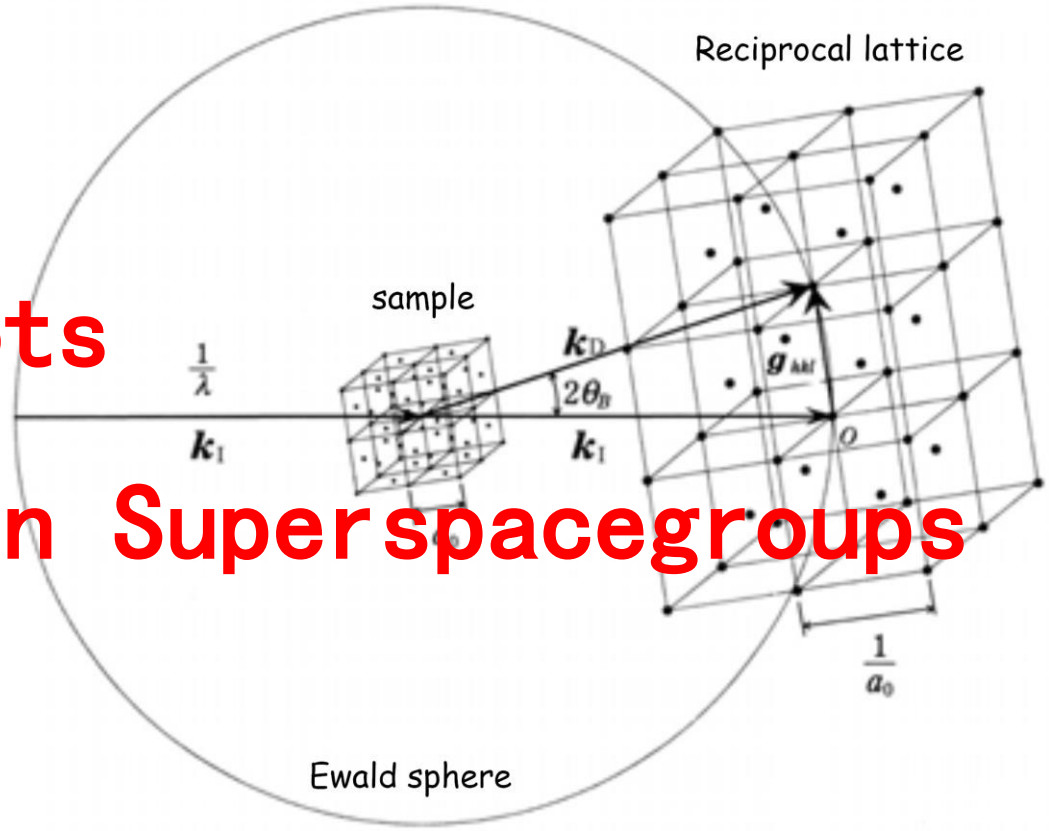
Croucher summer courses

Reflection Conditions

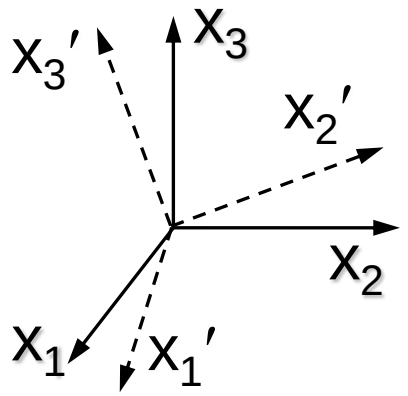
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Hongkong， 2024.6.19

Content

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Part 1. Reflection Conditions



Symmetry operation contains Rotation part **R** and translation part **T**

$$\mathbf{R} = (a_{ij}) = \begin{bmatrix} a_{11}a_{12}a_{13} \\ a_{21}a_{22}a_{23} \\ a_{31}a_{32}a_{33} \end{bmatrix} \quad a_{ij} = \cos(x_i', x_j) \quad ; \quad \mathbf{T} = (t_x\ t_y\ t_z)$$

For（x，-y, z+½）, **R** is （1 0 0， 0 -1 0， 0 0 1）; **T** is （0 0 ½）

Note: translation part **T** doesn't include the part due to the original shift.

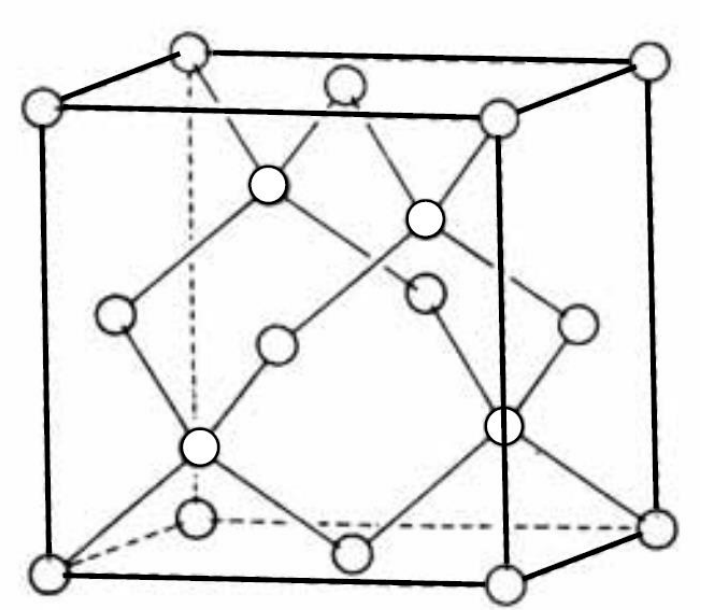
If the index of one reflection *hkl* keeps unchanged after the R-operation, $ht_x+kt_y+lt_z$ need be integer to have non-zero intensity.

For (x，-y, z+½), *h*0*l* : *l* = 2*n*.

Lattice extinction in 3D

Why no 100 reflection for Si?

Si: Cubic *Fd*-3*m*, a = 0.543 nm



Diamond structure

$$F_{hkl} = \sum_i f_i e^{i2\pi(hx_i + ky_i + lz_i)}$$

Body-centered cubic structure: (0,0,0) and (½, ½, ½)

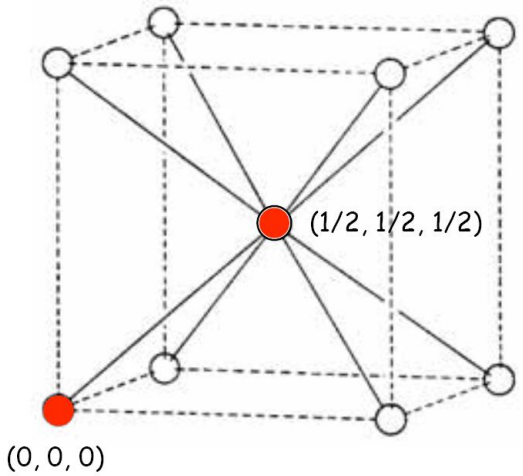
$$F_{hkl} = \sum_{i=1}^{N} f_i e^{i2\pi(hx_i+ky_i+lz_i)}$$

$$= \sum_{i=1}^{N/2} f_i \left(e^{i2\pi(hx_i+ky_i+lz_i)} + e^{i2\pi(h(x_i+\frac{1}{2})+k(y_i+\frac{1}{2})+l(z_i+\frac{1}{2}))}\right)$$

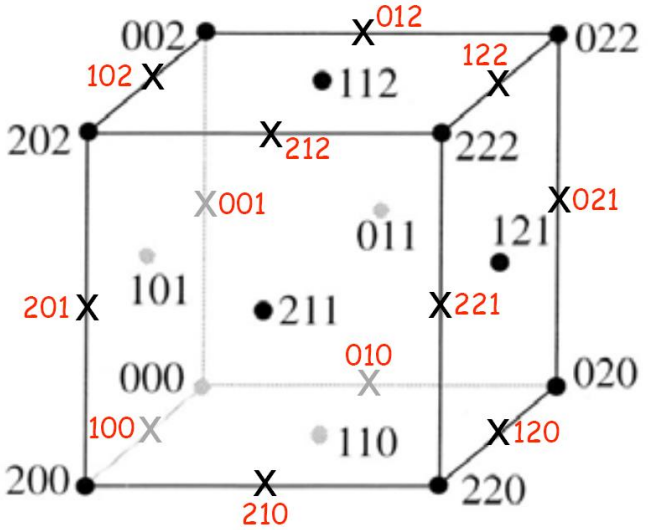
$$= \sum_{i=1}^{N/2} f_i e^{i2\pi(hx_i+ky_i+lz_i)}(1+e^{i\pi(h+k+l)}) = f(1+e^{i\pi(h+k+l)})$$

