Tech Talk

Mastering Space Group Tables for Electron Diffraction Pattern Indexing

Xiaobing Hu

The NU*ANCE* Center, Northwestern University

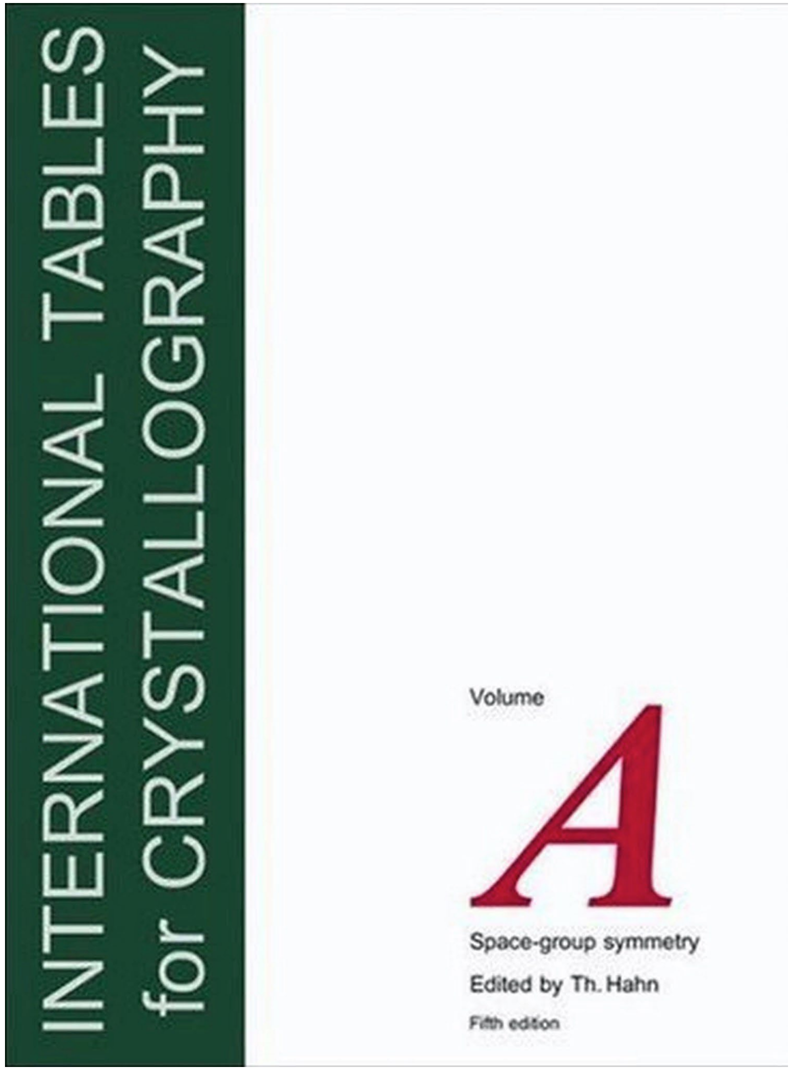
Department of Materials Sciences and Engineering, Northwestern University

February 19, 2025

Contact Information:
Email: xbhu@northwestern.edu
Office: Tech Building Ground Floor JG14
Phone: 847-467-4992

Outline

- ➢Index of electron diffraction patterns
- ➢Introduction of lattice, point and space group
- ➢ Contribution of diffraction intensity from unit cell
- ➢How to use space group table?



✓ Index of electron diffraction patterns

Things to be considered when indexing the reflections

- Planar distance match targeted phase
- **Lattice extinction rules**
- Indexed plane (hkl) must within the zone-axis [uvw]
  h*u + k*v + l*w=0
- Intersection angle between two planes within an individual zone-axis matches

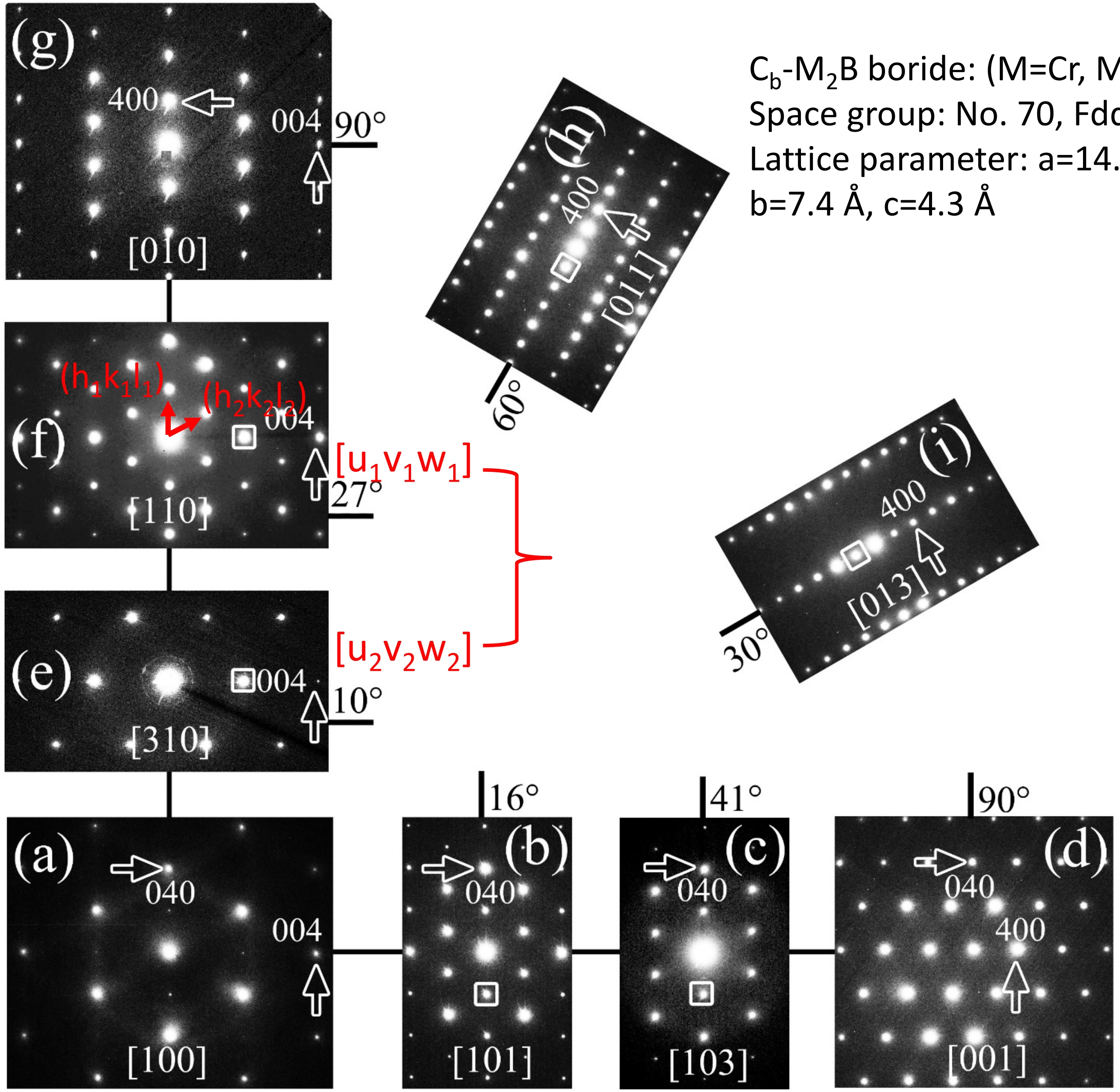
  $(h_1k_1l_1)$ $(h_2k_2l_2)$
- Intersection angles between two zone-axis matches

Along $[u_1v_1w_1]$ direction: read tilting angle X_1, Y_1 from microscope;
Along $[u_2v_2w_2]$ direction: read tilting angle X_2, Y_2 from microscope;

Experimental measured intersection angle θ:

$$\cos\theta = \cos(x_1 - x_2) * \cos(y_1 - y_2)$$

C_b-M_2B boride: (M=Cr, Mo, Fe)
Space group: No. 70, Fddd
Lattice parameter: a=14.7 Å, b=7.4 Å, c=4.3 Å

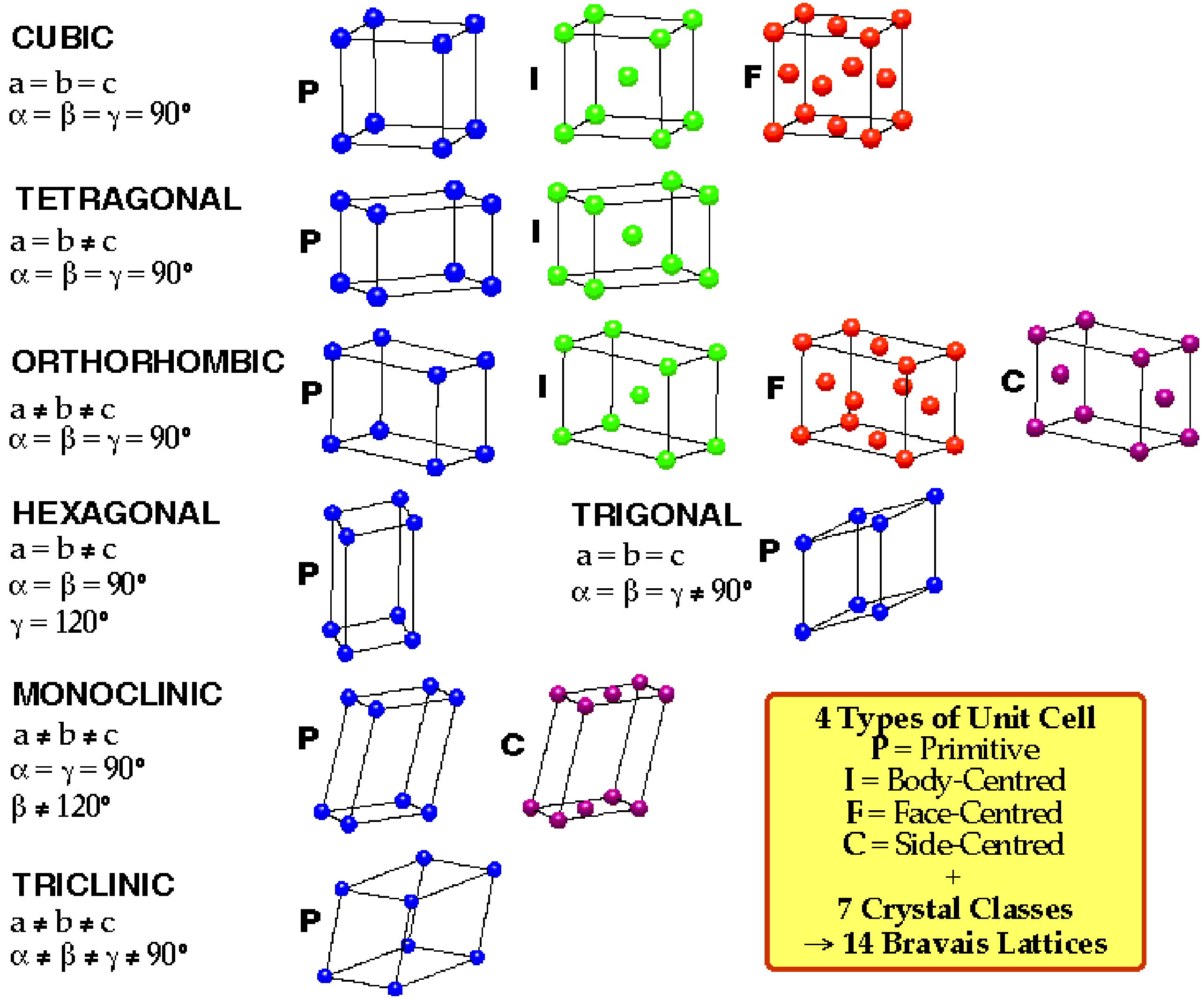


Hu, et al, Acta Materialia 68 (2014) 70-81

✓ Introduction of lattice, point and space group

Solid state matter has three state:

- Crystal structure (**having translational periodicity**)
- Quasi-crystal structure (no translation periodicity)
- Amorphous (only short-range order)



https://home.iitk.ac.in/~sangals/crystosim/crystaltut.html

NUANCE
Northwestern University Atomic and Nanoscale Characterization Experimental Center
Northwestern
EXPLORING INNER SPACE

