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21個 非對稱中心點群의 等價逆格子點

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Reciprocal Lattice Points Equivalent under the Operations of 21 Noncentrosymmetric Point Groups

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요 약

32개 點群은 中心對稱(centrosymmetric)을 갖는 11가지 點群(Laue群)과 21個의 非對稱中心(noncentrosymmmtric)點群으로 이루어졌다.

本 硏究에서는 21個 非對稱中心點群 各各의 等價回折面(等價逆格子點)들을 誘導하였다.

Abstract

The thirty two point groups consist of eleven Laue groups (centrosymmetric point groups) and twenty one noncentrosymmteric point groups.

In this paper, the reciprocal lattice points equivalent under the operations of 21 noncentrosymmetric point groups are derived

1. 서 론

結晶에는 1, 2, 3, 4, 6, $\bar{1}$, $\bar{2}$, $\bar{3}$, $\bar{4}$, $\bar{6}$ 等 10가지 回轉 基本對稱 要素가 있으며 이 10가지 對稱要素를 組合하면 32개 點群이 誘導된다.[1)]

點群은 格子의 對稱性을 나타내는데 Miller 指數의

對稱性은 點群의 對稱性에 따른다.

따라서 Miller 指數 hkl 의 函數인 回折强度의 對稱性도 點群 對稱으로 부터 誘導 될 수 있다.[2] 11가지 對稱中心點群의 等價面關係는 이미 發表되었으며[3] 지금까지 發表된 21個 非對稱中心點群의 等價面關係는 理解하기에 어려움이 있을뿐만 아니라 誤謬까지 包含되어있다.[4)~5)]

2. 이 론

21個의 非對稱中心點群에 包含된 對稱 要素들을 行列로 나타내면 Table 1과 같으며 Ewald球 内의 逆格子點들은 8가지 다른 Miller 指數種類 $hkl, \bar{h}kl, h\bar{k}l, hk\bar{l}, \overline{hk}l, h\overline{kl}, \bar{h}k\bar{l}, \overline{hkl}$로 分類할 수 있다.

이 8가지 Miller 指數들을 각 點群 對稱 行列에 操作하므로써 等價面들을 求할 수 있으며 이들 等價面關係式에서 重複되는것을 除去하면 21個 點群 各各의 非對稱領域内에 있는 等價面關係가 얻어지는데 이를 Table 2에 整理하여 놓았다.

그런데, tetragonal 에서 點群 $\bar{4}2m$은 $\bar{4}m2$로도 볼 수 있으며, 點群 3(R)은 hexagonal인 3(H)로도 되고, 點群 32는 321(H)와 312(H)로 分類되며, 點群 3m(R)은 3m1(H)와 31m(H)로 分類되고, hexagonal의 點群 $\bar{6}m2$는 點群 $\bar{6}2m$으로도 되므로 7가지가 더 添加되며 monoclinic의 點群 2와 m을 c-axis unique인 경우도 添加하여 Table 2에는 모두 30種類의 點群으로 分類하여 表示하였다.

Table 1. 21個 非對稱中心點群에 包含된 對稱의 軸(面)變換 行列.

對稱性	對稱方向	結晶系	面變換 行列
1	none	Triclinic	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
2	[100]	Orthorhombic Tetragonal Cubic	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$
	[010]	Monoclinic (b-axis unique) Orthorhombic Tetragonal Cubic	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$
	[001]	Monoclinic (c-axis unique) Orthorhombic Cubic	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
	[110]	Tetragonal Cubic	$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$

Table 1. (cont.)

	$[1\bar{1}0]$	Trigonal(R)	$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$
	[100]	Hexagonal	$\begin{bmatrix} 1 & 0 & 0 \\ -1 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$
	[210]	Hexagonal	$\begin{bmatrix} 1 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$
3	[001]	Trigonal(H)	$\begin{bmatrix} 0 & 1 & 0 \\ -1 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
	[111]	Trigonal(R) Cubic	$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$
$\bar{3}$	[001]	Trigonal(H)	$\begin{bmatrix} 0 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$
	[111]	Trigonal(R) Cubic	$\begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{bmatrix}$
4	[100]	Cubic	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}$
	[010]	Cubic	$\begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$
	[001]	Tetragonal Cubic	$\begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
$\bar{4}$	[100]	Cubic	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$
	[010]	Cubic	$\begin{bmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{bmatrix}$
	[001]	Tetragonal Cubic	$\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$

Table 1. (cont.)

