X-선 분말회절에 의한 결정구조 해석을 위한 결정면의 다중도 인자

徐日煥, 秋錦洪, 李珍昊, 林星秀, 柳保盈, 朴晶蘭
金憲俊*, 成百石*, 李正秀*, 金文執**

忠南大學校 物理學科, 大田 305-764
*韓國原子力硏究所 中性子物理硏究室, P.O.BOX 7 서울 淸凉 郵遞局
**順天鄕大學校 物理學科, 溫陽 336-600

Multiplicity Factors of Crystal Planes for Structure Analysis by X-ray Powder Diffraction

Il-Hwan Suh, Geum-Hong Choo, Jin-Ho Lee, Sung-Su Lim, Bo-Young Ryu, Jeong-Ran Park, Huhn Jun Kim,*
Baek-Seok Seong, Jeong-Soo Lee and Moon-Jib Kim**

Department of Physics, Chungnam National University Daejeon 305-764, Korea
**Neutron Physics Laboratory, Korea Atomic Energy Research Institute P.O.Box 7, Cheong Ryang, Seoul, Korea*
***Department of Physics, Soonchunhyang University Onyang 336-600, Korea*

要 約

同一한 面間距離와 同一한 强度를 갖는 面들의 數로써 定義되는 한 面形(form)의 多重度 因子를 11個의 Laue群의 對稱性에 基礎하여 圖表化하였다.

Abstract

The multiplicity factor, which is defined as the number of different planes in a form having identical interplanar spacing and identical intensity, is tabulated here for the eleven Laue groups on the basis of their symmetries.

1. Introduction

The multiplicity factor, which is one of the six factors affecting the relative intensity of the diffraction lines on a powder patterns[1], has been reported in many literatures. They are, however, neither described in detail nor easily understandable.[1~5]

In the present paper, the multiplicities for all crystal forms of the eleven Laue groups are tabulated explicitly.

2. Theory

The equivalent plane relation in each Laue group can be deduced from its symmetry and there are fourteen different kinds of planes for positive Miller indices: *hkℓ*, *hkh*, *hkk*, *hhℓ*, *hhh*, *0kℓ*, *h0ℓ*, *hk0*, *0kk*, *h0h*, *hh0*, *h00*, *0k0*, *00ℓ*. The substitution of these planes into the equivalent plane relation results in the multiplicities for the crystal forms.

Table 1 shows the information on the 11 Laue groups(column 2) where alternative possibilities are separated by dashed lines. Crystal system is given in column 1. Column 3 describes the equivalent plane relation, but only one of each centrosymmetric pair is given[6]. Column 4 shows the different kinds of crystal forms and all the corresponding multiplicities are given in the last column. Substituting the crystal form given in column 4 into the equivalent plane relation in column 3, a set of all symmetrically equivalent planes is obtained.

Since there is only one Laue group in triclinic, monoclinic and orthorhombic systems, the multiplicities for their crystal forms are unique. However, for the monoclinic crystal, its unique axis must be confirmed before referring to the table 1.

In each of the tetragonal, trigonal, hexagonal and cubic systems, there are certain planes which are equivalent by the higher-symmetry Laue class but not by the lower-symmetry Laue class. Since such forms have the same interplanar spacing, they give rise to the same line in a powder diffraction pattern even in the lower-symmetry Laue class. Therefore, the intensities of the forms in parentheses in the lower-symmetry Laue class are stronger than their own ones. In order to obtain their real intensities, the crystal forms which are not connected by the symmetry of the lower-symmetry Laue class must be found by comparing the two equivalent plane relations(in column 3) of the lower-symmetry and the highest-symmetry Laue classes in a system and then, the intensities of the additional forms with the same interplanar spacing but with the different intensity must be subtracted from the experimentally obtained ones.

Acknowledgment

This work was supporrted by the Korean Science and Engineering Foundation (KOSEF) through the Science Research Center(SRC) of Excellence Program.

References

1. Cullity, B.D., Elements of X-ray Diffraction, p.126, p.523, Addison-Wesley publishing Company(1978).
2. Nuffield, E.W., X-ray Diffraction Methods, pp.108-110, John Wiley & Sons, Inc., New York. London. Sydney(1966).
3. Azaroff, Leonid V., Elements of X-ray Crystallography, p.201, McGraw-Hill Book Company(1968).
4. Klug, H.P. and Alexander, L.E., X-ray diffracion procedures, pp.162-164, John Wiley & Sons, New York, London. Sydney. Toronto (1974).
5. International Tables for X-Ray Crystallography, Vol. 1, Edited by Norman F.M. Henry and Kathleen Lonsdale, pp. 31-34, The Kynoch Press, Birmingham, England(1969).
6. Lee, J.H., M.S. Thesis, Chungnam National University. Daejeon, 305-764 Korea(1992).