F=2f if h+k+l = 2n
F=0 if h+k+l = 2n+1

Forbidden reflections



Real space



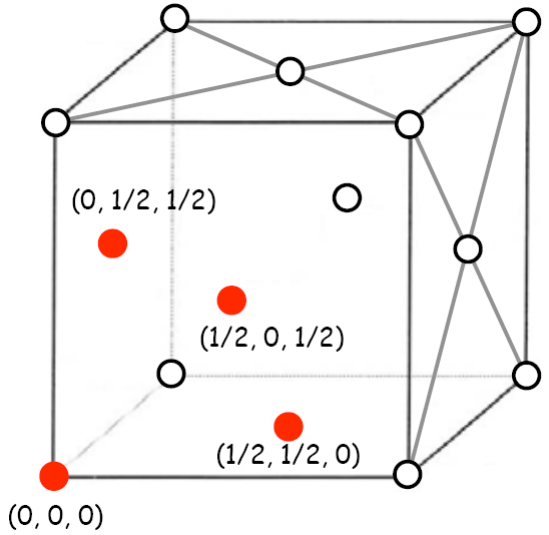
reciprocal space

Face-centered cubic structure: (0,0,0), (½, ½, 0), (½, 0, ½) and (0, ½, ½)

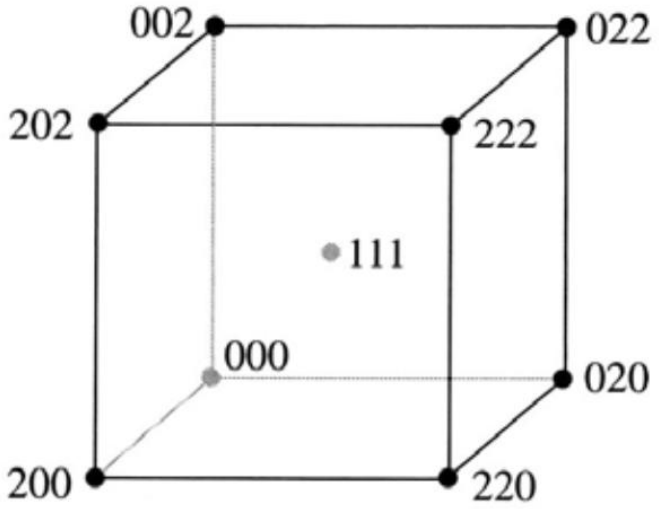
$$F_{hkl} = f\left(1 + e^{i\pi(h+k)} + e^{i\pi(h+l)} + e^{i\pi(k+l)}\right)$$

F=4f if h, k, l are all even or all odd;
F=0 if h, k, l are mixed even and odd.

Forbidden reflections



Real space



reciprocal space

Table 2.2.13.1. *Integral reflection conditions for centred cells (lattices)*

Reflection condition	Centring type of cell	Centring symbol
None	Primitive	P R *(rhombohedral axes)
$h + k = 2n$	C-face centred	C
$k + l = 2n$	A-face centred	A
$h + l = 2n$	B-face centred	B
$h + k + l = 2n$	Body centred	I
$h + k, h + l$ and $k + l = 2n$ or: h, k, l all odd or all even ('unmixed')	All-face centred	F
$-h + k + l = 3n$	Rhombohedrally centred, obverse setting (standard)	R* (hexagonal axes)
$h - k + l = 3n$	Rhombohedrally centred, reverse setting	
$h - k = 3n$	Hexagonally centred	H†

Glide extinction in 2D

Symmetry operation with any translation will create forbidden reflections.

x_i, y_i, z_i $\quad$ $-x_i, y_i, z_i+½$

$$F_{hkl} = \sum_{i=1}^{N} f_i e^{i2\pi(hx_i+ky_i+lz_i)}$$

$$= \sum_{i=1}^{N/2} f_i (e^{i2\pi(hx_i+ky_i+lz_i)} + e^{i2\pi(h(-x_i)+ky_i+l(z_i+\frac{1}{2}))})$$

$$= \sum_{i=1}^{N/2} f_i e^{i2\pi(ky_i+lz_i)} (e^{i2\pi hx_i} + e^{i\pi(-2hx_i+l)})$$

For 0kl reflection, if l = 2n, F=2f
if l= 2n+1, F=0

a, b, c, n, e, d-glide

Table 2.2.13.2. *Zonal and serial reflection conditions for glide planes and screw axes (cf. Chapter 1.3)*

(*a*) Glide planes

Type of reflections	Reflection condition	Glide plane: Orientation of plane	Glide plane: Glide vector	Glide plane: Symbol	Crystallographic coordinate system to which condition applies
$0kl$	$k = 2n$	(100)	$\mathbf{b}/2$	b	Monoclinic (a unique), Tetragonal; Orthorhombic, Cubic
	$l = 2n$		$\mathbf{c}/2$	c	
	$k + l = 2n$		$\mathbf{b}/2 + \mathbf{c}/2$	n	
	$k + l = 4n$ $(k, l = 2n)^*$		$\mathbf{b}/4 \pm \mathbf{c}/4$	d	
$h0l$	$l = 2n$	(010)	$\mathbf{c}/2$	c	Monoclinic (b unique), Tetragonal; Orthorhombic, Cubic
	$h = 2n$		$\mathbf{a}/2$	a	
	$l + h = 2n$		$\mathbf{c}/2 + \mathbf{a}/2$	n	
	$l + h = 4n$ $(l, h = 2n)^*$		$\mathbf{c}/4 \pm \mathbf{a}/4$	d	
$hk0$	$h = 2n$	(001)	$\mathbf{a}/2$	a	Monoclinic (c unique), Tetragonal; Orthorhombic, Cubic
	$k = 2n$		$\mathbf{b}/2$	b	
	$h + k = 2n$		$\mathbf{a}/2 + \mathbf{b}/2$	n	
	$h + k = 4n$ $(h, k = 2n)^*$		$\mathbf{a}/4 \pm \mathbf{b}/4$	d	
$h\bar{h}0l$ $0k\bar{k}l$ $\bar{h}0hl$	$l = 2n$	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ $\}\{11\bar{2}0\}$	$\mathbf{c}/2$	c	Hexagonal
$hh.\overline{2h}.l$ $\overline{2h}.hhl$ $h.\overline{2h}.hl$	$l = 2n$	$(1\bar{1}00)$ $(01\bar{1}0)$ $(\bar{1}010)$ $\}\{1\bar{1}00\}$	$\mathbf{c}/2$	c	Hexagonal
hhl hkk hkh	$l = 2n$ $h = 2n$ $k = 2n$	$(1\bar{1}0)$ $(01\bar{1})$ $(\bar{1}01)$ $\}\{1\bar{1}0\}$	$\mathbf{c}/2$ $\mathbf{a}/2$ $\mathbf{b}/2$	c, n a, n b, n	Rhombohedral†
$hhl, h\bar{h}l$	$l = 2n$	$(1\bar{1}0), (110)$	$\mathbf{c}/2$	c, n	Tetragonal‡; Cubic§
	$2h + l = 4n$		$\mathbf{a}/4 \pm \mathbf{b}/4 \pm \mathbf{c}/4$	d	
$hkk, hk\bar{k}$	$h = 2n$	$(01\bar{1}), (011)$	$\mathbf{a}/2$	a, n	
	$2k + h = 4n$		$\pm\mathbf{a}/4 + \mathbf{b}/4 \pm \mathbf{c}/4$	d	
$hkh, \bar{h}kh$	$k = 2n$	$(\bar{1}01), (101)$	$\mathbf{b}/2$	b, n	
	$2h + k = 4n$		$\pm\mathbf{a}/4 \pm \mathbf{b}/4 + \mathbf{c}/4$	d	

Screw axis extinction in 1D

x_i, y_i, z_i $\quad$ $-x_i, -y_i, z_i+½$

For 00l reflection, if l = 2n, F=2f

if l= 2n+1, F=0

Screw axis: 2_1, 3_p, 4_p, 6_p

* Glide planes *d* with orientations (100), (010) and (001) occur only in orthorhombic and cubic *F* space groups. Combination of the integral reflection condition (*hkl:* all odd or all even) with the zonal conditions for the *d* glide planes leads to the further conditions given between parentheses.

† For rhombohedral space groups described with 'rhombohedral axes' the three reflection conditions ($l = 2n, h = 2n, k = 2n$) imply interleaving of *c* and *n* glides, *a* and *n* glides, *b* and *n* glides, respectively. In the Hermann–Mauguin space-group symbols, *c* is always used, as in $R3c$ (161) and $R\bar{3}c$ (167), because *c* glides occur also in the hexagonal description of these space groups.

