Korea J. Cryst., Vol. 1, P. 57~59, 1990

点群 422의 操作下에 等價逆格子点

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Reciprocal Lattice Points Equivalent under the Operations of the Point Group 422

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(Received 15 January 1990; accepted 2 February 1990)

요 약

International Tables of X-Ray Crystallography Vol. IV(1974) Table 2.3.2.에 誤字가 있다. 点群 422의 等價反射面들은 $hkl=\bar{h}\bar{k}l=h\bar{k}\bar{l}=\bar{h}k\bar{l}=kh\bar{l}=\bar{k}hl=k\bar{h}l=\overline{kh}\bar{l}$이다.

Abstract

We point out an error in the Table 2.3.2 of International Tables of X-Ray Crystallography Vol. IV(1974). The equivalent reflections of the point group 422 should be $hkl=\bar{h}\bar{k}l=h\bar{k}\bar{l}=\bar{h}k\bar{l}=kh\bar{l}=\bar{k}hl=k\bar{h}l=\overline{kh}\bar{l}$.

INTRODUCTION

There are ten basic rotational symmetry elements in crystalline solids grown in laboratory or obtained in nature. They are 1-, 2-, 3-, 4-, 6-, $\bar{1}$-, $\bar{2}$-, $\bar{3}$-, $\bar{4}$-, and $\bar{6}$-fold symmetries. Consistent combinations of the basic rotational symmetry elements give rise to 32 point groups or crystal classes, and seven point groups out of them belong to tetragonal system[1]. They are 4, $\bar{4}$, $\frac{4}{m}$, 422, 4mm, $\bar{4}$2m and $\frac{4}{m}$mm. Here the families of equivalent planes of the point group 422 will be derived.

THEORY

The Bragg law $\lambda=2d_{hkl}\sin\theta_{hkl}$ is the necessary condition for diffraction that can be visualized relatively easily on the Ewald sphere with the reciprocal lattices concept.

The reciprocal lattice vector defined by $\vec{d}^*_{hkl}=h\vec{a}^*+k\vec{b}^*+l\vec{c}^*$ is normal to (hkl) and $|\vec{d}^*_{hkl}|$ is the reciprocal of d_{hkl}.

Therefore the reciprocal lattice point designated by the vector $\vec{d}^*_{hkl}$ represents a family of plane (hkl)[2].

Let us try to find out the equivalent reciprocal lattice points, i.e., families of equivalent planes in the point group 422, where the first letter 4 stands for a tetrad axis along c-axis, the second letter 2 for diad axes perpendicular to the tetrad axis and the third letter 2 for diad axes bisecting the above two 2-fold symmetry axes.

4-fold symmetry along c-axis can be represented by a 3×3 matrix as follows :

$$\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Operating this symmetry on any arbitrary position and then continuing the operation iteratively, we get equivalent positions :

$$\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -y \\ x \\ z \end{bmatrix}$$

$$\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} -y \\ x \\ z \end{bmatrix} = \begin{bmatrix} -x \\ -y \\ z \end{bmatrix}$$

$$\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} -x \\ -y \\ z \end{bmatrix} = \begin{bmatrix} y \\ -x \\ z \end{bmatrix}$$

Applying 2−fold symmetry along a−axis to the above four positions, we get additional four positions :

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \\ -y \\ -z \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} -y \\ x \\ z \end{bmatrix} = \begin{bmatrix} -y \\ -x \\ -z \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} -x \\ -y \\ z \end{bmatrix} = \begin{bmatrix} -x \\ y \\ -z \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} y \\ -x \\ z \end{bmatrix} = \begin{bmatrix} y \\ x \\ -z \end{bmatrix}$$

The third 2−fold symmetry bisecting a− and b−axis is represented by

$$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

Operation of this symmetry on each of the above eight positions results in one of themselves. Therefore there are only eight equivalent positions : (x y z), (−x −y z), (−x y −z), (x −y −z), (−y −x −z), (y x −z), (y −x z) and (−y x z).

Substituting the eight positions to structure factor equation one can ascertain that the eight plane groups $(h\ k\ l)$, $(-h\ -k\ l)$, $(-h\ k\ -l)$, $(h\ -k\ -l)$, $(-k\ -h\ -l)$, $(k\ h\ -l)$, $(k\ -h\ l)$ and $(-k\ h\ l)$ have identical structure factors. Therefore, the point group 422 belongs to the Laue group $\frac{4}{m}$ mm.

Omitting the scattering and temperature factors, its identical structure factors are as follows :

$$\begin{aligned} F(hkl) &= \exp 2\pi i(\ hx+ky+lz) \\ &= \ 〃\ (-hx-ky+lz) \\ &= \ 〃\ (-hx+ky-lz) \\ &= \ 〃\ (\ hx-ky-lz) \\ &= \ 〃\ (-hy-kx-lz) \\ &= \ 〃\ (\ hy+kx-lz) \\ &= \ 〃\ (\ hy-kx+lz) \\ &= \ 〃\ (-hy+kx+lz). \end{aligned}$$

CONCLUSION

In the point group 422 there are eight equivalent reflections if the Friedel's law is not assumed. They are (hkl), $(\bar{h}k\bar{l})$, $(h\bar{k}\bar{l})$, $(\bar{h}\bar{k}l)$, $(kh\bar{l})$, $(\bar{k}hl)$, $(k\bar{h}l)$ and $(\overline{khl})$.

Therefore the Table 2.3.2 in the International Table for X−Ray Crystallography Vol. IV, p.151 (1974)[3] should be corrected

from

point group	equivalent reflections
422	$hkl=\bar{h}k\bar{l}=h\bar{k}l=\cdots$

to

422	$hkl=\bar{h}k\bar{l}=h\bar{k}\bar{l}=\cdots$

References

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3) International Table for X−Ray Crystallography (1974). **IV**, 151, edited by J.A. Ibers and W.C. Hamiton. Birmingham : Kynoch Press.