Symmetry operations in space groups for crystallography

- Macroscopic Symmetry

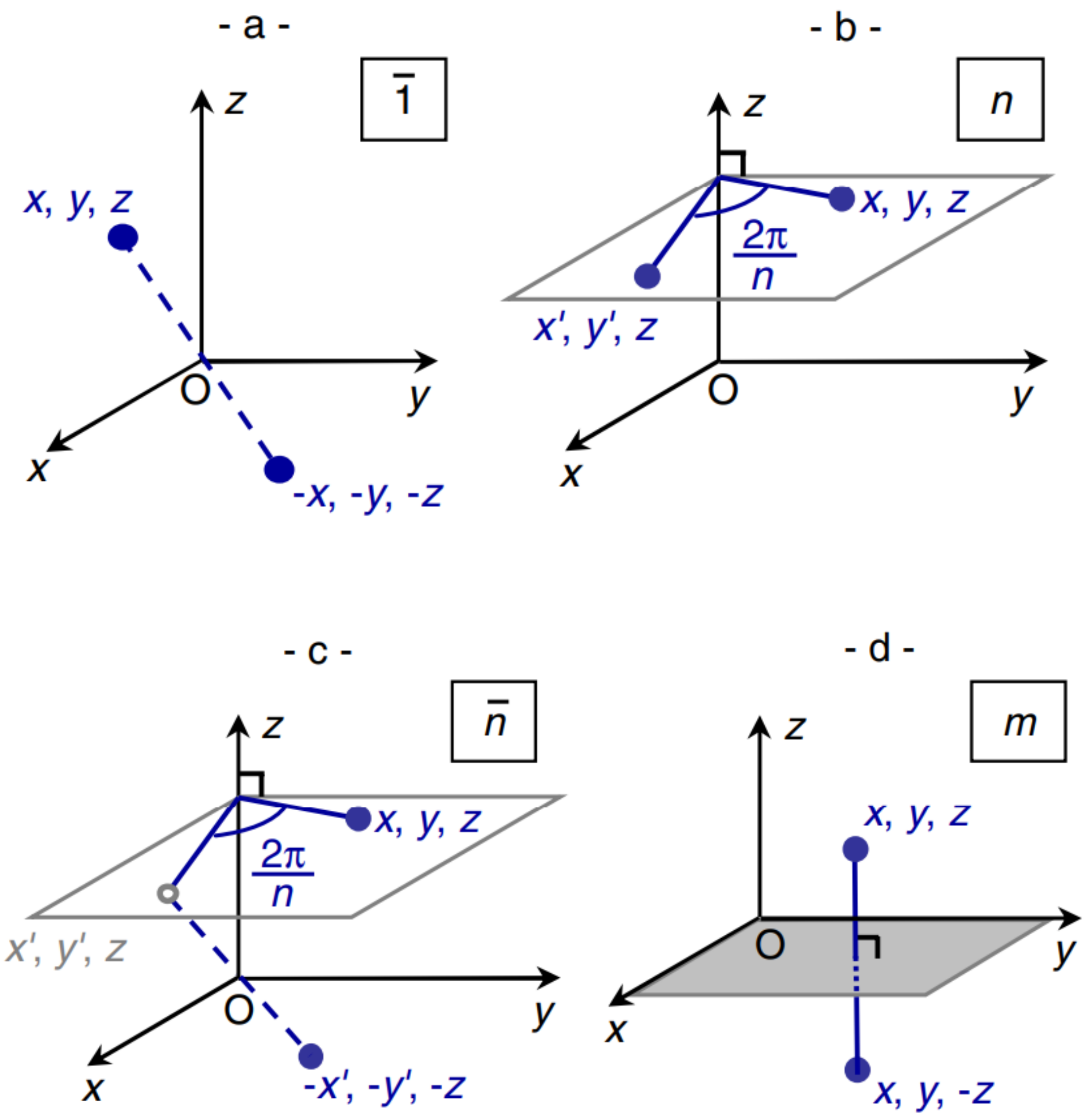
Basic operation:
Rotation----L1， L2， L3， L4， L6;
Reflection----m
Inversion----$\bar{1}$
Combined operation:
Rotoinversion = Rotation + Inversion
$\bar{\mathbf{4}}$, $\bar{\mathbf{6}}$

- Microscopic Symmetry **(Macroscopic Symmetry + partial glide)**

Glide reflection = Reflection + partial translation
a, **b**, **c**, **n**, **d**

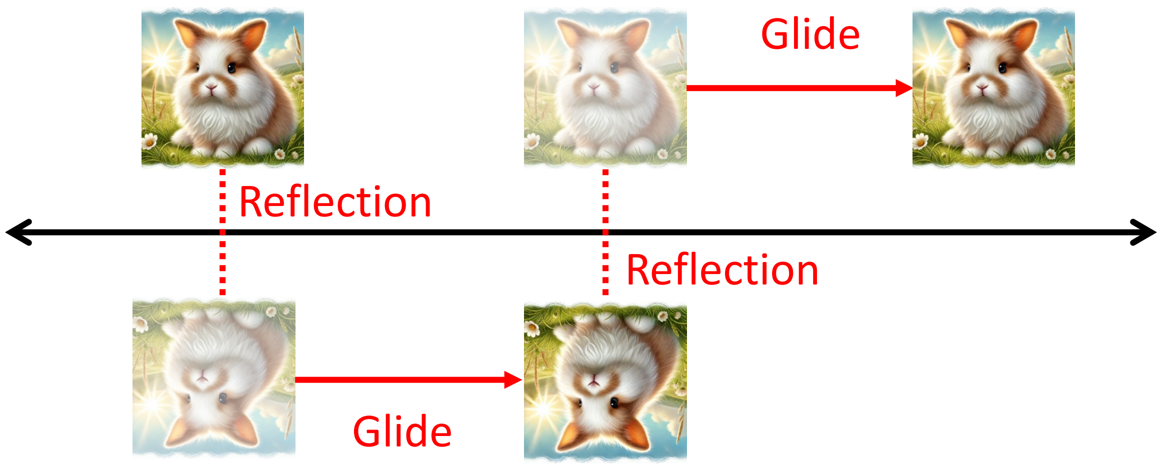
Screw rotation = Rotation + partial translation

Screw axis: 2_1, 3_1, 3_2, 4_1, 4_2, 4_3, 6_1, 6_2, 6_3, 6_4, 6_5



Symmetry planes and their symbols

Schematic of glide reflection operation

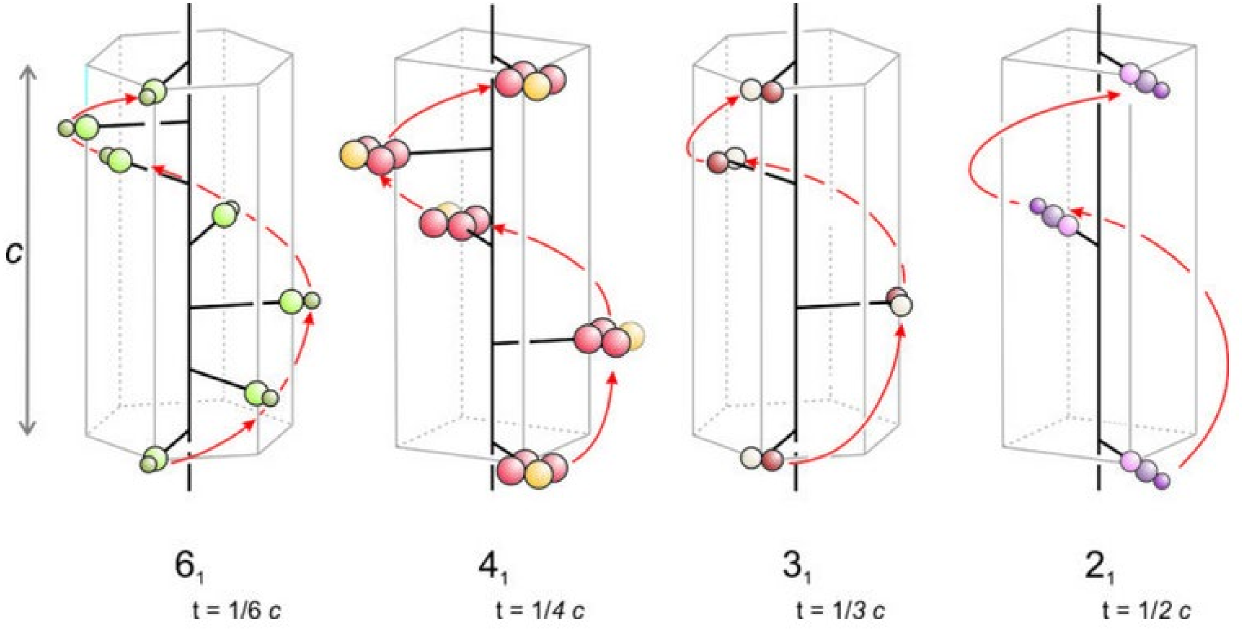


Printed Symbol	Symmetry Plane	Graphic Symbol: Normal to Plane of Projection	Graphic Symbol: Parallel to the Plane of Projection	Nature of Glide Translation [1]
m	Reflection plane (mirror)			None
a, b	Axial glide plane			a/2 or b/2
c	Axial glide plane		none	c/2
n	Diagonal glide plane (net)			(a + b)/2 or (b + c)/2 or (a + c)/2
d	"Diamond" glide plane		3/8 1/8	(a ± b)/4 or (b ± c)/4 or (a ± c)/4
e	"Double" glide plane			(a/2 + c/2) or (b/2 + c/2) or (a/2 + b/2)

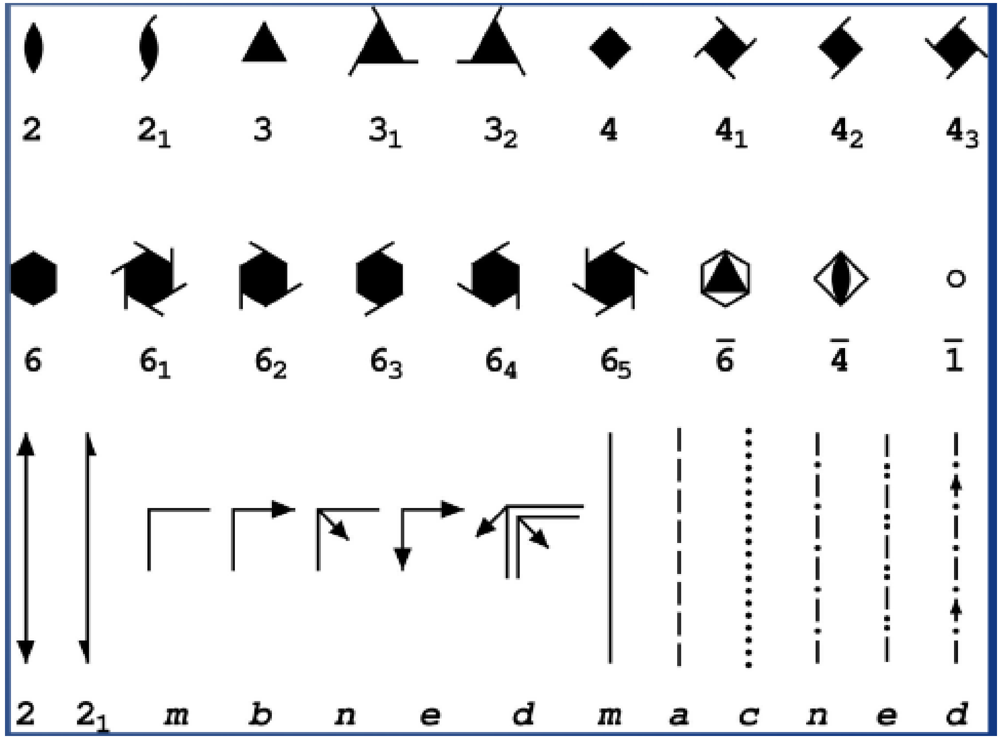
[1] "a, b, c" lengths of the unit.