‡ For tetragonal *P* space groups, the two reflection conditions (*hhl* and $h\bar{h}l$ with $l = 2n$) imply interleaving of *c* and *n* glides. In the Hermann–Mauguin space-group symbols, *c* is always used, irrespective of which glide planes contain the origin: *cf.* $P4cc$ (103), $P\bar{4}2c$ (112) and $P4/nnc$ (126).

§ For cubic space groups, the three reflection conditions ($l = 2n, h = 2n, k = 2n$) imply interleaving of *c* and *n* glides, *a* and *n* glides, and *b* and *n* glides, respectively. In the Hermann–Mauguin space-group symbols, either *c* or *n* is used, depending upon which glide plane contains the origin, *cf.* $P\bar{4}3n$ (218), $Pn\bar{3}n$ (222), $Pm\bar{3}n$ (223) *vs* $F\bar{4}3c$ (219), $Fm\bar{3}c$ (226), $Fd\bar{3}c$ (228).

(*b*) Screw axes

Type of reflections	Reflection conditions	Screw axis			Crystallographic coordinate system to which condition applies
		Direction of axis	Screw vector	Symbol	
*h*00	$h = 2n$	[100]	**a**/2	2_1	Monoclinic (*a* unique), Orthorhombic, Tetragonal; Cubic
				4_2	
	$h = 4n$		**a**/4	$4_1, 4_3$	
0*k*0	$k = 2n$	[010]	**b**/2	2_1	Monoclinic (*b* unique), Orthorhombic, Tetragonal; Cubic
				4_2	
	$k = 4n$		**b**/4	$4_1, 4_3$	
00*l*	$l = 2n$	[001]	**c**/2	2_1	Monoclinic (*c* unique), Orthorhombic; Cubic
				4_2	Tetragonal; Cubic
	$l = 4n$		**c**/4	$4_1, 4_3$	Tetragonal; Cubic
000*l*	$l = 2n$	[001]	**c**/2	6_3	Hexagonal
	$l = 3n$		**c**/3	$3_1, 3_2, 6_2, 6_4$	Hexagonal
	$l = 6n$		**c**/6	$6_1, 6_5$	Hexagonal

Pc

hkl: --
h0l: l=2n
0k0: --

$Pca2_1$

Hkl: --
0kl:
h0l:
hk0:
h00:
0k0:
00l:

Pbcn

hkl:
0kl:
h0l:
hk0:
h00:
0k0:
00l:

Ccme

hkl:
0kl:
h0l:
hk0:
h00:
0k0:
00l:

I4/mcm

hkl:
hk0:
0kl:
hhl:
00l:
0k0:
hh0:

Pc

hkl: --
h0l: l=2n
0k0: --

$Pca2_1$

Hkl: --
0kl: l=2n
h0l: h=2n
hk0:
h00: h=2n
0k0:
00l: l=2n

Pbcn

hkl:
0kl: k=2n
h0l: l=2n
hk0: h+k=2n
h00: h=2n
0k0: h=2n
00l: h=2n

Ccme

hkl: h+k=2n
0kl: l=2n,k=2n
h0l: h=2n
hk0: h,k=2n
h00: h=2n
0k0: h=2n
00l: h=2n

I4/mcm

hkl: h+k+l=2n
hk0: h+k =2n
0kl: l=2n, k=2n
hhl: l=2n
00l: l=2n
0k0: k =2n
hh0:

Determine Space groups by Laue class and extinction

Diffraction symbols: Laue class and reflection conditions

Total 122 Diffraction symbols from 230 space groups,

58 uniquely determine the related space group.

Extinction symbols: systematic absences only

Example: *Cc*, *C*2/*c* belong to the same Diffraction symbol

Laue class: 12/*m*1

Reflection conditions:

hkl: h+k=2n;

h0l: h, l=2n; 0kl: k=2n; hk0: h+k=2n;

h00: h=2n; 0k0: k=2n; 00l: l=2n.

Diffraction symbol: 12/*m*1*C*1*c*1

Extinction symbol: *C*1*c*1

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups*

TRICLINIC. Laue class $\bar{1}$

Reflection conditions	Extinction symbol	Point group	
		1	$\bar{1}$
None	*P*–	*P*1 (1)	*P*$\bar{1}$ (2)

$P2_1$, $P2_1/m$ belong to the same diffraction symbol (0k0, k=2n), $P2_1/c$ is unequivocally determined by its diffraction symbol.

MONOCLINIC, Laue class 2/*m*

Unique axis *b*				Laue class 1 2/*m* 1		
Reflection conditions				Point group		
hkl 0*kl* *hk*0	*h*0*l* *h*00 00*l*	0*k*0	Extinction symbol	2	*m*	2/*m*
			*P*1–1	**P121** (3)	**P1m1** (6)	**P1 2/m 1** (10)
		k	*P*12$_1$1	**P12$_1$1** (4)		**P1 2$_1$/m 1** (11)
	h		*P*1*a*1		*P*1*a*1 (7)	*P*1 2/*a* 1 (13)
	h	*k*	*P*1 2$_1$/*a* 1			*P*1 2$_1$/*a* 1 (14)
	l		*P*1*c*1		**P1c1** (7)	**P1 2/c 1** (13)
	l	*k*	*P*1 2$_1$/*c* 1			**P1 2$_1$/c 1** (14)
	h + *l*		*P*1*n*1		*P*1*n*1 (7)	*P*1 2/*n* 1 (13)
	h + *l*	*k*	*P*1 2$_1$/*n* 1			*P*1 2$_1$/*n* 1 (14)
h + *k*	*h*	*k*	*C*1–1	**C121** (5)	**C1m1** (8)	**C1 2/m 1** (12)
h + *k*	*h*, *l*	*k*	*C*1*c*1		**C1c1** (9)	**C1 2/c 1** (15)
k + *l*	*l*	*k*	*A*1–1	*A*121 (5)	*A*1*m*1 (8)	*A*1 2/*m* 1 (12)
k + *l*	*h*, *l*	*k*	*A*1*n*1		*A*1*n*1 (9)	*A*1 2/*n* 1 (15)
h + *k* + *l*	*h* + *l*	*k*	*I*1–1	*I*121 (5)	*I*1*m*1 (8)	*I*1 2/*m* 1 (12)
h + *k* + *l*	*h*, *l*	*k*	*I*1*a*1		*I*1*a*1 (9)	*I*1 2/*a* 1 (15)

Unique axis *c*				Laue class 1 1 2/*m*		
Reflection conditions				Point group		
hkl 0*kl* *h*0*l*	*hk*0 *h*00 0*k*0	00*l*	Extinction symbol	2	*m*	2/*m*
			*P*11–	*P*112 (3)	*P*11*m* (6)	*P*11 2/*m* (10)
		l	*P*112$_1$	*P*112$_1$ (4)		*P*11 2$_1$/*m* (11)
	h		*P*1*a*1		*P*1*a*1 (7)	*P*1 2/*a* 1 (13)
	h	*k*	*P*1 2$_1$/*a* 1			*P*1 2$_1$/*a* 1 (14)
	l		*P*1*c*1		*P*1*c*1 (7)	*P*1 2/*c* 1 (13)
	l	*k*	*P*1 2$_1$/*c* 1			*P*1 2$_1$/*c* 1 (14)
	h + *l*		*P*1*n*1		*P*1*n*1 (7)	*P*1 2/*n* 1 (13)
	h + *l*	*k*	*P*1 2$_1$/*n* 1			*P*1 2$_1$/*n* 1 (14)
h + *k*	*h*	*k*	*C*1–1	*C*121 (5)	*C*1*m*1 (8)	*C*1 2/*m* 1 (12)
h + *k*	*h*, *l*	*k*	*C*1*c*1		*C*1*c*1 (9)	*C*1 2/*c* 1 (15)
k + *l*	*l*	*k*	*A*1–1	*A*121 (5)	*A*1*m*1 (8)	*A*1 2/*m* 1 (12)
k + *l*	*h*, *l*	*k*	*A*1*n*1		*A*1*n*1 (9)	*A*1 2/*n* 1 (15)
h + *k* + *l*	*h* + *l*	*k*	*I*1–1	*I*121 (5)	*I*1*m*1 (8)	*I*1 2/*m* 1 (12)
h + *k* + *l*	*h*, *l*	*k*	*I*1*a*1		*I*1*a*1 (9)	*I*1 2/*a* 1 (15)

ORTHORHOMBIC, Laue class *mmm* $(2/m\ 2/m\ 2/m)$

In this table, the symbol *e* in the space-group symbol represents the two glide planes given between parentheses in the corresponding extinction symbol. Only for one of the two cases does a bold printed symbol correspond with the standard symbol.