6	[001]	Haxagonal	$\begin{bmatrix} 1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
$\bar{6}$	[001]	Haxagonal	$\begin{bmatrix} -1 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$
m	[100]	Orthorhombic Tetragonal Cubic	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
	[100]	Trigonal(H) Haxagonal	$\begin{bmatrix} -1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
	[010]	Monoclinic (b-axis unique) Orthorhombic Cubic	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
	[001]	Monoclinic (c-axis unique) Orthorhombic Tetragonal Cubic	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$
	[110]	Tetragonal Cubic	$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
	$[1\bar{1}0]$	Trigonal(R) Cubic	$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
	[210]	Trigonal(H) Hexagonal	$\begin{bmatrix} -1 & -1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

Table 2. 28個 非對稱中心點群의 等價逆格子點
R: rhombohedral coordinate axis
H: hexagonal coordinate axis

System	Point groups	Space groups	Equivalent reflections
Tri-clinic	1	P1	hkl, $\bar{h}kl$, $h\bar{k}l$, $hk\bar{l}$ $\overline{hk}l$, $\bar{h}k\bar{l}$, $h\overline{kl}$, $\overline{hkl}$

Table 2. (cont.)

Monoclinic	2 (b-axis unique)	P2 $P2_1$ C2	$hkl = \bar{h}k\bar{l}$, $\bar{h}kl = hk\bar{l}$ $h\bar{k}l = \bar{h}\bar{k}\bar{l}$, $\bar{h}\bar{k}l = h\bar{k}\bar{l}$
	m (b-axis unique)	Pm Pc Cm Cc	$hkl = h\bar{k}l$, $\bar{h}kl = \bar{h}\bar{k}l$ $hk\bar{l} = h\bar{k}\bar{l}$, $\bar{h}k\bar{l} = \bar{h}\bar{k}\bar{l}$
	2 (c-axis unique)	P2 $P2_1$ C2	$hkl = \bar{h}\bar{k}l$, $\bar{h}kl = h\bar{k}l$ $hk\bar{l} = \bar{h}\bar{k}\bar{l}$, $\bar{h}k\bar{l} = h\bar{k}\bar{l}$
	m (c-axis unique)	Pm Pc Cm Cc	$hkl = hk\bar{l}$, $\bar{h}kl = \bar{h}k\bar{l}$ $h\bar{k}l = h\bar{k}\bar{l}$, $\bar{h}\bar{k}l = \bar{h}\bar{k}\bar{l}$
Orthorhombic	222 (22)	P222 P2221 $P2_12_12$ $P2_12_12_1$ $C222_1$ C222 F222 I222 $I2_12_12_1$	$hkl = \bar{h}\bar{k}l = \bar{h}k\bar{l} = h\bar{k}\bar{l}$ $\bar{h}kl = h\bar{k}l = hk\bar{l} = \bar{h}\bar{k}\bar{l}$