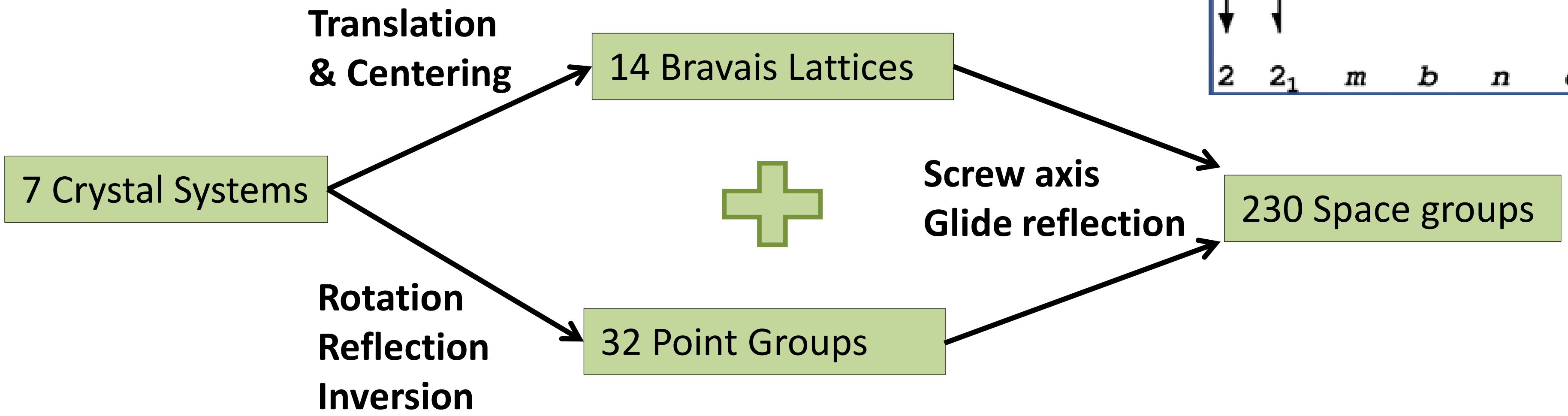
Glide planes: A combination of a reflection and a translation parallel to the reflection plane. The translational component can be half of the translation unit (planes a, b, c, n, e) or a quarter (planes d), always in a parallel direction to the plane.

Schematic of screw axis operation



Schematic of screw axis operation





Mathematical descriptions of operation elements

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = W * \begin{pmatrix} x \\ y \\ z \end{pmatrix} + t$$

Operation matrix

Translation vector

Post-operation

Original location

For a 6_1 screw-axis along [001] direction

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{bmatrix} 1 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} * \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \frac{1}{6} \end{pmatrix}$$

For the n glide plane (110) plane

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{bmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} * \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$$

For 2-fold ration axis [100] direction

$$W = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{bmatrix}$$

For 2-fold ration axis [010] direction

$$W = \begin{bmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{bmatrix}$$

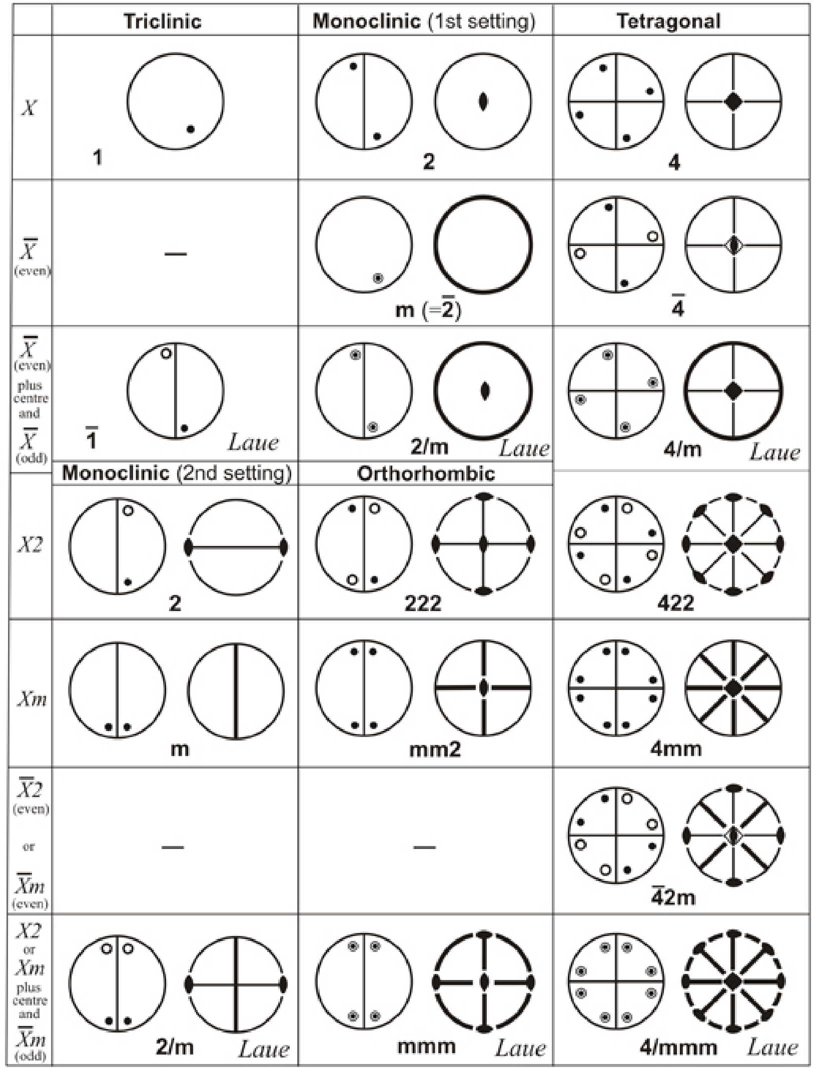
For a position operated by two continuous 2-fold ration [100] and [010] direction

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{bmatrix} * \begin{bmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{bmatrix} * \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$= \begin{bmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{bmatrix} * \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

This is a 2-fold ration axis [001] direction

32 Point group (plane group; without consideration of translation)



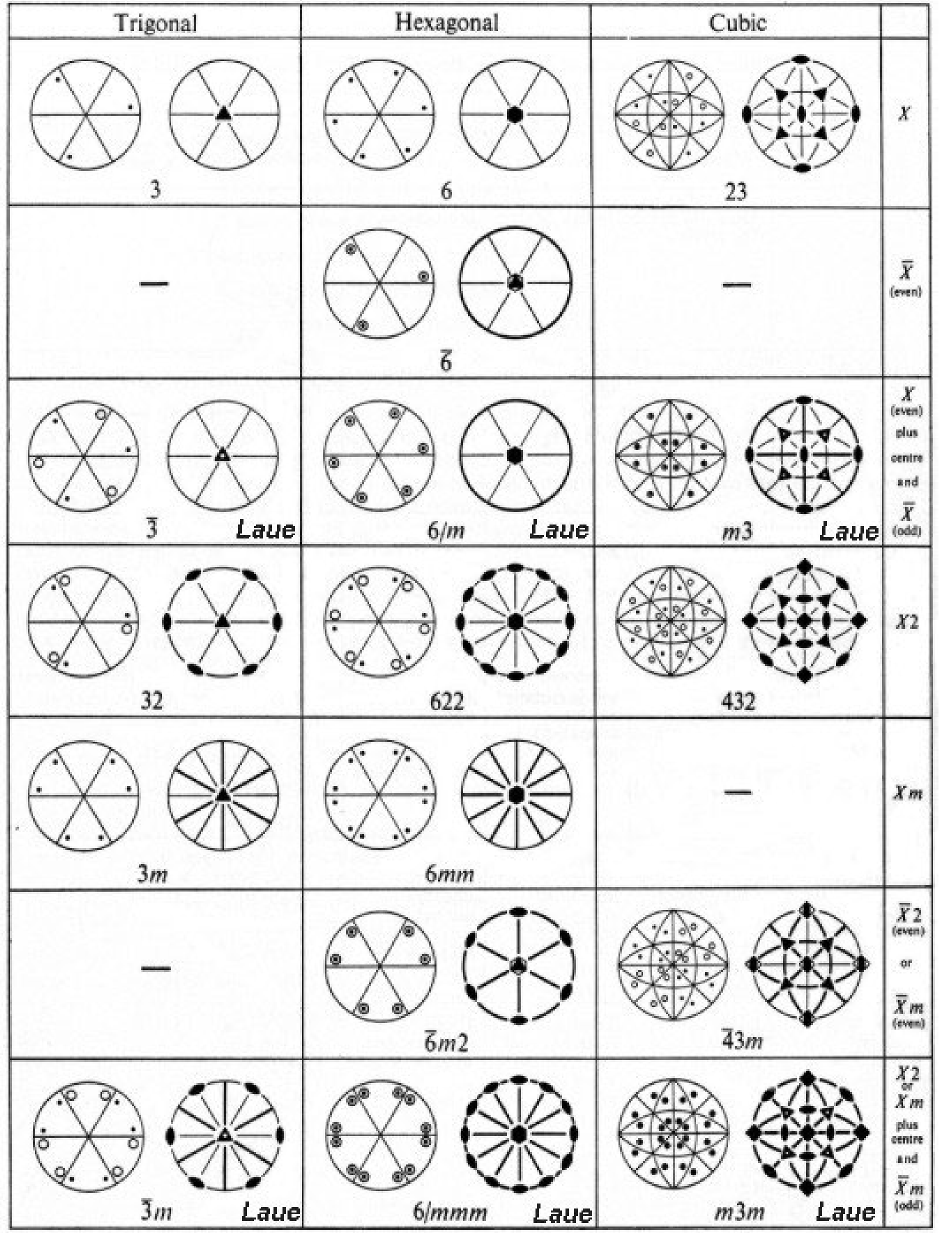


Table 2.1.2.1. *Crystal families, crystal systems, conventional coordinate systems and Bravais lattices in one, two and three dimensions*

Crystal family	Symbol*	Crystal system	Crystallographic point groups†	No. of space groups	Conventional coordinate system: Restrictions on cell parameters	Conventional coordinate system: Parameters to be determined	Bravais lattices*
One dimension							
–	–	–	1, m	2	None	a	p
Two dimensions							
Oblique (monoclinic)	m	Oblique	1, 2	2	None	a, b γ‡	mp
Rectangular (orthorhombic)	o	Rectangular	m, $2mm$	7	$\gamma = 90°$	a, b	op oc
Square (tetragonal)	t	Square	4, $4mm$	3	$a = b$ $\gamma = 90°$	a	tp
Hexagonal	h	Hexagonal	3, 6 $3m$, $6mm$	5	$a = b$ $\gamma = 120°$	a	hp
Three dimensions							
Triclinic (anorthic)	a	Triclinic	1, $\bar{1}$	2	None	$a, b, c,$ α, β, γ	aP
Monoclinic	m	Monoclinic	2, m, $2/m$	13	b-unique setting $\alpha = \gamma = 90°$	a, b, c β‡	mP mS (mC, mA, mI)
					c-unique setting $\alpha = \beta = 90°$	$a, b, c,$ γ‡	mP mS (mA, mB, mI)
Orthorhombic	o	Orthorhombic	222, $mm2$, mmm	59	$\alpha = \beta = \gamma = 90°$	a, b, c	oP oS (oC, oA, oB) oI oF
Tetragonal	t	Tetragonal	4, $\bar{4}$, $4/m$ 422, $4mm$, $\bar{4}2m$, $4/mmm$	68	$a = b$ $\alpha = \beta = \gamma = 90°$	a, c	tP tI
Hexagonal	h	Trigonal	3, $\bar{3}$ 32, $3m$, $\bar{3}m$	18	$a = b$ $\alpha = \beta = 90°, \ \gamma = 120°$	a, c	hP
				7	$a = b = c$ $\alpha = \beta = \gamma$ (rhombohedral axes, primitive cell) $a = b$ $\alpha = \beta = 90°, \gamma = 120°$ (hexagonal axes, triple obverse cell)	a, α	hR
		Hexagonal	6, $\bar{6}$, $6/m$ 622, $6mm$, $\bar{6}2m$, $6/mmm$	27	$a = b$ $\alpha = \beta = 90°, \gamma = 120°$	a, c	hP
Cubic	c	Cubic	23, $m\bar{3}$ 432, $\bar{4}3m$, $m\bar{3}m$	36	$a = b = c$ $\alpha = \beta = \gamma = 90°$	a	cP cI cF

NUANCE
Northwestern University Atomic and Nanoscale Characterization Experimental Center
Northwestern
EXPLORING INNER SPACE

✓ Contribution of diffraction intensity from unit cell

Scattering amplitude from **unit cell** can be described as :

$$A_{cell}=\frac{e^{2\pi ikr}}{r}\sum f_i(\theta)e^{2\pi i\boldsymbol{K}*\boldsymbol{R_i}}$$

$f(\theta)$: atomic scattering factor

$\frac{e^{2\pi ikr}}{r}$: descripting the scattered wave

$\boldsymbol{R_i}$ is the vector which defines the location of each atom within the unit cell.

$\boldsymbol{R_i}=x_i$***a** + y_i***b** + z_i***c**

$\boldsymbol{K}$ is the diffraction vector of unit, where $\boldsymbol{K}=\boldsymbol{g}$ atom within the unit cell.