Reflection conditions								Laue class *mmm* $(2/m\ 2/m\ 2/m)$		
								Point group		
hkl	*0kl*	*h0l*	*hk0*	*h00*	*0k0*	*00l*	Extinction symbol	222	*mm2* *m2m* *2mm*	*mmm*
							$P--\,-$	***P222*** (16)	***Pmm2*** (25)	***Pmmm*** (47)
									Pm2m (25)	
									P2mm (25)	
						l	$P--2_1$	***P222$_1$*** (17)		
					k		$P-2_1-$	*P22$_1$2* (17)		
					k	l	$P-2_12_1$	*P22$_1$2$_1$* (18)		
				h			$P2_1--$	*P2$_1$22* (17)		
				h		l	$P2_1-2_1$	*P2$_1$22$_1$* (18)		
				h	k		$P2_12_1-$	***P2$_1$2$_1$2*** (18)		
				h	k	l	$P2_12_12_1$	***P2$_1$2$_1$2$_1$*** (19)		
			h	h			$P--a$		*Pm2a* (28)	
									P2$_1$ma (26)	***Pmma*** (51)
			k		k		$P--b$		*Pm2$_1$b* (26)	
									P2mb (28)	*Pmmb* (51)
			$h+k$	h	k		$P--n$		*Pm2$_1$n* (31)	
									P2$_1$mn (31)	***Pmmn*** (59)
		h		h			$P-a-$		***Pma2*** (28)	*Pmam* (51)
									P2$_1$am (26)	
		h	h	h			$P-aa$		*P2aa* (27)	*Pmaa* (49)
		h	k	h	k		$P-ab$		*P2$_1$ab* (29)	*Pmab* (57)
		h	$h+k$	h	k		$P-an$		*P2an* (30)	*Pman* (53)
		l				l	$P-c-$		***Pmc2$_1$*** (26)	
									P2cm (28)	*Pmcm* (51)
		l	h	h		l	$P-ca$		*P2$_1$ca* (29)	*Pmca* (57)
		l	k		k	l	$P-cb$		*P2cb* (32)	*Pmcb* (55)
		l	$h+k$	h	k	l	$P-cn$		*P2$_1$cn* (33)	*Pmcn* (62)

Different settings (standard & non-standard) for *Pmma*

Reflection conditions								Laue class *mmm* ($2/m\ 2/m\ 2/m$)		
								Point group		
hkl	0*kl*	*h*0*l*	*hk*0	*h*00	0*k*0	00*l*	Extinction symbol	222	*mm*2 *m*2*m* 2*mm*	*mmm*
	$k+l$	l	k		k	l	*Pncb*			*Pncb* (50)
	$k+l$	l	$h+k$	h	k	l	*Pncn*			*Pncn* (52)
	$k+l$	$h+l$		h	k	l	*Pnn* –		***Pnn2*** (34)	***Pnnm*** (58)
	$k+l$	$h+l$	h	h	k	l	*Pnna*			***Pnna*** (52)
	$k+l$	$h+l$	k	h	k	l	*Pnnb*			*Pnnb* (52)
	$k+l$	$h+l$	$h+k$	h	k	l	*Pnnn*			***Pnnn*** (48)
$h+k$	k	h	$h+k$	h	k		*C* – – –	***C222*** (21)	***Cmm2*** (35) *Cm2m* (38) *C2mm* (38)	***Cmmm*** (65)
$h+k$	k	h	$h+k$	h	k	l	*C*– –2_1	***C222***$_1$ (20)		
$h+k$	k	h	h, k	h	k		*C*– –(*ab*)		*Cm2e* (39) *C2me* (39)	***Cmme*** (67)
$h+k$	k	h, l	$h+k$	h	k	l	*C*–*c* –		***Cmc2***$_1$ (36) *C2cm* (40)	***Cmcm*** (63)
$h+k$	k	h, l	h, k	h	k	l	*C*–*c*(*ab*)		*C2ce* (41)	***Cmce*** (64)
$h+k$	k, l	h	$h+k$	h	k	l	*Cc* – –		*Ccm*2_1 (36) *Cc2m* (40)	*Ccmm* (63)
$h+k$	k, l	h	h, k	h	k	l	*Cc* –(*ab*)		*Cc2e* (41)	*Ccme* (64)
$h+k$	k, l	h, l	$h+k$	h	k	l	*Ccc* –		***Ccc2*** (37)	***Cccm*** (66)
$h+k$	k, l	h, l	h, k	h	k	l	*Ccc*(*ab*)			***Ccce*** (68)
$h+l$	l	$h+l$	h	h		l	*B* – – –	*B*222 (21)	*Bmm*2 (38) *Bm*2*m* (35) *B*2*mm* (38)	*Bmmm* (65)

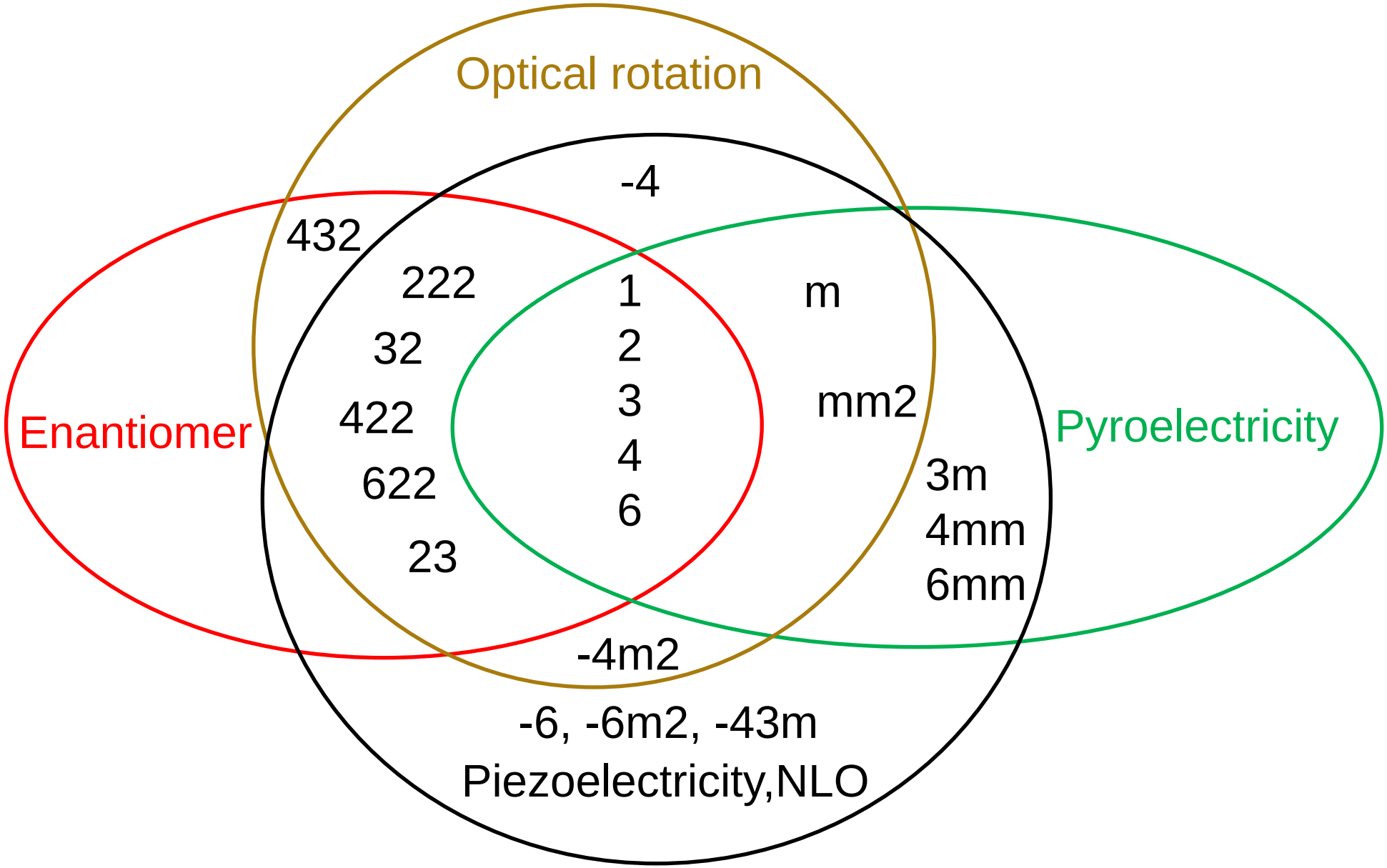
Symmetry of special projections

Along [001] $c\,2\,m\,m$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $p\,2\,g\,m$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

