown Eq. (5) and in the cubic system only Miller indices are required for the calculation of their interplanar angles.

References

1) International Tables for X-ray Crystallography, Vo.l. II, Edited by John S. Kasper and Kathleen Lonsdale, pp. 106-119, D.Reidel Publishing Company, Dordrecht/Boston/Lancaster (1985).
2) Elements of X-ray Diffraction, by B. D. Cullity, p. 502, Addison-Wesley Publishing Company, Inc. (1978).
3) International Tables for Crystallography Volume C, Edited by A. J. C. Wilson, pp. 2-9, Kluwer Academic Publishers, Dordrecht/Boston/London (1995).