$\boldsymbol{g}=h$***a*** + y_i***b*** + z_i***c***

$$A_{cell}=\frac{e^{2\pi ikr}}{r}\sum f_i(\theta)e^{2\pi i\boldsymbol{K}*\boldsymbol{R_i}}$$
$$=\frac{e^{2\pi ikr}}{r}\sum f_i(\theta)e^{2\pi i(hx_i+ky_i+lz_i)}$$
$$=\frac{e^{2\pi ikr}}{r}F_{hkl}$$

F_{hkl}: structure factor of unit cell

$$F_{hkl}=\sum f_i(\theta)e^{2\pi i(hx_i+ky_i+lz_i)}$$

- ❖ applies whether there is one atom or one hundred atoms in the unit cell
- ❖ no matter where they are located, and it applies to all crystal lattices

Diffraction pattern intensity $I \propto A_{cell}^2 \propto F_{hkl}^2$

Example I: Face centered cubic (FCC) lattice

F_{hkl}: structure factor of unit cell

$$F_{hkl} = \sum f_i(\theta) e^{2\pi i(hx_i+ky_i+lz_i)}$$

For FCC lattice

$$e^{\theta i} = \cos\theta + i\sin\theta$$
$$e^{\pi i} = \cos\pi + i\sin\pi = -1$$
$$e^{2\pi i} = \cos 2\pi + i\sin 2\pi = 1$$

$$F_{hkl} = \sum f_i(\theta) e^{2\pi i(hx_i+ky_i+lz_i)}$$
$$= f\{1 + e^{\pi i(h+k)} + e^{\pi i(h+l)} + e^{\pi i(k+l)}\}$$

- If h, k, l are all even or odd integers

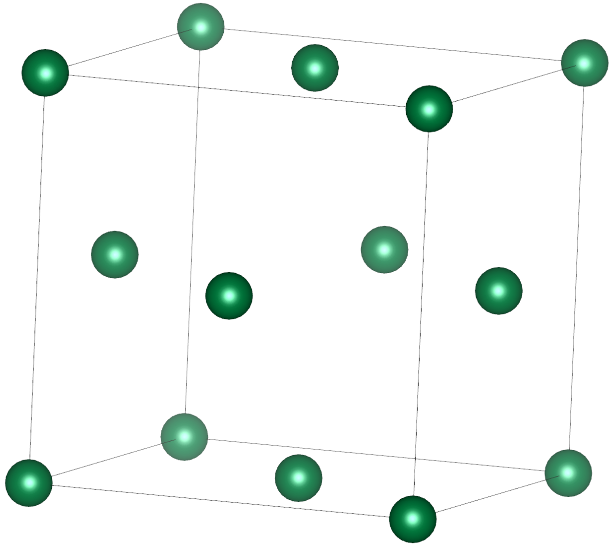
$$F_{hkl} = f\{1 + e^{2\pi i} + e^{2\pi i} + e^{2\pi i}\} = 4f$$

- If h, k, l are in mixed even and odd integers

$$F_{hkl} = f\{1 + 2e^{\pi i} + e^{2\pi i}\} = 0$$

For FCC lattice, only lattice plane {h, k, l} existing rule:
(h, k, l) must be all even or odd integers

Schematic of FCC lattice



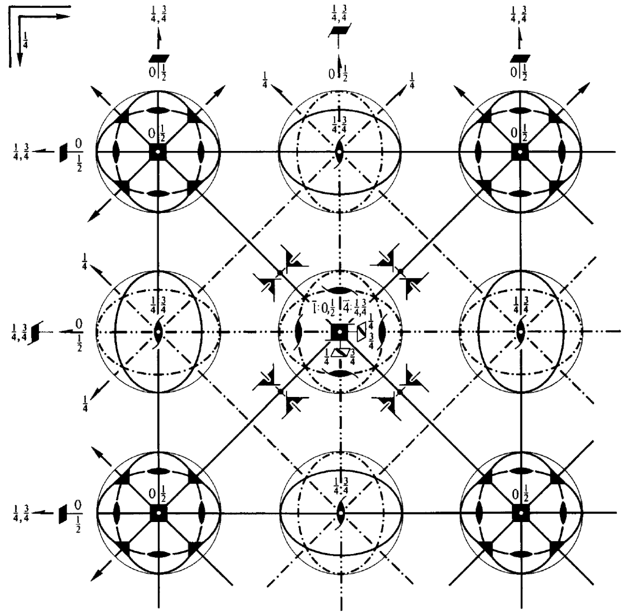
FCC lattice: Space group Fm$\bar{3}$m, group number 225
Atom locations:
(x, y, z)=(0,0,0), $(0,\frac{1}{2},\frac{1}{2})$, $(\frac{1}{2},\frac{1}{2},0)$, $(\frac{1}{2},0,\frac{1}{2})$

For FCC lattice, only lattice plane {h, k, l} existing rule:
(h, k, l) must be all even or odd integers

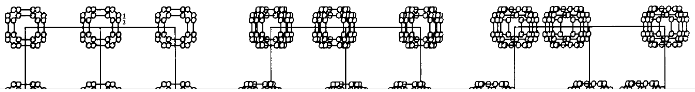
International Tables for Crystallography (2006). Vol. A, Space group 225, pp. 688–691.

$Fm\bar{3}m$ O_h^5 $m\bar{3}m$ Cubic

No. 225 $F\ 4/m\ \bar{3}\ 2/m$ Patterson symmetry $Fm\bar{3}m$



Upper left quadrant only



Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates: $(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$						Reflection conditions: h,k,l permutable
									General:
192	*l*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$			hkl : $h+k,h+l,k+l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$			$0kl$: $k,l=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$			hhl : $h+l=2n$
			(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$			$h00$: $h=2n$
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$			
			(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$			
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x,y,\bar{z}$	(27) $x,\bar{y},z$	(28) $\bar{x},y,z$			
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x,y$	(31) $z,x,\bar{y}$	(32) $z,\bar{x},y$			
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z},x$	(35) $\bar{y},z,x$	(36) $y,z,\bar{x}$			
			(37) $\bar{y},\bar{x},z$	(38) y,x,z	(39) $\bar{y},x,\bar{z}$	(40) $y,\bar{x},\bar{z}$			
			(41) $\bar{x},\bar{z},y$	(42) $x,\bar{z},\bar{y}$	(43) x,z,y	(44) $\bar{x},z,\bar{y}$			
			(45) $\bar{z},\bar{y},x$	(46) $\bar{z},y,\bar{x}$	(47) $z,\bar{y},\bar{x}$	(48) z,y,x			
									Special: as above, plus
96	*k*	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	z,x,x	$z,\bar{x},\bar{x}$	no extra conditions
			$\bar{z},\bar{x},x$	$\bar{z},x,\bar{x}$	x,z,x	$\bar{x},z,\bar{x}$	$x,\bar{z},\bar{x}$	$\bar{x},\bar{z},x$	
			$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	$x,\bar{x},z$	$\bar{x},x,z$	$x,z,\bar{x}$	$\bar{x},z,x$	
			$\bar{x},\bar{z},\bar{x}$	$x,\bar{z},x$	$z,x,\bar{x}$	$z,\bar{x},x$	$\bar{z},x,x$	$\bar{z},\bar{x},\bar{x}$	
96	*j*	$m..$	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	$z,0,y$	$z,0,\bar{y}$	no extra conditions
			$\bar{z},0,y$	$\bar{z},0,\bar{y}$	$y,z,0$	$\bar{y},z,0$	$y,\bar{z},0$	$\bar{y},\bar{z},0$	
			$y,0,\bar{z}$	$\bar{y},0,\bar{z}$	$y,0,z$	$\bar{y},0,z$	$0,z,\bar{y}$	$0,z,y$	
			$0,\bar{z},\bar{y}$	$0,\bar{z},y$	$z,y,0$	$z,\bar{y},0$	$\bar{z},y,0$	$\bar{z},\bar{y},0$	
48	*i*	$m.m2$	$\frac{1}{2},y,y$	$\frac{1}{2},\bar{y},y$	$\frac{1}{2},y,\bar{y}$	$\frac{1}{2},\bar{y},\bar{y}$	$y,\frac{1}{2},y$	$y,\frac{1}{2},\bar{y}$	no extra conditions
			$\bar{y},\frac{1}{2},y$	$\bar{y},\frac{1}{2},\bar{y}$	$y,y,\frac{1}{2}$	$\bar{y},y,\frac{1}{2}$	$y,\bar{y},\frac{1}{2}$	$\bar{y},\bar{y},\frac{1}{2}$	
48	*h*	$m.m2$	$0,y,y$	$0,\bar{y},y$	$0,y,\bar{y}$	$0,\bar{y},\bar{y}$	$y,0,y$	$y,0,\bar{y}$	no extra conditions
			$\bar{y},0,y$	$\bar{y},0,\bar{y}$	$y,y,0$	$\bar{y},y,0$	$y,\bar{y},0$	$\bar{y},\bar{y},0$	
48	*g*	$2.mm$	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},x$	$\frac{3}{4},\frac{1}{4},\bar{x}$	hkl : $h=2n$
			$\frac{1}{4},x,\frac{3}{4}$	$\frac{3}{4},\bar{x},\frac{3}{4}$	$x,\frac{1}{4},\frac{3}{4}$	$\bar{x},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\bar{x}$	$\frac{1}{4},\frac{3}{4},x$	
32	*f*	$.3m$	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			no extra conditions
			$x,x,\bar{x}$	$\bar{x},\bar{x},\bar{x}$	$x,\bar{x},x$	$\bar{x},x,x$			
24	*e*	$4m.m$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	no extra conditions
24	*d*	$m.mm$	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{1}{4},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$	hkl : $h=2n$
8	*c*	$\bar{4}3m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$					hkl : $h=2n$
4	*b*	$m\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$						no extra conditions
4	*a*	$m\bar{3}m$	$0,0,0$						no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [111] $p6mm$
$\mathbf{a}'=\frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $c2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Example II: Ordered FCC lattice ($L1_2$ type)

F_{hkl}: structure factor of unit cell

$$F_{hkl} = \sum f_i(\theta) e^{2\pi i(hx_i + ky_i + lz_i)}$$

For $L1_2$ lattice

$$F_{hkl} = \sum f_i(\theta) e^{2\pi i(hx_i + ky_i + lz_i)}$$
$$= f_{Al} + f_{Ni} * \{e^{\pi i(h+k)} + e^{\pi i(h+l)} + e^{\pi i(k+l)}\}$$

FCC lattice: Space group $Pm\bar{3}m$, group number 221

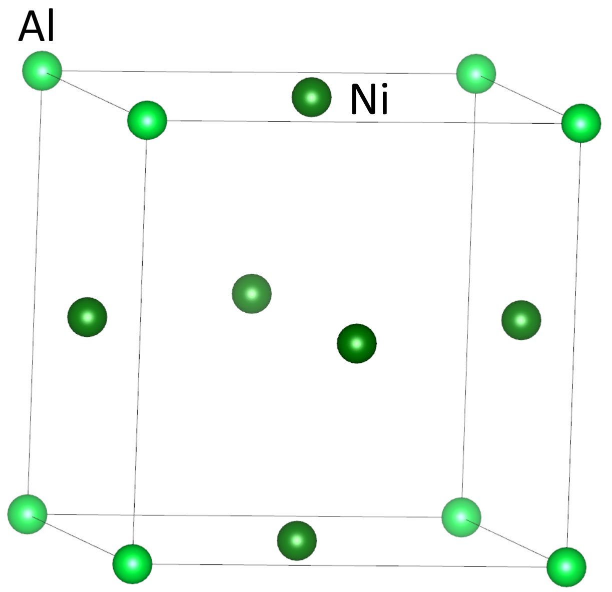
Atom locations:

Al(x, y, z)=(0,0,0)

Ni (x, y, z)=$(0,\frac{1}{2},\frac{1}{2})$, $(\frac{1}{2},\frac{1}{2},0)$, $(\frac{1}{2},0,\frac{1}{2})$

$$e^{\theta i} = \cos\theta + i\sin\theta$$
$$e^{\pi i} = \cos\pi + i\sin\pi = -1$$
$$e^{2\pi i} = \cos 2\pi + i\sin 2\pi = 1$$

Schematic of Ni_3Al lattice



- If h, k, l are all even or odd integers:

$$F_{hkl} = f_{Al} + f_{Ni} * \{e^{2\pi i} + e^{2\pi i} + e^{2\pi i}\} = f_{Al} + 3f_{Ni}$$ → Diffraction patterns with larger intensity

- If h, k, l are in mixed even and odd integers:

$$F_{hkl} = f_{Al} + f_{Ni}\{2e^{\pi i} + e^{2\pi i}\} = f_{Al} - f_{Ni}$$ → Diffraction patterns with reduced intensity

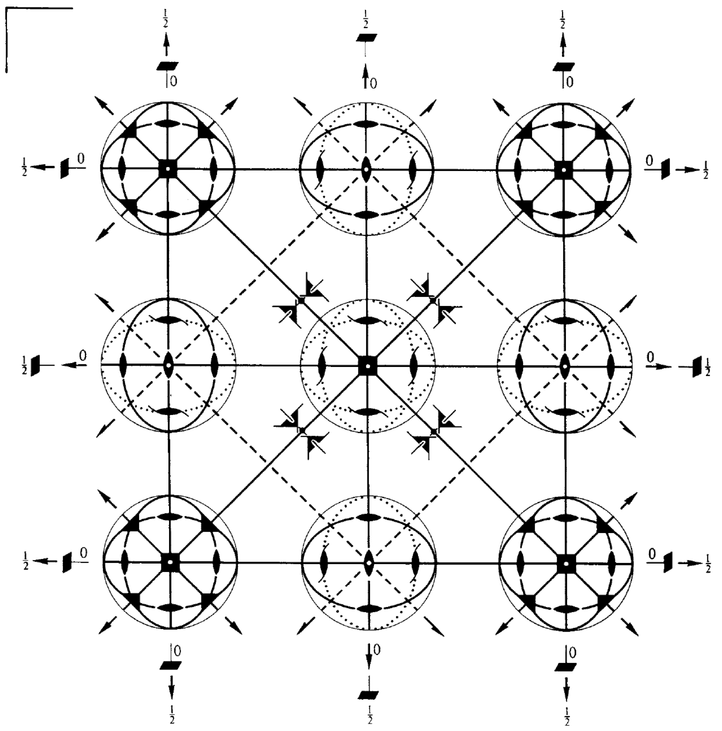
For $L1_2$ type, all lattice planes existed but with different intensities.