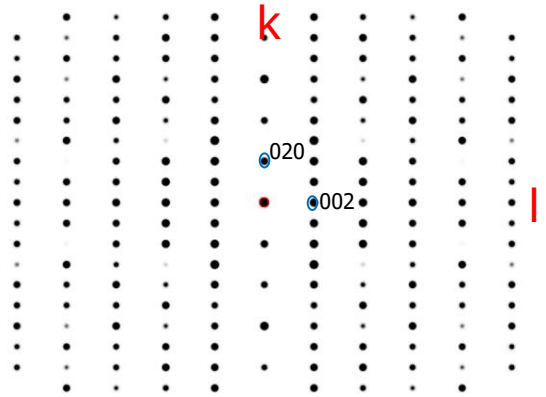
Along [010] $p\,2\,m\,m$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0, y, 0$

Point group symmetry ←→Physical property

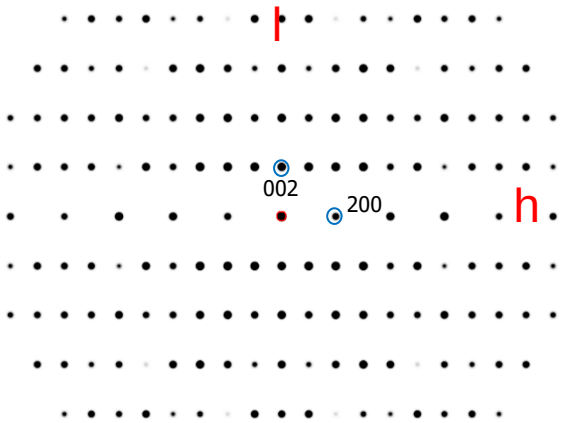


Space group determination

- Symmetry in diffraction pattern – Laue class
- Systematic absences: hkl, hk0, h0l, 0kl, h00, 0k0, 00l



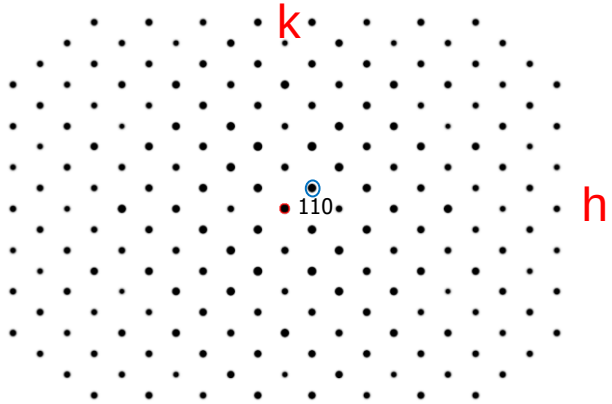
[100]



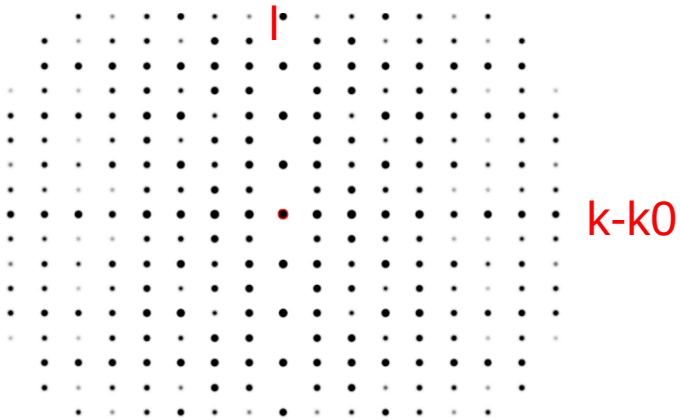
[010]

hkl:
0kl: l =2n
h0l: l = 2n
hk0: h+k = 2n
h00: h = 2n
0k0: k = 2n
00l: l = 2n

56: *Pccn*



[001]



[110]

Part 2. Phase relations

If two reflections (*h k l*), (*h'k'l'*) are related by the rotation part of a symmetry, their structure factor phases is related by the translation part.

$$\textbf{Phase}(h'k'l') = \textbf{Phase}(h\,k\,l) + 360^\circ\ (h\cdot t_1 + k\cdot t_2 + l\cdot t_3)$$

Note: the rotation part includes those due to the orignal shift.

Friedel's law without anomalous scattering

$$F(hkl) = \sum_{j=1}^{N} f_j(hkl) \exp 2\pi i(hx_j + ky_j + lz_j)$$

Amplitude relations:

$|F(hkl)| = |F(-h\ -k\ -l)|$

Phase relations:

$\phi(hkl) = -\phi(-h\ -k\ -l)$

Phase restriction

For centrosymmetric structures, (*-h -k -l*) and (*h k l*) is also related by the inversion center.

If the origin is at the inversion center, its translation part is 0.

Thus, $\phi(-h\ -k\ -l) = \phi(h\ k\ l)$.

Friedel's law : $\phi(-h\ -k\ -l) = -\phi(h\ k\ l)$

How to fulfill both?

$\phi(h\ k\ l) = 0$ or 180 （$-0^o = 0^o$ and $-180^o = 180^o$）

2-fold rotation（-x，y，–z）

$P_{hkl} = P_{-hk-l}$

Phases for h0l and –h0-l have to be 0^o or 180^o due to the Friedel's law.

Mirror（x，-y，z）

$P_{hkl} = P_{h-kl}$

Phases for 0k0 and 0-k0 have to be 0^o or 180^o due to the Friedel's law.

2_1 screw axis（-x，y+½，–z）

$P_{hkl} = P_{-hk-l} + 360^\circ (h \cdot t_1 + k \cdot t_2 + l \cdot t_3)$

$= P_{-hk-l} + 180^\circ * k$

For 0k0 with k odd, their phases need be the same and differ by 180°, thus they are extinct。

Phases for h0l and –h0-l have to be 0^o or 180^o due to the Friedel's law.

Glide（x+½，-y，z）

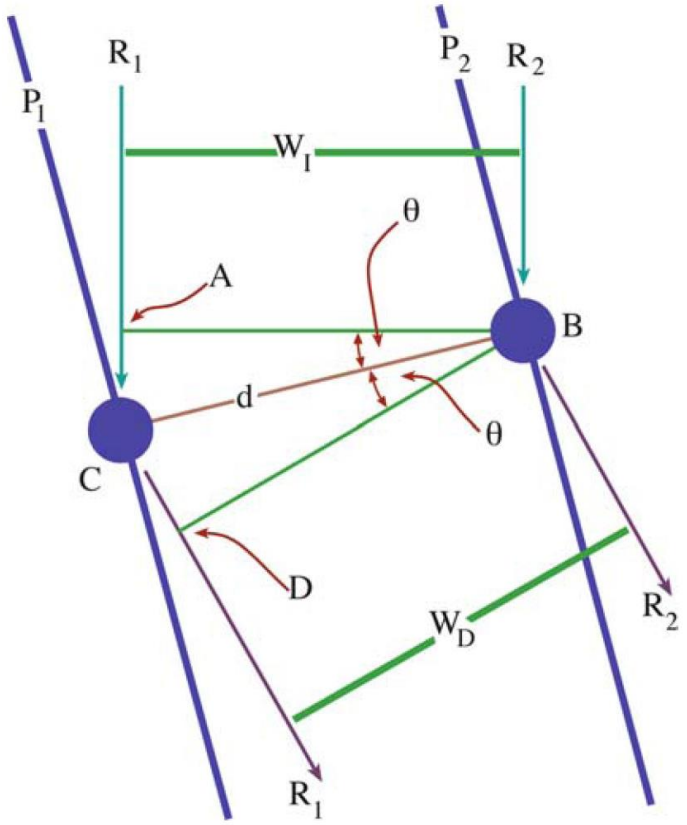
$P_{hkl} = P_{h-kl} + 360^\circ (h \cdot t_1 + k \cdot t_2 + l \cdot t_3)$

$= P_{h-kl} + 180^\circ * h$

For h0l with h odd, their phases need be the same and differ by 180°, thus they are extinct。

Phases for 0k0 and 0-k0 have to be 0^o or 180^o due to the Friedel's law.