	$mm2$ ($2m$)	Pmm2 $Pmc2_1$ Pcc2 Pma2 $Pca2_1$ Pnc2 $Pmn2_1$ Pba2 $Pna2_1$ Pnn2 Cmm2 $Cmc2_1$ Ccc2 Amm2 Abm2 Ama2 Aba2 Fmm2 Fdd2 Imm2 Iba2 Ima2	$hkl = \bar{h}kl = h\bar{k}l = \bar{h}\bar{k}l$ $hk\bar{l} = \bar{h}k\bar{l} = h\bar{k}\bar{l} = \bar{h}\bar{k}\bar{l}$
Teragonal	4	P4 $P4_1$ $P4_2$ $P4_3$ I4 $I4_1$	$hkl = \bar{h}\bar{k}l = k\bar{h}l = \bar{k}hl$ $hk\bar{l} = \bar{h}\bar{k}\bar{l} = k\bar{h}\bar{l} = \bar{k}h\bar{l}$
	$\bar{4}$	$P\bar{4}$ $I\bar{4}$	$hkl = \bar{h}\bar{k}l = k\bar{h}\bar{l} = \bar{k}h\bar{l}$ $hk\bar{l} = \bar{h}\bar{k}\bar{l} = k\bar{h}l = \bar{k}hl$
	422 (42)	P422 $P42_12$ $P4_122$ $P4_12_12$ $P4_222$ $P4_22_12$ $P4_322$ $P4_32_12$ I422 $I4_122$	$hkl = \bar{h}k\bar{l} = h\bar{k}\bar{l} = \bar{h}\bar{k}l = kh\bar{l} = \bar{k}hl = k\bar{h}l = \bar{k}\bar{h}l$
	$4mm$ ($4m$)	P4mm P4bm $P4_2cm$ $P4_2nm$ P4cc P4nc $P4_2mc$ $P4_2bc$ I4mm I4cm $I4_1md$ $I4_1cd$	$hkl = h\bar{k}l = \bar{h}kl = \bar{h}\bar{k}l = khl = \bar{k}hl = k\bar{h}l = \bar{k}\bar{h}l$ $hk\bar{l} = h\bar{k}\bar{l} = \bar{h}k\bar{l} = \bar{h}\bar{k}\bar{l} = kh\bar{l} = \bar{k}h\bar{l} = k\bar{h}\bar{l} = \bar{k}\bar{h}\bar{l}$
	$\bar{4}2m$ ($\bar{4}m$)	$P\bar{4}2m$ $P\bar{4}2c$ $P\bar{4}2_1m$ $P\bar{4}2_1c$ $I\bar{4}2m$ $I\bar{4}2d$	$hkl = \bar{h}k\bar{l} = h\bar{k}\bar{l} = \bar{h}\bar{k}l = khl = \bar{k}\bar{h}l = \bar{k}h\bar{l} = k\bar{h}\bar{l}$ $hk\bar{l} = \bar{h}kl = h\bar{k}l = \bar{h}\bar{k}\bar{l} = kh\bar{l} = \bar{k}\bar{h}\bar{l} = \bar{k}hl = k\bar{h}l$
	$\bar{4}m2$	$P\bar{4}m2$ $P\bar{4}c2$ $P\bar{4}b2$ $P\bar{4}n2$ $I\bar{4}m2$ $I\bar{4}c2$	$hkl = \bar{h}kl = h\bar{k}l = \bar{h}\bar{k}l = kh\bar{l} = \bar{k}h\bar{l} = k\bar{h}\bar{l} = \bar{k}\bar{h}\bar{l}$
Tri-gonal/ Rhombohedral	3(R)	R3	$hkl = klh = lhk$ $\bar{h}kl = kl\bar{h} = l\bar{h}k$ $\bar{h}\bar{k}l = \bar{k}l\bar{h} = l\bar{h}\bar{k}$ $\bar{h}\bar{k}\bar{l} = \bar{k}\bar{l}\bar{h} = \bar{l}\bar{h}\bar{k}$

Table 2. (cont.)