For $L1_2$ type, all lattice planes existed but with different intensities.

International Tables for Crystallography (2006). Vol. A, Space group 221, pp. 672–674.

$Pm\bar{3}m$ $\quad O_h^1$ $\quad m\bar{3}m$ $\quad$ Cubic

No. 221 $\quad P\ 4/m\ \bar{3}\ 2/m$ $\quad$ Patterson symmetry $Pm\bar{3}m$



Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity	Wyckoff letter	Site symmetry	Coordinates						Reflection conditions
									h,k,l permutable General:
48	n	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$			no conditions
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$			
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$			
			(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$			
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$			
			(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$			
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x,y,\bar{z}$	(27) $x,\bar{y},z$	(28) $\bar{x},y,z$			
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x,y$	(31) $z,x,\bar{y}$	(32) $z,\bar{x},y$			
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z},x$	(35) $\bar{y},z,x$	(36) $y,z,\bar{x}$			
			(37) $\bar{y},\bar{x},z$	(38) y,x,z	(39) $\bar{y},x,\bar{z}$	(40) $y,\bar{x},\bar{z}$			
			(41) $\bar{x},\bar{z},y$	(42) $x,\bar{z},\bar{y}$	(43) x,z,y	(44) $\bar{x},z,\bar{y}$			
			(45) $\bar{z},\bar{y},x$	(46) $\bar{z},y,\bar{x}$	(47) $z,\bar{y},\bar{x}$	(48) z,y,x			
									Special: no extra conditions
24	m	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	z,x,x	$z,\bar{x},\bar{x}$	
			$\bar{z},\bar{x},x$	$\bar{z},x,\bar{x}$	x,z,x	$\bar{x},z,\bar{x}$	$x,\bar{z},\bar{x}$	$\bar{x},\bar{z},x$	
			$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	$x,\bar{x},z$	$\bar{x},x,z$	$x,z,\bar{x}$	$\bar{x},z,x$	
			$\bar{x},\bar{z},\bar{x}$	$x,\bar{z},x$	$z,x,\bar{x}$	$z,\bar{x},x$	$\bar{z},x,x$	$\bar{z},\bar{x},\bar{x}$	
24	l	$m..$	$\tfrac12,y,z$	$\tfrac12,\bar{y},z$	$\tfrac12,y,\bar{z}$	$\tfrac12,\bar{y},\bar{z}$	$z,\tfrac12,y$	$z,\tfrac12,\bar{y}$	
			$\bar{z},\tfrac12,y$	$\bar{z},\tfrac12,\bar{y}$	$y,z,\tfrac12$	$\bar{y},z,\tfrac12$	$y,\bar{z},\tfrac12$	$\bar{y},\bar{z},\tfrac12$	
			$y,\tfrac12,\bar{z}$	$\bar{y},\tfrac12,\bar{z}$	$y,\tfrac12,z$	$\bar{y},\tfrac12,z$	$\tfrac12,z,\bar{y}$	$\tfrac12,z,y$	
			$\tfrac12,\bar{z},\bar{y}$	$\tfrac12,\bar{z},y$	$z,y,\tfrac12$	$z,\bar{y},\tfrac12$	$\bar{z},y,\tfrac12$	$\bar{z},\bar{y},\tfrac12$	
24	k	$m..$	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	$z,0,y$	$z,0,\bar{y}$	
			$\bar{z},0,y$	$\bar{z},0,\bar{y}$	$y,z,0$	$\bar{y},z,0$	$y,\bar{z},0$	$\bar{y},\bar{z},0$	
			$y,0,\bar{z}$	$\bar{y},0,\bar{z}$	$y,0,z$	$\bar{y},0,z$	$0,z,\bar{y}$	$0,z,y$	
			$0,\bar{z},\bar{y}$	$0,\bar{z},y$	$z,y,0$	$z,\bar{y},0$	$\bar{z},y,0$	$\bar{z},\bar{y},0$	
12	j	$m.m2$	$\tfrac12,y,y$	$\tfrac12,\bar{y},y$	$\tfrac12,y,\bar{y}$	$\tfrac12,\bar{y},\bar{y}$	$y,\tfrac12,y$	$y,\tfrac12,\bar{y}$	
			$\bar{y},\tfrac12,y$	$\bar{y},\tfrac12,\bar{y}$	$y,y,\tfrac12$	$\bar{y},y,\tfrac12$	$y,\bar{y},\tfrac12$	$\bar{y},\bar{y},\tfrac12$	
12	i	$m.m2$	$0,y,y$	$0,\bar{y},y$	$0,y,\bar{y}$	$0,\bar{y},\bar{y}$	$y,0,y$	$y,0,\bar{y}$	
			$\bar{y},0,y$	$\bar{y},0,\bar{y}$	$y,y,0$	$\bar{y},y,0$	$y,\bar{y},0$	$\bar{y},\bar{y},0$	
12	h	$mm2..$	$x,\tfrac12,0$	$\bar{x},\tfrac12,0$	$0,x,\tfrac12$	$0,\bar{x},\tfrac12$	$\tfrac12,0,x$	$\tfrac12,0,\bar{x}$	
			$\tfrac12,x,0$	$\tfrac12,\bar{x},0$	$x,0,\tfrac12$	$\bar{x},0,\tfrac12$	$0,\tfrac12,\bar{x}$	$0,\tfrac12,x$	
8	g	$.3m$	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			
			$x,x,\bar{x}$	$\bar{x},\bar{x},\bar{x}$	$x,\bar{x},x$	$\bar{x},x,x$			
6	f	$4m.m$	$x,\tfrac12,\tfrac12$	$\bar{x},\tfrac12,\tfrac12$	$\tfrac12,x,\tfrac12$	$\tfrac12,\bar{x},\tfrac12$	$\tfrac12,\tfrac12,x$	$\tfrac12,\tfrac12,\bar{x}$	
6	e	$4m.m$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	
3	d	$4/mm.m$	$\tfrac12,0,0$	$0,\tfrac12,0$	$0,0,\tfrac12$				
3	c	$4/mm.m$	$0,\tfrac12,\tfrac12$	$\tfrac12,0,\tfrac12$	$\tfrac12,\tfrac12,0$				
1	b	$m\bar{3}m$	$\tfrac12,\tfrac12,\tfrac12$						
1	a	$m\bar{3}m$	$0,0,0$						

Symmetry of special projections

Along [001] $p4mm$ $\quad$ $\mathbf{a}'=\mathbf{a}$ $\quad$ $\mathbf{b}'=\mathbf{b}$ $\quad$ Origin at $0,0,z$

Along [111] $p6mm$ $\quad$ $\mathbf{a}'=\tfrac13(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\quad$ $\mathbf{b}'=\tfrac13(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$ $\quad$ Origin at x,x,x

Along [110] $p2mm$ $\quad$ $\mathbf{a}'=\tfrac12(-\mathbf{a}+\mathbf{b})$ $\quad$ $\mathbf{b}'=\mathbf{c}$ $\quad$ Origin at $x,x,0$

Example III: Ordered BCC lattice (B2 type)

F_{hkl}: structure factor of unit cell

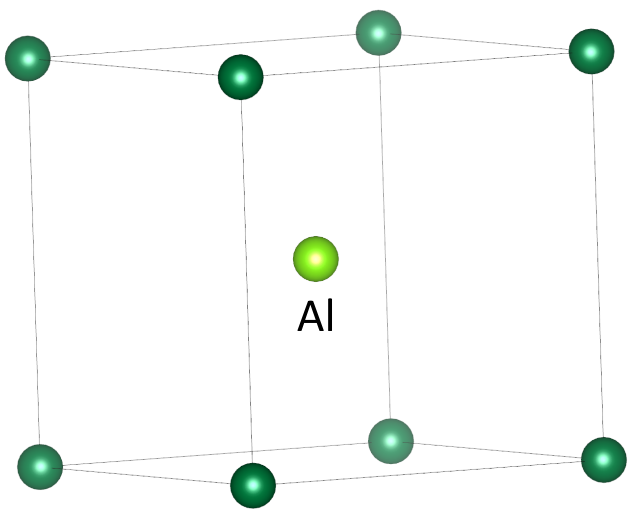
$$F_{hkl} = \sum f_i(\theta) e^{2\pi i(hx_i+ky_i+lz_i)}$$

For B2 lattice

$$F_{hkl} = \sum f_i(\theta) e^{2\pi i(hx_i+ky_i+lz_i)}$$
$$= f_{Al} + f_{Ni} * e^{\pi i(h+k+l)}$$

$$e^{\theta i} = \cos\theta + i\sin\theta$$
$$e^{\pi i} = \cos\pi + i\sin\pi = -1$$
$$e^{2\pi i} = \cos 2\pi + i\sin 2\pi = 1$$

Schematic of NiAl lattice



- If (h + k+ l) are even integers:

$F_{hkl} = f_{Al} + f_{Ni}$ → Diffraction patterns with larger intensity

- If (h + k+ l) are odd integers:

$F_{hkl} = f_{Al} - f_{Ni}$ → Diffraction patterns with reduced intensity

For B2 type, all lattice planes existed but with different intensities.

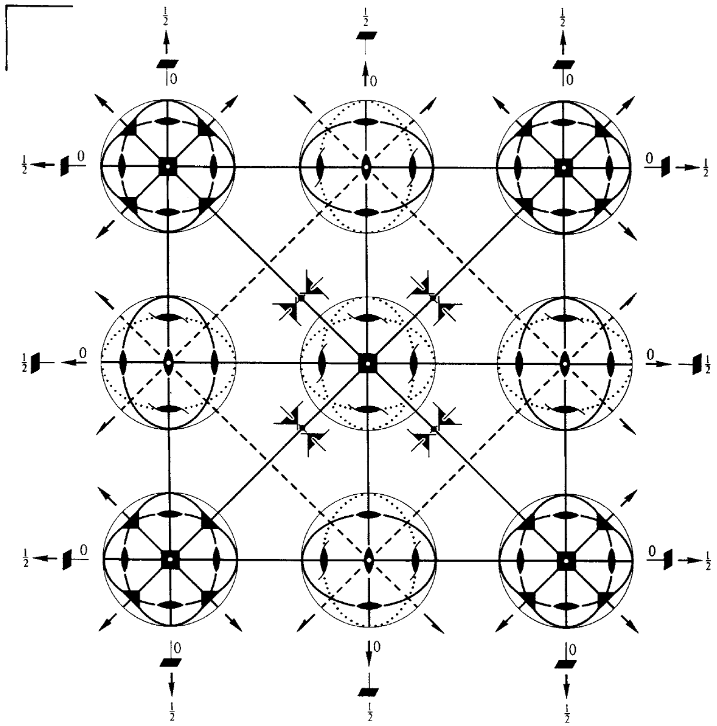
FCC lattice: Space group Pm$\bar{3}$m, group number 221
Atom locations:
Al(x, y, z)=(0,0,0)
Ni (x, y, z)=($\frac{1}{2}$,$\frac{1}{2}$, $\frac{1}{2}$)

For B2 type, all lattice planes existed but with different intensities.

International Tables for Crystallography (2006). Vol. A, Space group 221, pp. 672–674.