Part 3. Shape of reciprocal spot



$$\mathrm{AC} + \mathrm{CD} = 2d\sin\theta = n\lambda$$

$$A(\mathbf{K}) = F(\mathbf{K})\sum_{n_x} e^{i2\pi n_x \mathbf{k}\bullet\mathbf{a}} \sum_{n_y} e^{i2\pi n_y \mathbf{k}\bullet\mathbf{b}} \sum_{n_z} e^{i2\pi n_z \mathbf{k}\bullet\mathbf{c}}$$

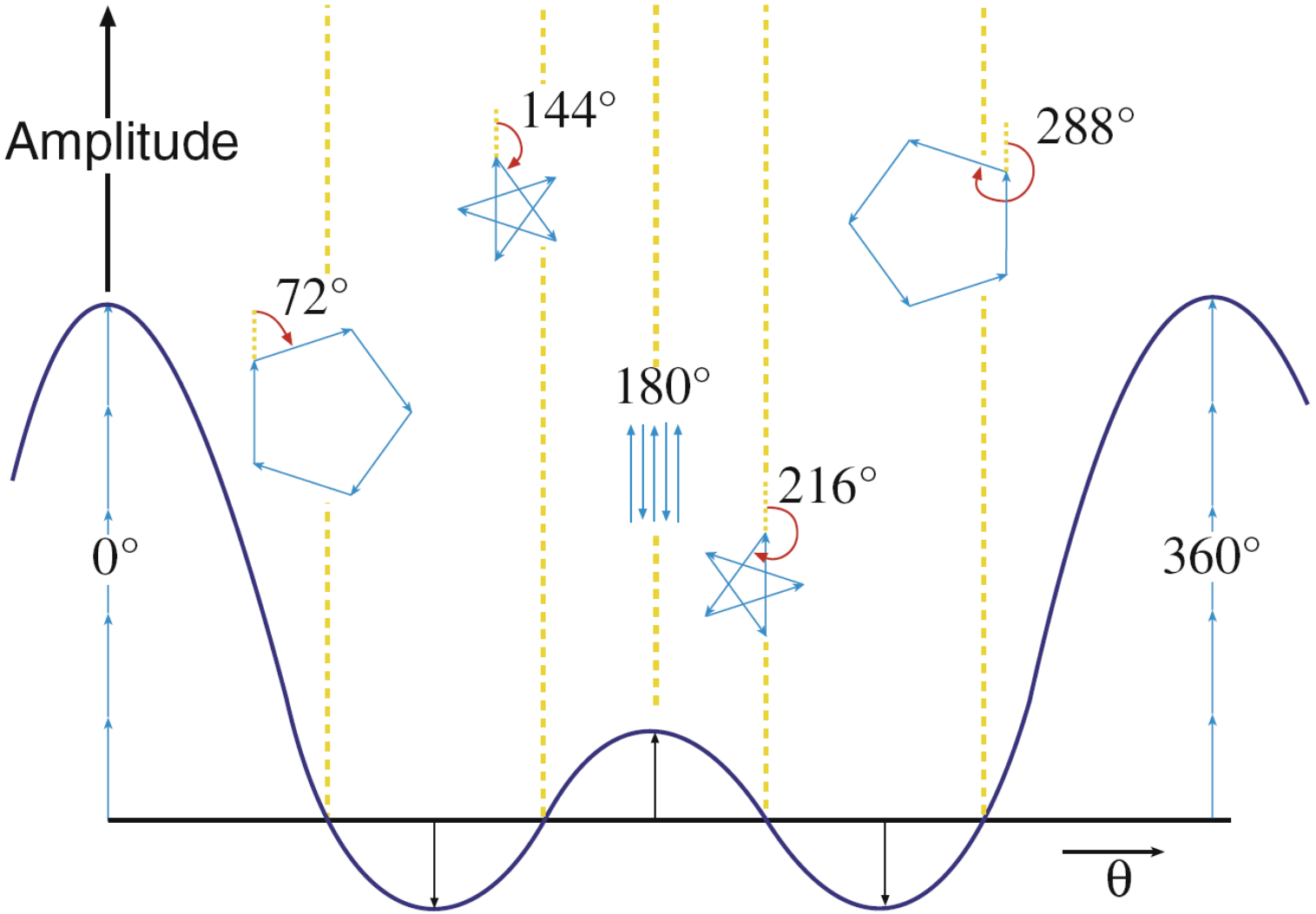
$$= F(\mathbf{K}) \frac{1-e^{i2\pi N_x \mathbf{k}\bullet\mathbf{a}}}{1-e^{i2\pi \mathbf{k}\bullet\mathbf{a}}} \frac{1-e^{i2\pi N_y \mathbf{k}\bullet\mathbf{b}}}{1-e^{i2\pi \mathbf{k}\bullet\mathbf{b}}} \frac{1-e^{i2\pi N_z \mathbf{k}\bullet\mathbf{c}}}{1-e^{i2\pi \mathbf{k}\bullet\mathbf{c}}}$$

$$F(\mathbf{K}) = \sum_i f_i e^{i2\pi \mathbf{k}\bullet\mathbf{r}_i}$$

$$I = A^*(\mathbf{K}) \cdot A(\mathbf{K})$$

$$= |F(\mathbf{K})|^2 \frac{\sin^2(\pi N_x \mathbf{K}\bullet\mathbf{a})}{\sin^2(\pi \mathbf{K}\bullet\mathbf{a})} \frac{\sin^2(\pi N_y \mathbf{K}\bullet\mathbf{b})}{\sin^2(\pi \mathbf{K}\bullet\mathbf{b})} \frac{\sin^2(\pi N_z \mathbf{K}\bullet\mathbf{c})}{\sin^2(\pi \mathbf{K}\bullet\mathbf{c})}$$

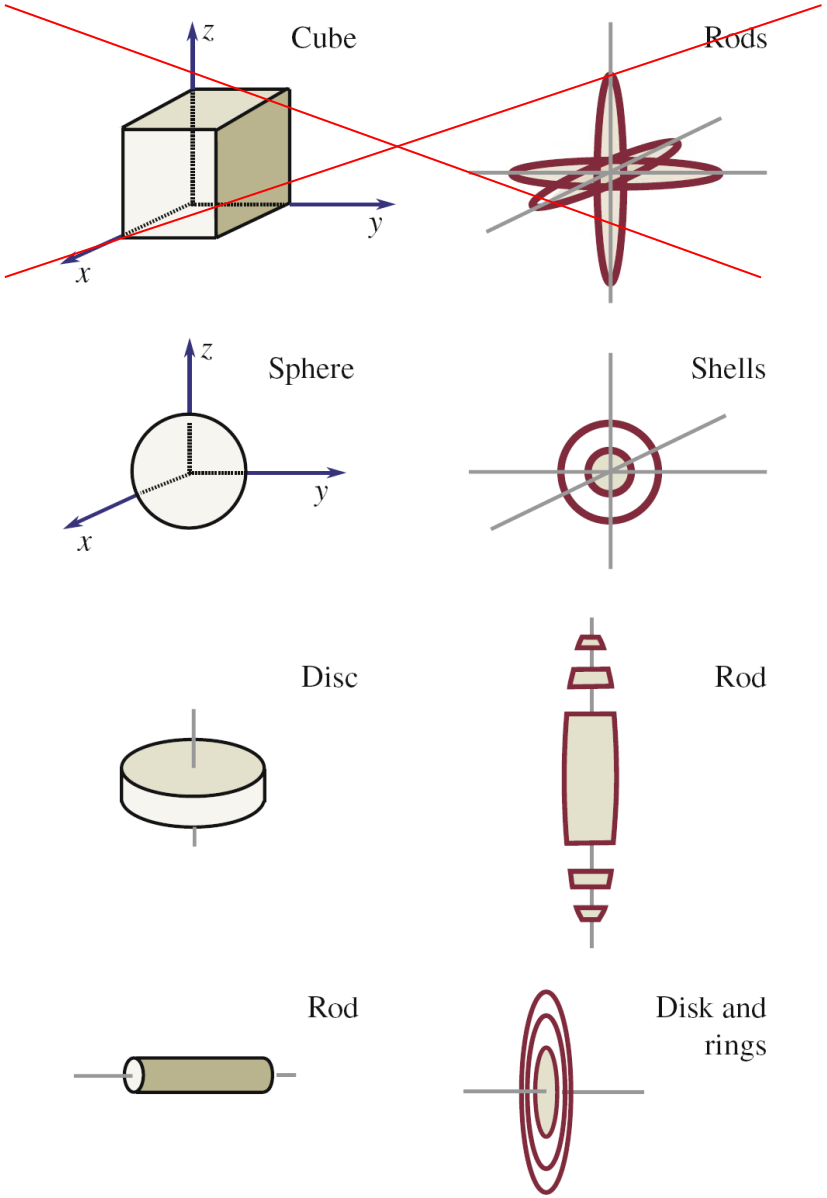
N_x-1 nodes located at $h\mathbf{a}^* + n/N_x\ \mathbf{a}^*$

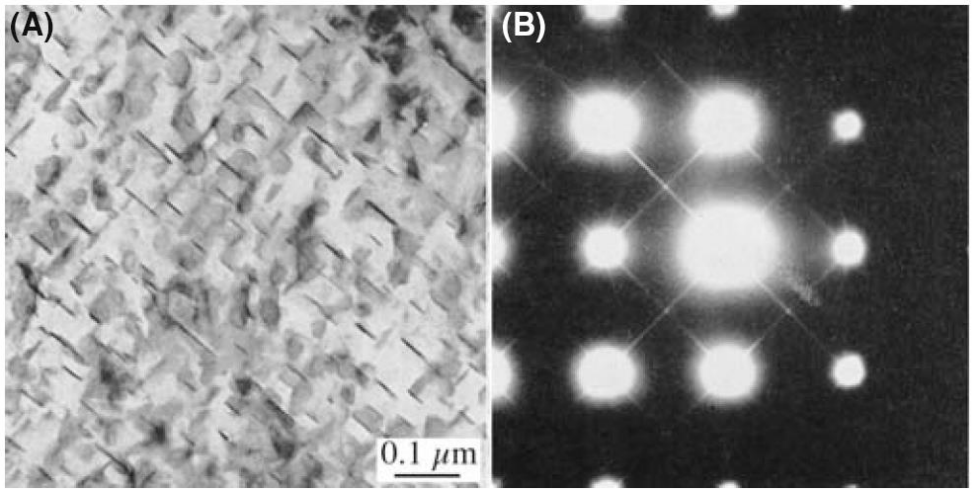


What is Fourier transform of this?

