

InterplanarA: A Computer Program for the Calculation of the Crystallographic Interplanar Angles

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InterplanarA: 結晶學的 面間 角의 計算을 위한 a Computer Program

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초 록

실격자(real lattice)에서 이차원적인 (hkl)면의 총 집합이 역격자(reciprocal lattice)에서 한 개의 점(點)으로 나타내어지며 원점에서 이 역격자점을 이은 vector의 방향은 (hkl)면의 방향이다. 따라서 두 역격자 vectors간의 각도가 결정학적 두 면간의 각도이므로 이들 각도들을 계산해보면 역격자의 개념을 이해하는데 도움이 된다. 이 논문에서는 6개의 실격자 상수 $a, b, c, \alpha, \beta, \gamma$ 를 사용하여 두 결정학적 면 ($h_1k_1l_1$)과 ($h_2k_2l_2$)간의 각도를 계산하는 한 computer program 'InterplanarA'를 소개하였다.

1. Crystallographic Problem

The Miller indices (hkl) represent all the planes that are parallel to each other with the same interplanar distance in single crystals, and they are expressed as vectors in the reciprocal lattice. Accordingly, the interplanar angle between two planes is the angle between the corresponding two reciprocal lattice vectors with tail at the origin. To understand the concept of the reciprocal lattices, it is beneficial if the interplanar angles in the real lattices are easily calculated.

The interplanar angles have been studied only in three books to the best of our knowledge. Donnay, J. D. H. and Donnay Gabrielle (1985) expressed the

crystallographic interplanar angles in terms of only reciprocal lattice constants: $a^*, b^*, c^*, \alpha^*, \beta^*, \gamma^*$ and Cullity, B. D. (1978) in terms of real lattice constants $a, b, c, \alpha, \beta, \gamma$ together with interplanar spacing and unit cell volume V . Koch E. (1995) provided how to calculate the angle between crystal planes ($h_1k_1l_1$) and ($h_2k_2l_2$) using reciprocal lattice parameters without providing any explicit expression for each of the seven crystal systems. Thus, to compute the interplanar angle using the above-mentioned formulas, either the reciprocal lattice parameters or the interplanar distance $d(hkl)$ and the unit cell volume V should be calculated first for triclinic, monoclinic and trigonal systems.

In this paper, the interplanar angle ϕ between crystal planes ($h_1k_1l_1$) and ($h_2k_2l_2$) is described only with the six real cell constants $a, b, c, \alpha, \beta, \gamma$

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together with two Miller indices $(h_1k_1l_1)$ and $(h_2k_2l_2)$ so that the calculation of the angle becomes convenient and straightforward.

2. Theory of Solution

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 and $d(hkl)$ is the interplanar distance. Therefore, the interplanar angle ϕ 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 $\vec{d}_2^*(h_2k_2l_2)$: $\vec{d}_1^* \cdot \vec{d}_2^* = d_1^* \cdot d_2^* \cos\phi$, 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 $\vec{d}_1^* \cdot \vec{d}_2^*$ and the absolute values of $\vec{d}_1^*(h_1k_1l_1)$, $\vec{d}_2^*(h_2k_2l_2)$ are calculated as follows:

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

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,

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

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

$$\begin{aligned} &= \frac{1}{V^2} \{ h_1h_2(\vec{b} \times \vec{c})^2 + k_1k_2(\vec{c} \times \vec{a})^2 + l_1l_2(\vec{a} \times \vec{b})^2 \\ &+ (h_1k_2 + h_2k_1)[(\vec{b} \cdot \vec{c})(\vec{c} \cdot \vec{a}) - c^2(\vec{b} \cdot \vec{a})] \end{aligned}$$

$$\begin{aligned} &+ (h_1l_2 + h_2l_1)[(\vec{b} \cdot \vec{a})(\vec{c} \cdot \vec{b}) - b^2(\vec{c} \cdot \vec{a})] \\ &+ (k_1l_2 + k_2l_1)[(\vec{c} \cdot \vec{a})(\vec{a} \cdot \vec{b}) - a^2(\vec{c} \cdot \vec{b})] \} \\ &= \frac{1}{V^2} \{ h_1h_2b^2c^2\sin^2\alpha + k_1k_2c^2a^2\sin^2\beta \\ &+ l_1l_2a^2b^2\sin^2\gamma + (h_1k_2 + h_2k_1) \\ &[(bcc\cos\alpha)(cac\cos\beta) - c^2(bacos\gamma)] \\ &+ (h_1l_2 + h_2l_1)[(bacos\gamma)(cbc\cos\alpha) \\ &- b^2(cacos\beta)] + (k_1l_2 + k_2l_1) \\ &[(cacos\beta)(abc\cos\gamma) - a^2(cbc\cos\alpha)] \} \end{aligned}$$

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

Similarly

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

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

The interplanar angle ϕ for each of the seven crystal systems is obtained as follows.