$Pm\bar{3}m$ O_h^1 $m\bar{3}m$ Cubic

No. 221 $P\ 4/m\ \bar{3}\ 2/m$ Patterson symmetry $Pm\bar{3}m$



Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

Reflection conditions: h,k,l permutable

General:

	Wyckoff	Site	Coordinates			
48	n	1	(1) x,y,z (5) z,x,y (9) y,z,x (13) $y,x,\bar{z}$ (17) $x,z,\bar{y}$ (21) $z,y,\bar{x}$ (25) $\bar{x},\bar{y},\bar{z}$ (29) $\bar{z},\bar{x},\bar{y}$ (33) $\bar{y},\bar{z},\bar{x}$ (37) $\bar{y},\bar{x},z$ (41) $\bar{x},\bar{z},y$ (45) $\bar{z},\bar{y},x$	(2) $\bar{x},\bar{y},z$ (6) $z,\bar{x},\bar{y}$ (10) $\bar{y},z,\bar{x}$ (14) $\bar{y},\bar{x},\bar{z}$ (18) $\bar{x},z,y$ (22) $z,\bar{y},x$ (26) $x,y,\bar{z}$ (30) $\bar{z},x,y$ (34) $y,\bar{z},x$ (38) y,x,z (42) $x,\bar{z},\bar{y}$ (46) $\bar{z},y,\bar{x}$	(3) $\bar{x},y,\bar{z}$ (7) $\bar{z},\bar{x},y$ (11) $y,\bar{z},\bar{x}$ (15) $y,\bar{x},z$ (19) $\bar{x},\bar{z},\bar{y}$ (23) $\bar{z},y,x$ (27) $x,\bar{y},z$ (31) $z,x,\bar{y}$ (35) $\bar{y},z,x$ (39) $\bar{y},x,\bar{z}$ (43) x,z,y (47) $z,\bar{y},\bar{x}$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{z},x,\bar{y}$ (12) $\bar{y},\bar{z},x$ (16) $\bar{y},x,z$ (20) $x,\bar{z},y$ (24) $\bar{z},\bar{y},\bar{x}$ (28) $\bar{x},y,z$ (32) $z,\bar{x},y$ (36) $y,z,\bar{x}$ (40) $y,\bar{x},\bar{z}$ (44) $\bar{x},z,\bar{y}$ (48) z,y,x

no conditions

Special: no extra conditions

24	m	$..m$	x,x,z $\bar{z},\bar{x},x$ $x,x,\bar{z}$ $\bar{x},\bar{z},\bar{x}$	$\bar{x},\bar{x},z$ $\bar{z},x,\bar{x}$ $\bar{x},\bar{x},\bar{z}$ $x,\bar{z},x$	$\bar{x},x,\bar{z}$ x,z,x $x,\bar{x},z$ $z,x,\bar{x}$	$x,\bar{x},\bar{z}$ $\bar{x},z,\bar{x}$ $\bar{x},x,z$ $z,\bar{x},x$	z,x,x $x,\bar{z},\bar{x}$ $x,z,\bar{x}$ $\bar{z},x,x$	$z,\bar{x},\bar{x}$ $\bar{x},\bar{z},x$ $\bar{x},z,x$ $\bar{z},\bar{x},\bar{x}$
24	l	$m..$	$\frac{1}{2},y,z$ $\bar{z},\frac{1}{2},y$ $y,\frac{1}{2},\bar{z}$ $\frac{1}{2},\bar{z},\bar{y}$	$\frac{1}{2},\bar{y},z$ $\bar{z},\frac{1}{2},\bar{y}$ $\bar{y},\frac{1}{2},\bar{z}$ $\frac{1}{2},\bar{z},y$	$\frac{1}{2},y,\bar{z}$ $y,z,\frac{1}{2}$ $y,\frac{1}{2},z$ $z,y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\bar{z}$ $\bar{y},z,\frac{1}{2}$ $\bar{y},\frac{1}{2},z$ $z,\bar{y},\frac{1}{2}$	$z,\frac{1}{2},y$ $y,\bar{z},\frac{1}{2}$ $\frac{1}{2},z,\bar{y}$ $\bar{z},y,\frac{1}{2}$	$z,\frac{1}{2},\bar{y}$ $\bar{y},\bar{z},\frac{1}{2}$ $\frac{1}{2},z,y$ $\bar{z},\bar{y},\frac{1}{2}$
24	k	$m..$	$0,y,z$ $\bar{z},0,y$ $y,0,\bar{z}$ $0,\bar{z},\bar{y}$	$0,\bar{y},z$ $\bar{z},0,\bar{y}$ $\bar{y},0,\bar{z}$ $0,\bar{z},y$	$0,y,\bar{z}$ $y,z,0$ $y,0,z$ $z,y,0$	$0,\bar{y},\bar{z}$ $\bar{y},z,0$ $\bar{y},0,z$ $z,\bar{y},0$	$z,0,y$ $y,\bar{z},0$ $0,z,\bar{y}$ $\bar{z},y,0$	$z,0,\bar{y}$ $\bar{y},\bar{z},0$ $0,z,y$ $\bar{z},\bar{y},0$
12	j	$m.m2$	$\frac{1}{2},y,y$ $\bar{y},\frac{1}{2},y$	$\frac{1}{2},\bar{y},y$ $\bar{y},\frac{1}{2},\bar{y}$	$\frac{1}{2},y,\bar{y}$ $y,y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\bar{y}$ $\bar{y},y,\frac{1}{2}$	$y,\frac{1}{2},y$ $y,\bar{y},\frac{1}{2}$	$y,\frac{1}{2},\bar{y}$ $\bar{y},\bar{y},\frac{1}{2}$
12	i	$m.m2$	$0,y,y$ $\bar{y},0,y$	$0,\bar{y},y$ $\bar{y},0,\bar{y}$	$0,y,\bar{y}$ $y,y,0$	$0,\bar{y},\bar{y}$ $\bar{y},y,0$	$y,0,y$ $y,\bar{y},0$	$y,0,\bar{y}$ $\bar{y},\bar{y},0$
12	h	$mm2..$	$x,\frac{1}{2},0$ $\frac{1}{2},x,0$	$\bar{x},\frac{1}{2},0$ $\frac{1}{2},\bar{x},0$	$0,x,\frac{1}{2}$ $x,0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$ $\bar{x},0,\frac{1}{2}$	$\frac{1}{2},0,x$ $0,\frac{1}{2},\bar{x}$	$\frac{1}{2},0,\bar{x}$ $0,\frac{1}{2},x$
8	g	$.3m$	x,x,x $x,x,\bar{x}$	$\bar{x},\bar{x},x$ $\bar{x},\bar{x},\bar{x}$	$\bar{x},x,\bar{x}$ $x,\bar{x},x$	$x,\bar{x},\bar{x}$ $\bar{x},x,x$		
6	f	$4m.m$	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x$	$\frac{1}{2},\frac{1}{2},\bar{x}$
6	e	$4m.m$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$
3	d	$4/mm.m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$			
3	c	$4/mm.m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			
1	b	$m\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					
1	a	$m\bar{3}m$	$0,0,0$					

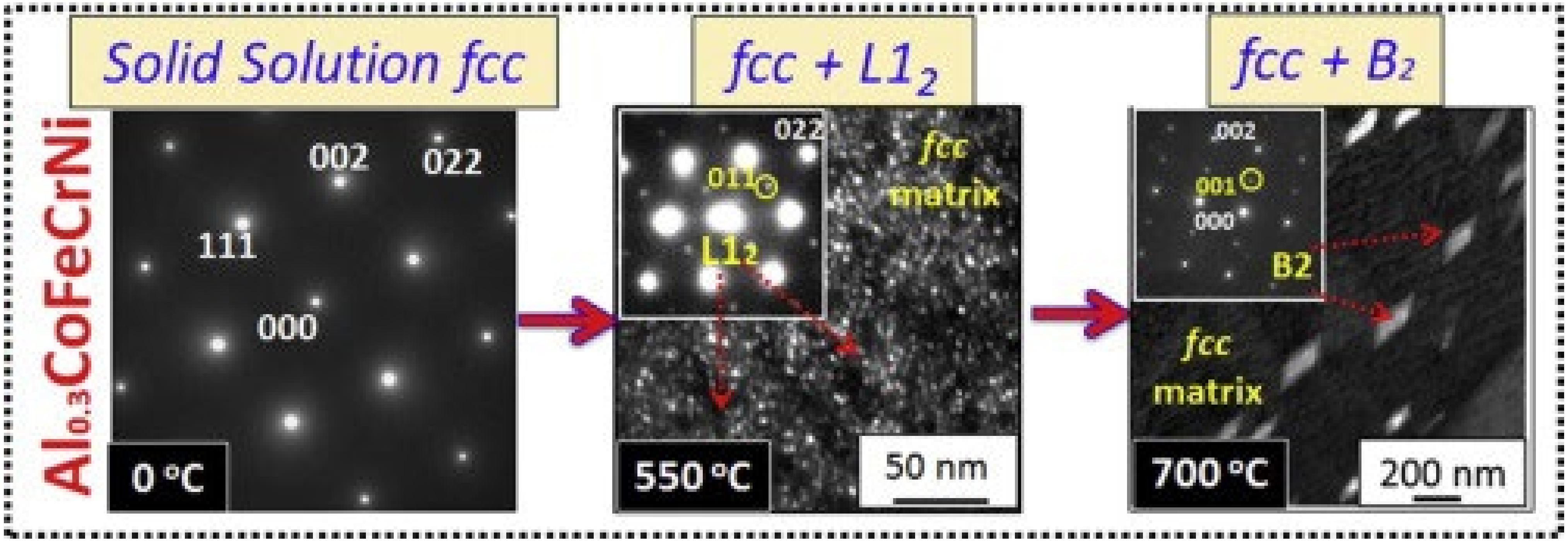
Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

Electron diffraction patterns of FCC and ordered FCC lattice



Ordered FCC (B2 type)

- If (h + k+ l) are even integers:

F_{hkl} =$f_{Al} + f_{Ni}$

- **If (h + k+ l) are odd integers:**

$\boldsymbol{F_{hkl} = f_{Al} - f_{Ni}}$

FCC lattice

- If h, k, l are all even or odd integers

F_{hkl} =f$\{1 + e^{2\pi i} + e^{2\pi i} + e^{2\pi i}\}$=4f

- If h, k, l are in mixed even and odd integers

F_{hkl} =f$\{1 + 2e^{\pi i} + e^{2\pi i}\}$=0

Ordered FCC (L1$_2$ type)

- If h, k, l are all even or odd integers:

F_{hkl} =$f_{Al} + f_{Ni} * \{e^{2\pi i} + e^{2\pi i} + e^{2\pi i}\}$= $f_{Al} + 3f_{Ni}$

- **If h, k, l are in mixed even and odd integers:**

$\boldsymbol{F_{hkl} = f_{Al} + f_{Ni}\{2e^{\pi i} + e^{2\pi i}\} = f_{Al} - f_{Ni}}$

Gwalani, et al, Scripta Materialia 123 (2016) 130-134

✓ How to read and use space group table?