Tri-gonal/ Rhombohedral	$3(H)$	P3 $P3_1$ $P3_2$ R3(H)	$\bar{h}kl = kh+\bar{k}l = h+\overline{kh}l$ $\bar{h}k\bar{l} = kh+\overline{kl} = h+\overline{khl}$
	$32(R)$	R32	$hkl = klh = lhk = \overline{khl} = \overline{lkh} = \overline{hlk}$ $\bar{h}kl = kl\bar{h} = l\bar{h}k = \bar{k}h\bar{l} = \bar{l}\bar{k}h = h\bar{l}\bar{k}$
	$321(H)$	P321 $P3_121$ $P3_221$ R32(H)	$\bar{h}kl = kh+\bar{k}l = h+\overline{kh}l = \bar{h}h+\bar{k}l = k\bar{h}l = h+\bar{k}k\bar{l}$
	$312(H)$	P312 $P3_112$ $P3_212$	$hkl = k\bar{h}+\bar{k}l = \bar{h}+\bar{k}hl = h+k\overline{kl} = \bar{h}h+k\bar{l} = \overline{khl}$ $hk\bar{l} = k\bar{h}+\overline{kl} = \bar{h}+\bar{k}h\bar{l} = h+k\bar{k}l = \bar{h}h+kl = \overline{kh}l$
	$3m(R)$	R3m R3c	$hkl = klh = lhk = khl = lkh = hlk$ $\bar{h}kl = kl\bar{h} = l\bar{h}k = k\bar{h}l = lk\bar{h} = \bar{h}lk$ $\overline{hk}l = \bar{k}l\bar{h} = l\overline{hk} = \overline{kh}l = l\overline{kh} = \bar{h}l\bar{k}$ $\overline{hkl} = \overline{klh} = \overline{lhk} = \overline{khl} = \overline{lkh} = \overline{hlk}$
	$3m1(H)$	P3m1 P3c1 R3m(H) R3c(H)	$hkl = k\bar{h}+\bar{k}l = \bar{h}+\bar{k}hl = \bar{h}h+kl = \overline{kh}l = h+k\bar{k}l$ $hk\bar{l} = k\bar{h}+\overline{kl} = \bar{h}+\bar{k}h\bar{l} = \bar{h}h+k\bar{l} = \overline{khl} = h+k\overline{kl}$
	$31m(H)$	P31m P31c	$\bar{h}kl = kh+\bar{k}l = h+\overline{kh}l = h+\bar{k}kl = \bar{h}h+\bar{k}l = k\bar{h}l$ $\bar{h}k\bar{l} = kh+\overline{kl} = h+\overline{khl} = h+\bar{k}k\bar{l} = \bar{h}h+\overline{kl} = k\overline{hl}$
Hexagonal	6	P6 $P6_1$ $P6_2$ $P6_3$ $P6_4$ $P6_5$	$hkl = h+k\bar{h}l = k\bar{h}+\bar{k}l = \overline{hk}l = \bar{h}+\bar{k}hl = \bar{k}h+kl$ $hk\bar{l} = h+k\overline{hl} = k\bar{h}+\overline{kl} = \overline{hkl} = \bar{h}+\bar{k}h\bar{l} = \bar{k}h+k\bar{l}$
	$\bar{6}$ (3/m)	$P\bar{6}$	$\bar{h}kl = h+\overline{khl} = kh+\bar{k}l = \bar{h}k\bar{l} = h+\overline{kh}l = kh+\overline{kl}$
	622 (62)	P622 $P6_122$ $P6_222$ $P6_322$ $P6_422$ $P6_522$	$hkl = h+k\bar{h}l = k\bar{h}+\bar{k}l = \overline{hk}l = \bar{h}+\bar{k}hl = \bar{k}h+kl$ $= h\bar{h}+\overline{kl} = h+k\overline{kl} = kh\bar{l} = \bar{h}h+k\bar{l} = \bar{h}+\bar{k}k\bar{l} = \overline{khl}$

Table 2. (cont.)