. . . .

. . . .





The diffused scattering can also be understood as superstructures.

THE PERIODICITY RULE

If there is a structural periodicity in real space, then there will be an array of points or relrods in reciprocal space and an array of spots or streaks in the DP.

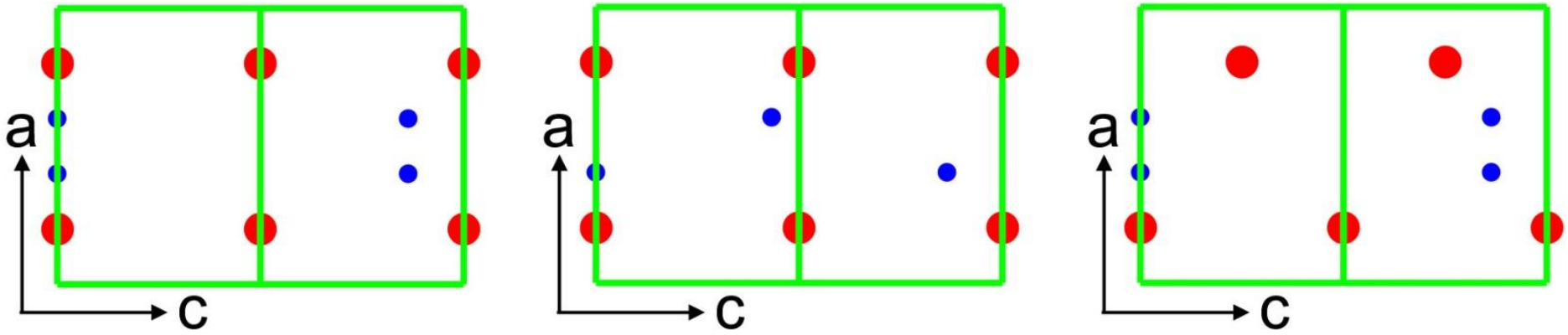
Part 4. (3+1)-D superspace group

International Tables for Crystallography 2006, Vol.C, Chapter 9.8

No.	Basic space group	Point group K_s	Bravais class No.	Group symbol	Special reflection conditions
1.1	$P1$	$(1, 1)$	1	$P1(\alpha\beta\gamma)$	
2.1	$P\bar{1}$	$(\bar{1}, \bar{1})$	1	$P\bar{1}(\alpha\beta\gamma)$	
3.1	$P2$	$(2, \bar{1})$	2	$P2(\alpha\beta 0)$	
3.2		$(2, \bar{1})$	3	$P2(\alpha\beta\frac{1}{2})$	
3.3		$(2, 1)$	5	$P2(00\gamma)$	
3.4		$(2, 1)$	5	$P2(00\gamma)s$	$00lm$: $m = 2n$
3.5		$(2, 1)$	6	$P2(\frac{1}{2}0\gamma)$	
4.1	$P2_1$	$(2, \bar{1})$	2	$P2_1(\alpha\beta 0)$	$00l0$: $l = 2n$
4.2		$(2, 1)$	5	$P2_1(00\gamma)$	$00lm$: $l = 2n$
4.3		$(2, 1)$	6	$P2_1(\frac{1}{2}0\gamma)$	$00Lm$: $L = 2n$
5.1	$B2$	$(2, \bar{1})$	4	$B2(\alpha\beta 0)$	
5.2		$(2, 1)$	7	$B2(00\gamma)$	
5.3		$(2, 1)$	7	$B2(00\gamma)s$	$00lm$: $m = 2n$
5.4		$(2, 1)$	8	$B2(0\frac{1}{2}\gamma)$	
6.1	Pm	$(m, 1)$	2	$Pm(\alpha\beta 0)$	
6.2		$(m, 1)$	2	$Pm(\alpha\beta 0)s$	$hk0m$: $m = 2n$
6.3		$(m, 1)$	3	$Pm(\alpha\beta\frac{1}{2})$	
6.4		$(m, \bar{1})$	5	$Pm(00\gamma)$	
6.5		$(m, \bar{1})$	6	$Pm(\frac{1}{2}0\gamma)$	
7.1	Pb	$(m, 1)$	2	$Pb(\alpha\beta 0)$	$hk0m$: $k = 2n$
7.2		$(m, 1)$	3	$Pb(\alpha\beta\frac{1}{2})$	$HK0m$: $K = 2n$
7.3		$(m, \bar{1})$	5	$Pb(00\gamma)$	$hk00$: $k = 2n$
7.4		$(m, \bar{1})$	6	$Pb(\frac{1}{2}0\gamma)$	$HK00$: $K = 2n$
8.1	Bm	$(m, 1)$	4	$Bm(\alpha\beta 0)$	
8.2		$(m, 1)$	4	$Bm(\alpha\beta 0)s$	$hk0m$: $m = 2n$
8.3		$(m, \bar{1})$	7	$Bm(00\gamma)$	
8.4		$(m, \bar{1})$	8	$Bm(0\frac{1}{2}\gamma)$	
9.1	Bb	$(m, 1)$	4	$Bb(\alpha\beta 0)$	$hk0m$: $k = 2n$
9.2		$(m, \bar{1})$	7	$Bb(00\gamma)$	$hk00$: $k = 2n$
10.1	$P2/m$	$(2/m, \bar{1}1)$	2	$P2/m(\alpha\beta 0)$	
10.2		$(2/m, \bar{1}1)$	2	$P2/m(\alpha\beta 0)0s$	$hk0m$: $m = 2n$
10.3		$(2/m, \bar{1}1)$	3	$P2/m(\alpha\beta\frac{1}{2})$	
10.4		$(2/m, 1\bar{1})$	5	$P2/m(00\gamma)$	

Nomenclature herein	Bravais lattice type: Int. Tables notation, untransformed cell axes	Bravais lattice type: Int. Tables notation, transformed cell axes
Monoclinic[b,c]		
PP	$P(00\gamma)$	$P(00\gamma)$
PA	$P(0\frac{1}{2}\gamma)$	$P(0\frac{1}{2}\gamma)$
PB	$P(\frac{1}{2}0\gamma)$	$P(\frac{1}{2}0\gamma)$
AP	$A(00\gamma)$	$A(00\gamma)$
AA	$A(01\gamma)$	$A(00\gamma)$
AB	$A(\frac{1}{2}0\gamma)$	$A(\frac{1}{2}0\gamma)$
BP	$B(00\gamma)$	$B(00\gamma)$
BA	$B(0\frac{1}{2}\gamma)$	$B(0\frac{1}{2}\gamma)$
BB	$B(10\gamma)$	$B(00\gamma)$
Orthorhombic[b]		
PP	$P(00\gamma)$	$P(00\gamma)$
PA	$P(0\frac{1}{2}\gamma)$	$P(0\frac{1}{2}\gamma)$
PB	$P(\frac{1}{2}0\gamma)$	$P(\frac{1}{2}0\gamma)$
PF	$P(\frac{1}{2}\frac{1}{2}\gamma)$	$P(\frac{1}{2}\frac{1}{2}\gamma)$
AP	$A(00\gamma)$	$A(00\gamma)$
AA	$A(01\gamma)$	$A(00\gamma)$
AB	$A(\frac{1}{2}0\gamma)$	$A(\frac{1}{2}0\gamma)$
AF	$A(\frac{1}{2}1\gamma)$	$A(\frac{1}{2}0\gamma)$
BP	$B(00\gamma)$	$B(00\gamma)$
BA	$B(0\frac{1}{2}\gamma)$	$B(0\frac{1}{2}\gamma)$
BB	$B(10\gamma)$	$B(00\gamma)$
BF	$B(1\frac{1}{2}\gamma)$	$B(0\frac{1}{2}\gamma)$
FP	$F(00\gamma)$	$F(00\gamma)$
FA	$F(01\gamma)$	$F(01\gamma)$
FB	$F(10\gamma)$	$F(10\gamma)$
FF	$F(11\gamma)$	$F(00\gamma)$
IC	$I(00\gamma)$	$I(00\gamma)$
II	$I(10\gamma)$	$I(00\gamma)$
CC	$C(00\gamma)$	$C(00\gamma)$
CI	$C(10\gamma)$	$C(10\gamma)$
Tetragonal		
PP	$P(00\gamma)$	$P(00\gamma)$
PI	$P(\frac{1}{2}\frac{1}{2}\gamma)$	$P(\frac{1}{2}\frac{1}{2}\gamma)$
IP	$I(00\gamma)$	$I(00\gamma)$
II	$I(10\gamma)$	$I(00\gamma)$
Hexagonal		
RP	$R(00\gamma)$	$R(00\gamma)$
R_oR_o	$R_o(10\gamma)$[d]	$R_o(00\gamma)$
R_oR_r	$R_o(01\gamma)$[d]	$R_o(00\gamma)$
PR	$P(\frac{1}{3}\frac{1}{3}\gamma)$	$P(\frac{1}{3}\frac{1}{3}\gamma)$
PP	$P(00\gamma)$	$P(00\gamma)$