Official label

Schoenflies notation to specify point groups in 3D

Hermann-Mauguin notation to specify point group

Crystal system

$P4/mbm$ D_{4h}^{5} $4/mmm$ Tetragonal

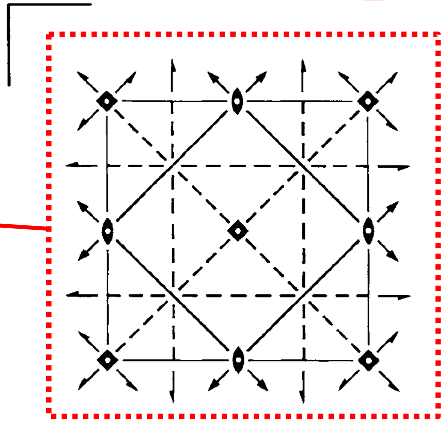
Space group number

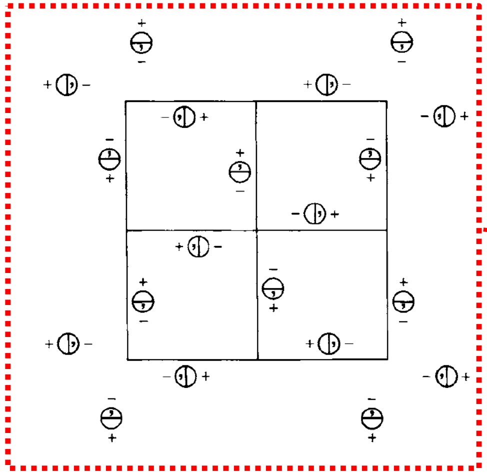
No. 127 $P\ 4/m\ 2_1/b\ 2/m$ Patterson symmetry $P4/mmm$

Full labels

symmetry of Patterson function

Location of symmetry elements





Set of equivalent points in general position

Origin at centre $(4/m)$ at $4/m\,1\,2_1/g$

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{2};\quad y \le \frac{1}{2} - x$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^{+}\quad 0,0,z$	(4) $4^{-}\quad 0,0,z$
(5) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(6) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$	(7) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x,0$	(8) $2\quad x,\bar{x}+\frac{1}{2},0$
(9) $\bar{1}\quad 0,0,0$	(10) $m\quad x,y,0$	(11) $\bar{4}^{+}\quad 0,0,z;\ 0,0,0$	(12) $\bar{4}^{-}\quad 0,0,z;\ 0,0,0$
(13) $a\quad x,\frac{1}{4},z$	(14) $b\quad \frac{1}{4},y,z$	(15) $m\quad x+\frac{1}{2},\bar{x},z$	(16) $g(\frac{1}{2},\frac{1}{2},0)\quad x,x,z$

General catalogs and features of various crystal structures

Crystal Family	Crystal system	Representative symmetry	Lattice parameters	Independent variants	Typical direction	Bravais lattice
Low symmetry	Triclinic	Only 1 or $\bar{1}$	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	6	[100]	P
	Monoclinic	One 2 or $\bar{2}$	Orientation I: $a \neq b \neq c$ $\alpha = \beta = 90°, \gamma \neq 90°$	4	[001]	P, B
			Orientation II: $a \neq b \neq c$ $\alpha = \gamma = 90°, \beta \neq 90°$		[010]	P, C
	Orthorhombic	Three 2 or $\bar{2}$	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	3	[100], [010], [001]	P, C, I, F
Middle symmetry	Tetragonal	One 4 or $\bar{4}$	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$	2	[001], [100], [110]	P, I
	Trigonal	One 3 or $\bar{3}$	Rhombohedral $a = b = c$ $\alpha = \beta = \gamma \neq 90°$	2	[111], [110]	R
			Trigonal $a = b \neq c$ $\alpha = \beta = 120°, \gamma \neq 120°$		[001], [100], [210]	P
	Hexagonal	One 6 or $\bar{6}$	$a = b \neq c$ $\alpha = \beta = 120°, \gamma \neq 120°$	2	[001], [100], [210]	P
High symmetry	Cubic	Four 4 or $\bar{4}$	$a = b = c$ $\alpha = \beta = \gamma = 90°$	1	[001], [111], [110]	P, I, F

- Full space group notation can tell us the existed critical symmetry elements.
- Short space group notation is more concise since combined symmetry elements can generate the other symmetry elements

Primitive lattice

$$P\,\frac{4}{m}\,\frac{2_1}{b}\,\frac{2}{m}$$

1	2	3

1st direction: [001]

4-fold rotation axis along [001]

m reflection perpendicular to [001]

2nd direction: [100]

2-fold screw rotation axis along [100]

b glide reflection perpendicular to [100]

3rd direction: [110]

2-fold rotation axis along [110]

m reflection perpendicular to [110]

Matrix operation for 4-fold axis along [001]

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = W1 * \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{bmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} * \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Matrix operation for b glide reflection perpendicular to [100]

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = W2 * \begin{pmatrix} x \\ y \\ z \end{pmatrix} + t = \begin{bmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} * \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{bmatrix} 0 \\ \frac{1}{2} \\ 0 \end{bmatrix}$$

For general for position having above two operations

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = W1 * \left\{ W2 * \begin{pmatrix} x \\ y \\ z \end{pmatrix} + t \right\} = \begin{bmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} * \left\{ \begin{bmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} * \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{bmatrix} 0 \\ \frac{1}{2} \\ 0 \end{bmatrix} \right\}$$

$$= \begin{bmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{bmatrix} * \left\{ \begin{bmatrix} \bar{x} \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{1}{2} \\ 0 \end{bmatrix} \right\} = \begin{bmatrix} \bar{y} \\ \bar{x} \\ z \end{bmatrix} + \begin{bmatrix} -\frac{1}{2} \\ 0 \\ 0 \end{bmatrix} = - \left\{ \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{bmatrix} * \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{bmatrix} \frac{1}{2} \\ 0 \\ 0 \end{bmatrix} \right\}$$

Operation of screw axis 2^1 along [110] direction

F_{hkl}: structure factor of unit cell

$$F_{hkl} = \sum f_i(\theta) e^{2\pi i(hx_i + ky_i + lz_i)}$$

$$e^{\theta i} = \cos\theta + i\sin\theta$$
$$e^{-\theta i} = \cos\theta - i\sin\theta$$
$$e^{\theta i} + e^{-\theta i} = 2\cos\theta$$

For atoms/cluster at the most general positions:

$$F_{hkl} = f * \{e^{2\pi i(hx+ky+lz)} + e^{2\pi i(-hx-ky+lz)} + e^{2\pi i(-hy+kx+lz)} + e^{2\pi i(hy-kx+lz)} + e^{\pi i(h+k)}[e^{2\pi i(-hx+ky-lz)} + e^{2\pi i(hx-ky-lz)} + e^{2\pi i(hy+kx-lz)} + e^{2\pi i(-hy-kx-lz)}] + e^{-2\pi i(hx+ky+lz)} + e^{-2\pi i(-hx-ky+lz)} + e^{-2\pi i(-hy+kx+lz)} + e^{-2\pi i(hy-kx+lz)} + e^{\pi i(h+k)}[e^{-2\pi i(-hx+ky-lz)} + e^{-2\pi i(hx-ky-lz)} + e^{2\pi i(hy+kx-lz)} + e^{-2\pi i(-hy-kx-lz)}]\}$$

$$= 2f * \{\cos 2\pi(hx+ky+lz) + \cos 2\pi(-hx-ky+lz) + \cos 2\pi(-hy+kx+lz) + \cos 2\pi(hy-kx+lz) + e^{\pi i(h+k)}[\cos 2\pi(-hx+ky-lz) + \cos 2\pi(hx-ky-lz) + \cos 2\pi(hy+kx-lz) + \cos 2\pi(hy+kx+lz)]\}$$

CONTINUED | No. 127 | $P4/mbm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Most general positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	l	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$0kl$: $k=2n$
			(5) $\bar{x}+\frac12,y+\frac12,\bar{z}$	(6) $x+\frac12,\bar{y}+\frac12,\bar{z}$	(7) $y+\frac12,x+\frac12,\bar{z}$	(8) $\bar{y}+\frac12,\bar{x}+\frac12,\bar{z}$	$h00$: $h=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	
			(13) $x+\frac12,\bar{y}+\frac12,z$	(14) $\bar{x}+\frac12,y+\frac12,z$	(15) $\bar{y}+\frac12,\bar{x}+\frac12,z$	(16) $y+\frac12,x+\frac12,z$	
							Special: as above, plus
8	k	$..m$	$x,x+\frac12,z$	$\bar{x},\bar{x}+\frac12,z$	$\bar{x}+\frac12,x,z$	$x+\frac12,\bar{x},z$	no extra conditions
			$\bar{x}+\frac12,x,\bar{z}$	$x+\frac12,\bar{x},\bar{z}$	$x,x+\frac12,\bar{z}$	$\bar{x},\bar{x}+\frac12,\bar{z}$	
8	j	$m..$	$x,y,\frac12$	$\bar{x},\bar{y},\frac12$	$\bar{y},x,\frac12$	$y,\bar{x},\frac12$	no extra conditions
			$\bar{x}+\frac12,y+\frac12,\frac12$	$x+\frac12,\bar{y}+\frac12,\frac12$	$y+\frac12,x+\frac12,\frac12$	$\bar{y}+\frac12,\bar{x}+\frac12,\frac12$	
8	i	$m..$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	no extra conditions
			$\bar{x}+\frac12,y+\frac12,0$	$x+\frac12,\bar{y}+\frac12,0$	$y+\frac12,x+\frac12,0$	$\bar{y}+\frac12,\bar{x}+\frac12,0$	
4	h	$m.2m$	$x,x+\frac12,\frac12$	$\bar{x},\bar{x}+\frac12,\frac12$	$\bar{x}+\frac12,x,\frac12$	$x+\frac12,\bar{x},\frac12$	no extra conditions
4	g	$m.2m$	$x,x+\frac12,0$	$\bar{x},\bar{x}+\frac12,0$	$\bar{x}+\frac12,x,0$	$x+\frac12,\bar{x},0$	no extra conditions
4	f	$2.mm$	$0,\frac12,z$	$\frac12,0,z$	$\frac12,0,\bar{z}$	$0,\frac12,\bar{z}$	hkl : $h+k=2n$
4	e	$4..$	$0,0,z$	$\frac12,\frac12,\bar{z}$	$0,0,\bar{z}$	$\frac12,\frac12,z$	hkl : $h+k=2n$
2	d	$m.mm$	$0,\frac12,0$	$\frac12,0,0$			hkl : $h+k=2n$
2	c	$m.mm$	$0,\frac12,\frac12$	$\frac12,0,\frac12$			hkl : $h+k=2n$
2	b	$4/m..$	$0,0,\frac12$	$\frac12,\frac12,\frac12$			hkl : $h+k=2n$
2	a	$4/m..$	$0,0,0$	$\frac12,\frac12,0$			hkl : $h+k=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \frac12\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac12(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4bm$ (100)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P42_12$ (90)	1; 2; 3; 4; 5; 6; 7; 8

$$= 2f * \{\cos 2\pi(hx + ky + lz) + \cos 2\pi(-hx - ky + lz) +$$
$$\cos 2\pi(-hy + kx + lz) + \cos 2\pi(hy - kx + lz) +$$
$$e^{\pi i(h+k)}[\cos 2\pi(-hx + ky - lz) + \cos 2\pi(hx - ky - lz) +$$
$$\cos 2\pi(hy + kx - lz) + \cos 2\pi(hy + kx + lz)]\}$$
$$= 4f * \cos 2\pi lz * \{\cos 2\pi(hx + ky) + \cos 2\pi(-hy + kx) +$$
$$e^{\pi i(h+k)}[\cos 2\pi(-hx + ky) + \cos 2\pi(hy + kx)]\}$$

$$\cos(\alpha + \beta) = \cos\alpha\cos\beta - \sin\alpha\sin\beta$$
$$\cos(\alpha - \beta) = \cos\alpha\cos\beta + \sin\alpha\sin\beta$$
$$\cos(\alpha + \beta) - \cos(\alpha - \beta) = 2\cos\alpha\cos\beta$$

$$e^{\theta i} = \cos\theta + i\sin\theta$$
$$e^{\pi i} = \cos\pi + i\sin\pi = -1$$
$$e^{2\pi i} = \cos 2\pi + i\sin 2\pi = 1$$

Let us consider crystal planes (hkl) with special cases:

- For (hkl) with special cases k=l=0, namely types of (h,0,0)

F= $4f * \{\cos 2\pi hx + \cos 2\pi hy + e^{\pi ih}[\cos 2\pi hx + \cos 2\pi hy]\}$

If h=even numbers, F=0; (reflection rule resulted from the screw axis 2^1 operation along [100] direction)

- For (hkl) with special cases h=0, namely types of (0,k,l)

F=$4f * \cos 2\pi lz * \{\cos 2\pi ky + \cos 2\pi kx + e^{\pi ik}[\cos 2\pi ky + \cos 2\pi kx]\}$

If k=even numbers, F=0; (reflection rule resulted from the b glide reflection operation perpendicular to [100] direction)

CONTINUED No. 127 $P4/mbm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry | Coordinates | Reflection conditions

16 *l* 1

				Reflection conditions
(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	General:
(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$0kl$: $k=2n$
(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	$h00$: $h=2n$
(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$	

For initial atoms located at general position (x, y, z):

$$F = 4f * \cos 2\pi lz * \{\cos 2\pi(hx + ky) + \cos 2\pi(-hy + kx) + e^{\pi i(h+k)}[\cos 2\pi(-hx + ky) + \cos 2\pi(hy + kx)]\}$$

Let us consider atoms/clusters located at special positions (x, y, z) with x=y=z=0

$$F = 8f * \{1 + e^{\pi i(h+k)}\}$$

- For (hkl) with h+k=even numbers, F=0

$$e^{\pi i} = \cos \pi + i \sin \pi = -1$$
$$e^{2\pi i} = \cos 2\pi + i \sin 2\pi = 1$$