Table 1. Multiplicity for the powder method

Crystal system	Laue group	Equivalent plane (only one of each centrosymmetric pair is given)	Crystal form	Multi-plicity
triclinic	$\bar{1}$	hkl	all planes	2
mono-clinic	2/m (b-axis unique)	hkl, $h\bar{k}l$	$hkl, \bar{h}kl, hhl, \bar{h}hl, hkh, \bar{h}kh, hkk$ $\bar{h}kk, hhh, \bar{h}hh, 0kl, hk0, 0kk, hh0$	4
			$h0l, \bar{h}0l, h0h, \bar{h}0h, h00, 0k0, 00l$	2
	2/m (c-axis unique)	hkl, $hk\bar{l}$	$hkl, \bar{h}kl, hhl, \bar{h}hl, hkh, \bar{h}kh, hkk$ $\bar{h}kk, hhh, \bar{h}hh, 0kl, h0l, 0kk, h0h$	4
			$hk0, \bar{h}k0, hh0, \bar{h}h0, h00, 0k0, 00l$	2
ortho-rhombic	mmm	hkl, $\bar{h}kl$, $h\bar{k}l$, $hk\bar{l}$	hkl, hhl, hkh, hkk, hhh	8
			$0kl, h0l, hk0, 0kk, h0h, hh0$	4
			$h00, 0k0, 00l$	2
tetra-gonal	4/m	hkl, $\bar{k}hl$, $hk\bar{l}$, $k\bar{h}l$	$(hkl), (hkh), (hkk)$ $hhl, hhh, h0l, h0h$	8
			$(hk0), hh0, h00$	4
			$00l$	2
	4/mmm	hkl, $\bar{k}hl$, $hk\bar{l}$, $k\bar{h}l$ $\bar{h}kl$, $kh\bar{l}$, $h\bar{k}l$, khl	hkl, hkh	16
			$hhl, hhh, h0l, hk0, h0h$	8
			$hh0, h00$	4
			$00l$	2
tri-gonal	$\bar{3}$(R)	hkl, lhk, klh	$(hkl), (\bar{h}kl), (\bar{h}hl), (hk0)$ $(\bar{h}k0)$ and all other planes	6
			hhh	2
	$\bar{3}$m(R)	hkl, lhk, klh hlk, lkh, khl	$hkl, \bar{h}kl, \bar{h}hl, hk0, \bar{h}k0$	12
			$hhl, \bar{h}kk, \bar{h}hh, hh0, \bar{h}h0, h00$	6
			hhh	2

tri-gonal	$\bar{3}$(H)	$hkil$, $ihkl$, $kihl$	(all planes)expect $h0\bar{h}0$, $hh2\bar{h}0$	6
			$000l$	2
	$\bar{3}$1m(H)	$hkil$, $ihkl$, $kihl$ $khil$, $hikl$, $ikhl$	$(hkil)$, $(hki\bar{l})$, $(hkih)$, $(hki\bar{h})$ $h0\bar{h}l$, $hki0$, $h0\bar{h}h$	12
			$(hh2\bar{h}l)$, $(h\bar{h}0l)$, $(hh2\bar{h}h)$, $(h\bar{h}0h)$ $hh2\bar{h}0$, $h0\bar{h}0$	6
			$000l$	2
	$\bar{3}$m1(H)	$hkil$, $ihkl$, $kihl$ $khi\bar{l}$, $\bar{h}\bar{i}\bar{k}l$, $\bar{i}\bar{k}\bar{h}l$	$(hkil)$, $(hkih)$, $(hkik)$ $hh2\bar{h}l$, $hh2\bar{h}h$, $hki0$	12
			$(0k\bar{k}l)$, $(h0\bar{h}l)$, $(0h\bar{h}h)$, $(h0\bar{h}h)$ $hh2\bar{h}0$, $h0\bar{h}0$	6
			$000l$	2
hexa-gonal	6/m	$hkil$, $\bar{k}\bar{i}\bar{h}l$, $ihkl$ $hki\bar{l}$, $kihl$, $\bar{i}\bar{h}\bar{k}l$	$(hkil)$, $(hkih)$, $(hkik)$ $hh2\bar{h}l$, $hh2\bar{h}h$, $h0\bar{h}l$, $h0\bar{h}h$	12
			$(hki0)$, $hh2\bar{h}0$, $h0\bar{h}0$	6
			$000l$	2
	6/mmm	$hkil$, $\bar{k}\bar{i}\bar{h}l$, $ihkl$ $hki\bar{l}$, $kihl$, $\bar{i}\bar{h}\bar{k}l$ $khil$, $\bar{i}\bar{k}\bar{h}l$, $hikl$ $khi\bar{l}$, $ikhl$, $\bar{h}\bar{i}\bar{k}l$	$hkil$, $hkih$	24
			$hh2\bar{h}l$, $hh2\bar{h}h$, $hki0$, $h0\bar{h}l$, $h0\bar{h}h$	12
			$h0\bar{h}0$ $hh2\bar{h}0$	6
			$000l$	2

cubic	m$\bar{3}$	hkl, $\bar{h}kl$, $h\bar{k}l$, $hk\bar{l}$ lhk, $\bar{l}hk$, $l\bar{h}k$, $lh\bar{k}$ klh, $\bar{k}lh$, $k\bar{l}h$, $kl\bar{h}$	(hkl), hhl	24
			$(hk0)$, $hh0$	12
			hhh	8
			$h00$	6
	m$\bar{3}$m	hkl, $\bar{h}kl$, $h\bar{k}l$, $hk\bar{l}$ lhk, $\bar{l}hk$, $l\bar{h}k$, $lh\bar{k}$ klh, $\bar{k}lh$, $k\bar{l}h$, $kl\bar{h}$ hlk, $\bar{h}lk$, $h\bar{l}k$, $hl\bar{k}$ lkh, $\bar{l}kh$, $l\bar{k}h$, $lk\bar{h}$ khl, $\bar{k}hl$, $k\bar{h}l$, $kh\bar{l}$	hkl	48
			hhl, $hk0$	24
			$hh0$	12
			hhh	8
			$h00$	6

R : rhombohedral coordinate axis
H : hexagonal coordinate axis