	$6mm$ (6m)	$P6mm$ $P6cc$ $P6_3cm$ $P6_3mc$	$hkl = h+k\bar{h}l = k\bar{h}+\bar{k}l = \overline{hk}l = \bar{h}+\bar{k}hl = \bar{k}h+kl$ $= \bar{h}h+kl = \bar{h}+\bar{k}kl = \overline{kh}l = h\bar{h}+\bar{k}l = h+k\bar{k}l = khl$ $hk\bar{l} = h+k\overline{hl} = k\bar{h}+\overline{kl} = \overline{hkl} = \bar{h}+\bar{k}h\bar{l} = \bar{k}h+k\bar{l}$ $= \bar{h}h+k\bar{l} = \bar{h}+\bar{k}k\bar{l} = \overline{khl} = h\bar{h}+\overline{kl} = h+k\overline{kl} = kh\bar{l}$
	$\bar{6}m2$ $(\bar{6}m)$	$P\bar{6}m2$ $P\bar{6}c2$ $P\bar{6}2c$	$hkl = \bar{h}+\bar{k}h\bar{l} = k\bar{h}+\bar{k}l = hk\bar{l} = \bar{h}+\bar{k}hl = k\bar{h}+\overline{kl}$ $= \bar{h}h+kl = h+k\overline{kl} = \overline{kh}l = \bar{h}h+kl = h+k\bar{k}l = \overline{khl}$
	$\bar{6}2m$ $(\bar{6}2)$	$P\bar{6}2m$ $P\bar{6}2c$	$\bar{h}kl = h+\overline{khl} = kh+\bar{k}l = \bar{h}k\bar{l} = h+\overline{khl} = kh+\overline{kl}$ $= \bar{h}h+\overline{kl} = h+\bar{k}kl = k\overline{hl} = \bar{h}h+\bar{k}l = h+\bar{k}k\bar{l} = k\bar{h}l$
Cubic	23	P23 F23 I23 $P2_13$ $I2_13$	$hkl = h\overline{kl} = klh = lhk = \overline{kl}h = \bar{l}h\bar{k}$ $= \bar{h}k\bar{l} = \overline{hk}l = k\overline{lh} = \overline{lh}k = \bar{k}l\bar{h} = l\overline{hk}$ $\bar{h}kl = \overline{hkl} = kl\bar{h} = l\bar{h}k = \overline{klh} = \overline{lhk}$ $= hk\bar{l} = h\bar{k}l = k\bar{l}h = \bar{l}hk = \bar{k}lh = lh\bar{k}$
	432	P432 $P4_232$ F432 $F4_132$ I432 $P4_332$ $P4_132$ $I4_132$	$hkl = hl\bar{k} = h\overline{kl} = h\bar{l}k = \bar{l}kh = \bar{h}k\bar{l} = lk\bar{h} = k\bar{h}l$ $= \overline{hk}l = \bar{k}hl = \bar{k}lh = \overline{lh}k = l\bar{k}h = \overline{kl}h = \bar{l}h\bar{k} = kh\bar{l}$ $= k\overline{lh} = \overline{lh}k = \bar{h}lk = \bar{k}l\bar{h} = l\overline{hk} = \overline{khl} = \overline{lkh} = \overline{hlk}$
	$\bar{4}3m$	$P\bar{4}3m$ $F\bar{4}3m$ $I\bar{4}3m$ $P\bar{4}3n$ $F\bar{4}3c$ $I\bar{4}3d$	$hkl = \overline{hl}k = h\overline{kl} = \bar{h}l\bar{k} = l\overline{kh} = \bar{h}k\bar{l} = \overline{lk}h = \bar{k}h\bar{l}$ $= \overline{hk}l = k\overline{hl} = klh = lhk = \overline{kh}l = \bar{k}lh = \bar{l}h\bar{k} = \bar{l}k\bar{h}$ $= k\overline{lh} = \overline{lh}k = h\overline{lk} = \bar{k}l\bar{h} = l\overline{hk} = khl = lkh = hlk$ $\bar{h}kl = h\bar{l}k = \overline{hkl} = hl\bar{k} = l\bar{k}h = hk\bar{l} = \overline{lkh} = \overline{khl}$ $= h\bar{k}l = kh\bar{l} = kl\bar{h} = l\bar{h}k = \bar{k}hl = \overline{klh} = \overline{lhk} = \bar{l}kh$ $= k\bar{l}h = \bar{l}hk = \overline{hlk} = \bar{k}lh = lh\bar{k} = k\bar{h}l = lk\bar{h} = \bar{h}lk$

3. 결 론

Table 2 의 제1列에는 結晶系, 제2列에는 非對稱中心點群, 제3列에는 各 非對稱點群에 屬한 空間群, 제4列에는 等價面이 羅列되어 있다.

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