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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*, α, β, γ를 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^*, α^*, β^*, γ^* and Cullity, B. D. (1978) in terms of real lattice constants *a*, *b*, *c*, α, β, γ 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*, α, β, γ

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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 $\vec{d}_2^*$ $(h_2k_2l_2)$: $\vec{d}_1^* \bullet \vec{d}_2^* = d_1^* \bullet d_2^* \cos\phi$, 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 $\vec{d}_1^* \bullet \vec{d}_2^*$ 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,

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

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

$$= \frac{1}{V^2}\{h_1h_2(\vec{b} \times \vec{c})^2 + k_1k_2(\vec{c} \times \vec{a})^2 + l_1l_2(\vec{a} \times \vec{b})^2 + (h_1k_2 + h_2k_1)[(\vec{b} \bullet \vec{c})(\vec{c} \bullet \vec{a}) - c^2(\vec{b} \bullet \vec{a})] + (h_1l_2 + h_2l_1)[(\vec{b} \bullet \vec{a})(\vec{c} \bullet \vec{b}) - b^2(\vec{c} \bullet \vec{a})] + (k_1l_2 + k_2l_1)[(\vec{c} \bullet \vec{a})(\vec{a} \bullet \vec{b}) - a^2(\vec{c} \bullet \vec{b})]\}$$

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

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

Similarly

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

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

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:

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

$$/[\{h_1^2b^2c^2\sin^2\alpha + k_1^2a^2c^2\sin^2\beta + l_1^2a^2b^2\sin^2\gamma$$
$$+ 2h_1k_1abc^2(\cos\alpha\cos\beta - \cos\gamma)$$
$$+ 2h_1l_1ab^2c(\cos\gamma\cos\alpha - \cos\beta)$$
$$+ 2k_1l_1a^2bc(\cos\beta\cos\gamma - \cos\alpha)\}^{1/2}$$
$$\times\{h_2^2b^2c^2\sin^2\alpha + k_2^2a^2c^2\sin^2\beta + l_2^2a^2b^2\sin^2\gamma$$
$$+ 2h_2k_2abc^2(\cos\alpha\cos\beta - \cos\gamma)$$
$$+ 2h_2l_2ab^2c(\cos\gamma\cos\alpha - \cos\beta)$$
$$+ 2k_2l_2a^2bc(\cos\beta\cos\gamma - \cos\alpha)\}^{1/2}] \qquad (1)$$

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

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

(3) The interplanar angle ϕ for orthorhombic system:

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

(4) The interplanar angle ϕ for tetragonal system:

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

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

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

(6) The interplanar angle ϕ for hexagonal system:

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

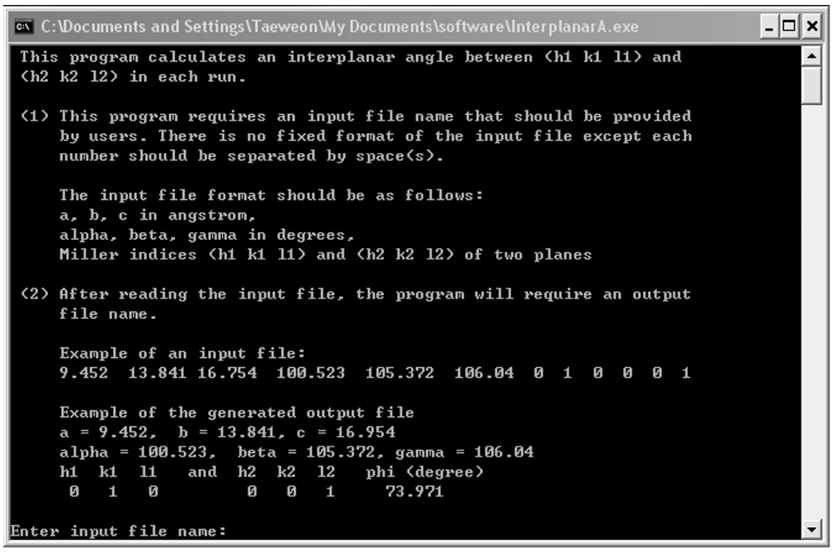

Fig. 1. The procedure to run the program "*InterplanarA*".

(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.

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