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

$$\begin{aligned} \cos\phi &= \frac{\vec{d}_1^* \cdot \vec{d}_2^*}{d_1^* d_2^*} = \{ h_1h_2b^2c^2\sin^2\alpha \\ &+ k_1k_2c^2a^2\sin^2\beta + l_1l_2a^2b^2\sin^2\gamma \\ &+ abc^2(h_1k_2 + h_2k_1)(\cos\alpha\cos\beta - \cos\gamma) \\ &+ ab^2c(h_1l_2 + h_2l_1)(\cos\gamma\cos\alpha - \cos\beta) \\ &+ a^2bc(k_1l_2 + k_2l_1)(\cos\beta\cos\gamma - \cos\alpha) \} \end{aligned}$$

$$\begin{aligned}
& /[\{h_1^2 b^2 c^2 \sin^2 \alpha + k_1^2 a^2 c^2 \sin^2 \beta + l_1^2 a^2 b^2 \sin^2 \gamma \\
& + 2h_1 k_1 a b c^2 (\cos \alpha \cos \beta - \cos \gamma) \\
& + 2h_1 l_1 a b^2 c (\cos \gamma \cos \alpha - \cos \beta) \\
& + 2k_1 l_1 a^2 b c (\cos \beta \cos \gamma - \cos \alpha)\}^{1/2} \\
& \times \{h_2^2 b^2 c^2 \sin^2 \alpha + k_2^2 a^2 c^2 \sin^2 \beta + l_2^2 a^2 b^2 \sin^2 \gamma \\
& + 2h_2 k_2 a b c^2 (\cos \alpha \cos \beta - \cos \gamma) \\
& + 2h_2 l_2 a b^2 c (\cos \gamma \cos \alpha - \cos \beta) \\
& + 2k_2 l_2 a^2 b c (\cos \beta \cos \gamma - \cos \alpha)\}^{1/2}] \quad (1)
\end{aligned}$$

(2) The interplanar angle ϕ for monoclinic system (b -axis unique):

$$\cos \phi = \frac{\frac{h_1 h_2}{a^2} + \frac{k_1 k_2 \sin^2 \beta}{b^2} + \frac{l_1 l_2}{c^2} - \frac{(h_1 l_2 + h_2 l_1) \cos \beta}{ac}}{\sqrt{\left(\frac{h_1^2}{a^2} + \frac{k_1^2 \sin^2 \cos \beta}{b^2} + \frac{l_1^2}{c^2} - \frac{2h_1 l_1 \cos \beta}{ac}\right) \left(\frac{h_2^2}{a^2} + \frac{k_2^2 \sin^2 \cos \beta}{b^2} + \frac{l_2^2}{c^2} - \frac{2h_2 l_2 \cos \beta}{ac}\right)}}$$

(3) The interplanar angle ϕ for orthorhombic system:

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

(4) The interplanar angle ϕ for tetragonal system:

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

(5) The interplanar angle ϕ for trigonal system (rhombohedral axes):

$$\begin{aligned}
& [\sin^2 \alpha (h_1 h_2 + k_1 k_2 + l_1 l_2) \\
& + (\cos^2 \alpha - \cos \alpha) (h_1 k_2 + h_2 k_1 \\
& + h_1 l_2 + h_2 l_1 + k_1 l_2 + k_2 l_1)] \\
\cos \phi = & \frac{\sqrt{\sin^2 \alpha (h_1^2 + k_1^2 + l_1^2)} \sqrt{\sin^2 \alpha (h_2^2 + k_2^2 + l_2^2)}}{\sqrt{[+ 2(\cos^2 \alpha - \cos \alpha) (h_1 k_1 + h_1 l_1 + k_1 l_1)]} \sqrt{[+ 2(\cos^2 \alpha - \cos \alpha) (h_2 k_2 + h_2 l_2 + k_2 l_2)]}}
\end{aligned}$$

(6) The interplanar angle ϕ for hexagonal system:

$$\cos \phi = \frac{h_1 h_2 + k_1 k_2 + \frac{1}{2}(h_1 k_2 + h_2 k_1) + \frac{3}{4} \frac{a^2}{c^2} l_1 l_2}{\sqrt{\left(h_1^2 + k_1^2 + h_1 k_1 + \frac{3}{4} \frac{a^2}{c^2} l_1^2\right) \left(h_2^2 + k_2^2 + h_2 k_2 + \frac{3}{4} \frac{a^2}{c^2} l_2^2\right)}}$$

```

C:\Documents and Settings\Taewon\My Documents\software\InterplanarA.exe
This program calculates an interplanar angle between <h1 k1 l1> and
<h2 k2 l2> in each run.

<1> This program requires an input file name that should be provided
by users. There is no fixed format of the input file except each
number should be separated by space(s).

The input file format should be as follows:
a, b, c in angstrom,
alpha, beta, gamma in degrees,
Miller indices <h1 k1 l1> and <h2 k2 l2> of two planes

<2> After reading the input file, the program will require an output
file name.

Example of an input file:
9.452 13.841 16.754 100.523 105.372 106.04 0 1 0 0 0 1

Example of the generated output file
a = 9.452, b = 13.841, c = 16.954
alpha = 100.523, beta = 105.372, gamma = 106.04
h1 k1 l1 and h2 k2 l2 phi <degree>
0 1 0 0 0 1 73.971

Enter input file name:

```

Fig. 1. The procedure to run the program "InterplanarA".

(7) The interplanar angle ϕ for cubic system:

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

The program *InterplanarA* for the calculation of the crystallographic interplanar angles has been written based on (Eq. 1).

3. How to Run the Program “InterplanarA”

Double-click on the executable, *interplanarA.exe*, and then follow the instructions on the screen as shown in Fig. 1.

4. Environment and Availability

The program is written in C-language, and it is executed on a Windows-based PC. Soft copy

of the program is available upon request from ihsuh@korea.ac.kr.

References

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

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