Symmetry operation in superspace



$\bar{x}_1, x_3, x_4$
$\bar{x}_1, x_3,$
$\bar{x}_1, \quad x_4$
(a)

$\bar{x}_1, x_3, x_4+½$
$\bar{x}_1, x_3,$
$\bar{x}_1, \quad x_4+½$
(b)

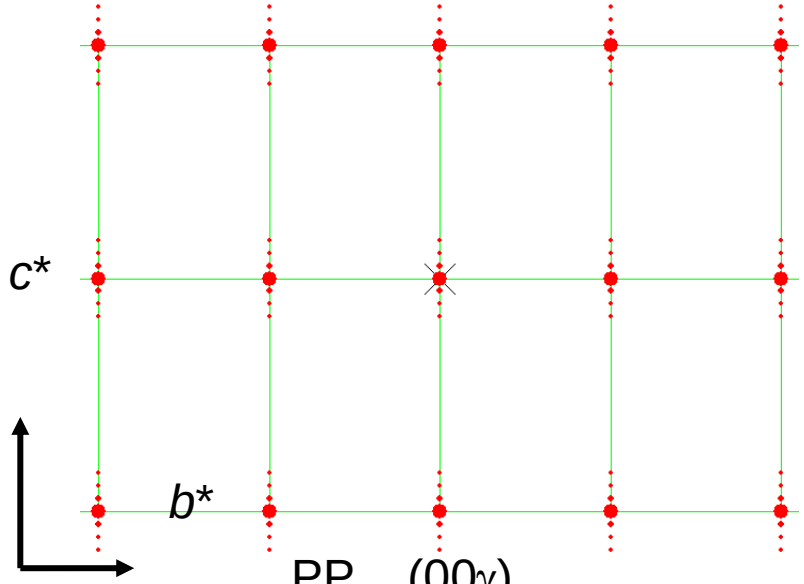
$\bar{x}_1, x_3+½, x_4$
$\bar{x}_1, x_3+½$
$\bar{x}_1, \quad x_4$
(c)

0*lm*: *m*=2*n*

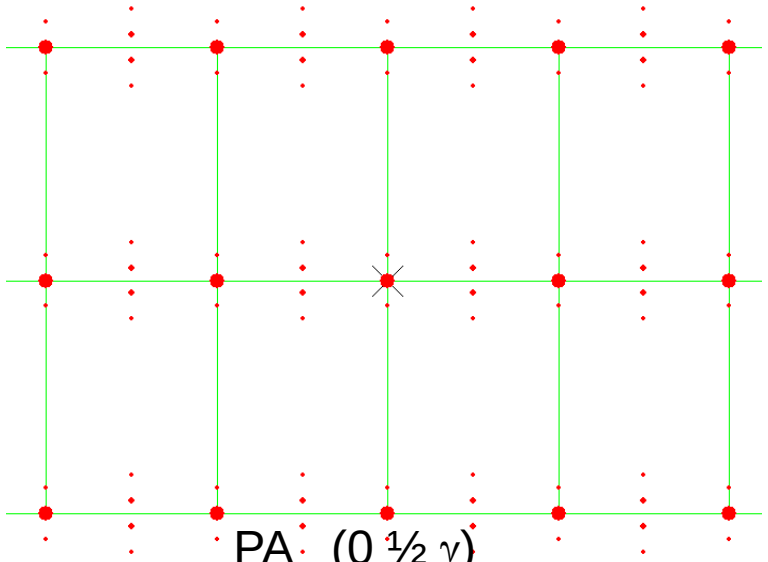
0*lm*: *l*=2*n*

2D incommensurate intergrowth structures

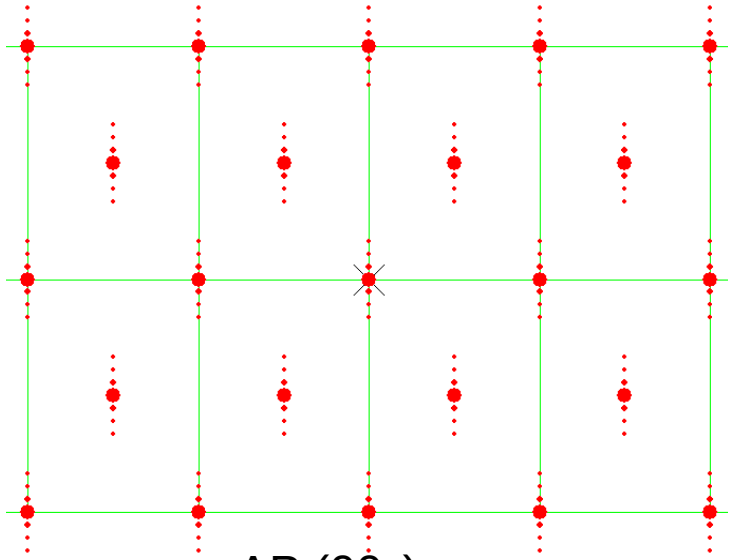
Lattice extinction in (2+1)-D space



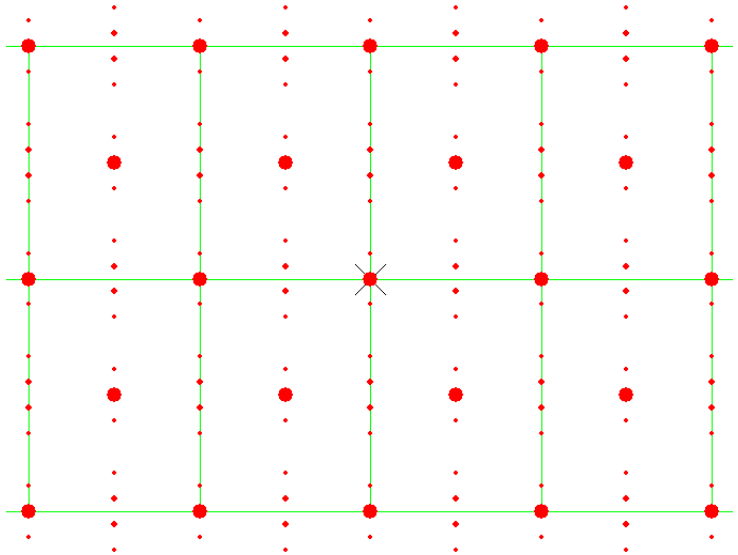
PP (00γ)



PA (0 ½ γ)



AP (00γ)



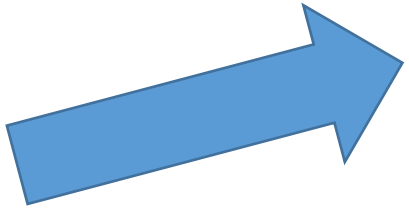
AA (01γ) or (00γ')

Reflection conditions of (3+1)-D superspace group

*I*2*mm*(00γ) *hklm*: *h*+*k*+*l*=2*n*

*I*4/*mmm*(00γ)00*ss* *hklm*:*h*+*k*+*l*=2*n*;

0klm:*m*=2*n*; *hhlm*:*m*=2*n*



l : (½ ½ ½ 0)+ --> *hklm*:*h*+*k*+*l*=2*n*

m_x: $-x_1$ x_2 x_3 x_4+½ --> *0klm*:*m*=2*n*

m_{x-y}: $-x_2$ x_1 x_3 x_4+½ --> *hhlm*:*m*=2*n*

*C*mmm(10γ)s00 *hklm*:*h*+*k*=2*n*; 0*klm*,*m*=2*n*

*P*4(00γ)*q* *00lm*:*m*=4*n*

*P*3(00γ)*t* *00lm*: *m*=3*n*