CONTINUED No. 127 $P4/mbm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity	Wyckoff letter	Site symmetry	Coordinates				Reflection conditions
							General:
16	l	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$0kl$: $k=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$h00$: $h=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$	
							Special: as above, plus
8	k	$..m$	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z$	$x+\frac{1}{2},\bar{x},z$	no extra conditions
			$\bar{x}+\frac{1}{2},x,\bar{z}$	$x+\frac{1}{2},\bar{x},\bar{z}$	$x,x+\frac{1}{2},\bar{z}$	$\bar{x},\bar{x}+\frac{1}{2},\bar{z}$	
8	j	$m..$	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	no extra conditions
			$\bar{x}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$y+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	
8	i	$m..$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	no extra conditions
			$\bar{x}+\frac{1}{2},y+\frac{1}{2},0$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},0$	$y+\frac{1}{2},x+\frac{1}{2},0$	$\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},0$	
4	h	$m.2m$	$x,x+\frac{1}{2},\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x,\frac{1}{2}$	$x+\frac{1}{2},\bar{x},\frac{1}{2}$	no extra conditions
4	g	$m.2m$	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x,0$	$x+\frac{1}{2},\bar{x},0$	no extra conditions
4	f	$2.mm$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	hkl : $h+k=2n$
4	e	$4..$	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hkl : $h+k=2n$
2	d	$m.mm$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl : $h+k=2n$
2	c	$m.mm$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h+k=2n$
2	b	$4/m..$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	a	$4/m..$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k=2n$

Special positions with x=y=z

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4bm$ (100)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P42_12$ (90)	1; 2; 3; 4; 5; 6; 7; 8

$$= f * \{8 + e^{\pi i(h+k)}[e^{2\pi i(-hx+ky-lz)} + e^{2\pi i(hx-ky-lz)} + e^{2\pi i(hy+kx-lz)} + e^{2\pi i(-hy-kx-lz)}] + $$
$$+ e^{\pi i(h+k)}[e^{-2\pi i(-hx+ky-lz)} + e^{-2\pi i(hx-ky-lz)} + e^{-2\pi i(hy+kx-lz)} + e^{-2\pi i(-hy-kx-lz)}]\}$$
$$= 8f * \{1 + e^{\pi i(h+k)}\}$$

- ❑ For any reflection (hkl), if h+k are odd numbers, F=16f

For (0kl) type, k must be odd number; (reflection rule resulted from the b glide reflection operation perpendicular to [100] direction)

For (h00) type, h must be odd number; (reflection rule resulted from the screw axis 2^1 operation along [100] direction)

- ❑ For any reflection (hkl), if h+k are even numbers, F=0

❖ **Only partial lattice translation** **(Face centered lattice, Body centered lattice, side centered lattice)** **and symmetry operation having partial translations** **(glide reflections and screw axes)** **can cause lattice extinction.**

CONTINUED   No. 127 $P4/mbm$

Reflection conditions

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	l	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$0kl$: $k=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$h00$: $h=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$	
							Special: as above, plus
8	k	$..m$	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z$	$x+\frac{1}{2},\bar{x},z$	no extra conditions
			$\bar{x}+\frac{1}{2},x,\bar{z}$	$x+\frac{1}{2},\bar{x},\bar{z}$	$x,x+\frac{1}{2},\bar{z}$	$\bar{x},\bar{x}+\frac{1}{2},\bar{z}$	
8	j	$m..$	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	no extra conditions
			$\bar{x}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$y+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	
8	i	$m..$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	no extra conditions
			$\bar{x}+\frac{1}{2},y+\frac{1}{2},0$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},0$	$y+\frac{1}{2},x+\frac{1}{2},0$	$\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},0$	
4	h	$m.2m$	$x,x+\frac{1}{2},\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x,\frac{1}{2}$	$x+\frac{1}{2},\bar{x},\frac{1}{2}$	no extra conditions
4	g	$m.2m$	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x,0$	$x+\frac{1}{2},\bar{x},0$	no extra conditions
4	f	$2.mm$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	hkl : $h+k=2n$
4	e	$4..$	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hkl : $h+k=2n$
2	d	$m.mm$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl : $h+k=2n$
2	c	$m.mm$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h+k=2n$
2	b	$4/m..$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	a	$4/m..$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I
[2] $P\bar{4}b2$ (117)   1; 2; 7; 8; 11; 12; 13; 14
[2] $P\bar{4}2_1m$ (113)   1; 2; 5; 6; 11; 12; 15; 16
[2] $P4bm$ (100)   1; 2; 3; 4; 13; 14; 15; 16
[2] $P42_12$ (90)   1; 2; 3; 4; 5; 6; 7; 8

Let us move on to a real structure

D5a-M_3B_2 boride: (M=Cr, Mo, Fe)
Space group: No. 127, P4/mbm
Lattice parameter: a=b=5.7 Å, c=3.0 Å

Atomic locations:
M: 4h, 0.173, 0.673, 0
M: 2a, 0, 0, 0
B: 4g, 0.388, 0.888, 0

For 4h position, $y=x+\frac{1}{2}$, $z=\frac{1}{2}$

$$F_{4h} = 4f * \cos 2\pi lz * \{\cos 2\pi(hx+ky) + \cos 2\pi(-hy+kx) + e^{\pi i(h+k)}[\cos 2\pi(-hx+ky) + \cos 2\pi(hy+kx)]\}$$

$$= 4f * \cos \pi l * \{\cos[2\pi(h+k)x + k\pi] + \cos[2\pi(k-h)x + h\pi]) + e^{\pi i(h+k)}[\cos[2\pi(k-h)x + k\pi] + \cos[2\pi(h+k)x + h\pi]]\}$$

CONTINUED No. 127 $P4/mbm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	l	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (9) $\bar{x},\bar{y},\bar{z}$ (13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (10) $x,y,\bar{z}$ (14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(3) $\bar{y},x,z$ (7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$ (11) $y,\bar{x},\bar{z}$ (15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(4) $y,\bar{x},z$ (8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$ (12) $\bar{y},x,\bar{z}$ (16) $y+\frac{1}{2},x+\frac{1}{2},z$	$0kl$: $k=2n$ $h00$: $h=2n$
							Special: as above, plus
8	k	$..m$	$x,x+\frac{1}{2},z$ $\bar{x}+\frac{1}{2},x,\bar{z}$	$\bar{x},\bar{x}+\frac{1}{2},z$ $x+\frac{1}{2},\bar{x},\bar{z}$	$\bar{x}+\frac{1}{2},x,z$ $x,x+\frac{1}{2},\bar{z}$	$x+\frac{1}{2},\bar{x},z$ $\bar{x},\bar{x}+\frac{1}{2},\bar{z}$	no extra conditions
8	j	$m..$	$x,y,\frac{1}{2}$ $\bar{x}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$ $x+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$\bar{y},x,\frac{1}{2}$ $y+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$ $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	no extra conditions
8	i	$m..$	$x,y,0$ $\bar{x}+\frac{1}{2},y+\frac{1}{2},0$	$\bar{x},\bar{y},0$ $x+\frac{1}{2},\bar{y}+\frac{1}{2},0$	$\bar{y},x,0$ $y+\frac{1}{2},x+\frac{1}{2},0$	$y,\bar{x},0$ $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},0$	no extra conditions
4	h	$m.2m$	$x,x+\frac{1}{2},\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x,\frac{1}{2}$	$x+\frac{1}{2},\bar{x},\frac{1}{2}$	no extra conditions
4	g	$m.2m$	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x,0$	$x+\frac{1}{2},\bar{x},0$	no extra conditions
4	f	$2.mm$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	hkl : $h+k=2n$
4	e	$4..$	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hkl : $h+k=2n$
2	d	$m.mm$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl : $h+k=2n$
2	c	$m.mm$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h+k=2n$
2	b	$4/m..$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	a	$4/m..$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k=2n$

Symmetry of special projections

Hu, et al, Scientific reports 4 (2014), 7367

Let us move on to a real structure

D5a-M_3B_2 boride: (M=Cr, Mo, Fe)
Space group: No. 127, P4/mbm
Lattice parameter: a=b=5.7 Å, c=3.0 Å

Atomic locations:
M: 4h, 0.173, 0.673, 0
M: 2a, 0, 0, 0
B: 4g, 0.388, 0.888, 0

For 4g position, $y = x + \frac{1}{2}$, z= 0

$$F_{4g} = 4f * \cos 2\pi lz * \{\cos 2\pi(hx+ky) + \cos 2\pi(-hy+kx) + e^{\pi i(h+k)}[\cos 2\pi(-hx+ky) + \cos 2\pi(hy+kx)]\}$$

$$= 4f * \{\cos[2\pi(h+k)x + k\pi] + \cos[2\pi(k-h)x + h\pi]) + e^{\pi i(h+k)}[\cos[2\pi(k-h)x + k\pi] + \cos[2\pi(h+k)x + h\pi]]\}$$

CONTINUED No. 127 $P4/mbm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	l	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (9) $\bar{x},\bar{y},\bar{z}$ (13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (10) $x,y,\bar{z}$ (14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(3) $\bar{y},x,z$ (7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$ (11) $y,\bar{x},\bar{z}$ (15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(4) $y,\bar{x},z$ (8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$ (12) $\bar{y},x,\bar{z}$ (16) $y+\frac{1}{2},x+\frac{1}{2},z$	$0kl$: $k=2n$ $h00$: $h=2n$
							Special: as above, plus
8	k	$..m$	$x,x+\frac{1}{2},z$ $\bar{x}+\frac{1}{2},x,\bar{z}$	$\bar{x},\bar{x}+\frac{1}{2},z$ $x+\frac{1}{2},\bar{x},\bar{z}$	$\bar{x}+\frac{1}{2},x,z$ $x,x+\frac{1}{2},\bar{z}$	$x+\frac{1}{2},\bar{x},z$ $\bar{x},\bar{x}+\frac{1}{2},\bar{z}$	no extra conditions
8	j	$m..$	$x,y,\frac{1}{2}$ $\bar{x}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$ $x+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$\bar{y},x,\frac{1}{2}$ $y+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$ $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	no extra conditions
8	i	$m..$	$x,y,0$ $\bar{x}+\frac{1}{2},y+\frac{1}{2},0$	$\bar{x},\bar{y},0$ $x+\frac{1}{2},\bar{y}+\frac{1}{2},0$	$\bar{y},x,0$ $y+\frac{1}{2},x+\frac{1}{2},0$	$y,\bar{x},0$ $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},0$	no extra conditions
4	h	$m.2m$	$x,x+\frac{1}{2},\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x,\frac{1}{2}$	$x+\frac{1}{2},\bar{x},\frac{1}{2}$	no extra conditions
4	g	$m.2m$	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x,0$	$x+\frac{1}{2},\bar{x},0$	no extra conditions
4	f	$2.mm$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	hkl : $h+k=2n$
4	e	$4..$	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hkl : $h+k=2n$
2	d	$m.mm$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl : $h+k=2n$
2	c	$m.mm$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h+k=2n$
2	b	$4/m..$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	a	$4/m..$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k=2n$

Symmetry of special projections

Let us move on to a real structure

D5a-M_3B_2 boride: (M=Cr, Mo, Fe)
Space group: No. 127, P4/mbm
Lattice parameter: a=b=5.7 Å, c=3.0 Å

Atomic locations:
M: 4h, 0.173, 0.673, 0
M: 2a, 0, 0, 0
B: 4g, 0.388, 0.888, 0

For 2a position, x=y=z=0

$$F_{2a} = 4f * \cos 2\pi l z * \{\cos 2\pi(hx+ky) + \cos 2\pi(-hy+kx) + e^{\pi i(h+k)}[\cos 2\pi(-hx+ky) + \cos 2\pi(hy+kx)]\}$$

$$= 4f * \{2 + 2e^{\pi i(h+k)}\}$$

CONTINUED No. 127 $P4/mbm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity	Wyckoff letter	Site symmetry	Coordinates				Reflection conditions
							General:
16	l	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$0kl$: $k=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$h00$: $h=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$	
							Special: as above, plus
8	k	$..m$	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z$	$x+\frac{1}{2},\bar{x},z$	no extra conditions
			$\bar{x}+\frac{1}{2},x,\bar{z}$	$x+\frac{1}{2},\bar{x},\bar{z}$	$x,x+\frac{1}{2},\bar{z}$	$\bar{x},\bar{x}+\frac{1}{2},\bar{z}$	
8	j	$m..$	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	no extra conditions
			$\bar{x}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$y+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	
8	i	$m..$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	no extra conditions
			$\bar{x}+\frac{1}{2},y+\frac{1}{2},0$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},0$	$y+\frac{1}{2},x+\frac{1}{2},0$	$\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},0$	
4	h	$m.2m$	$x,x+\frac{1}{2},\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x,\frac{1}{2}$	$x+\frac{1}{2},\bar{x},\frac{1}{2}$	no extra conditions
4	g	$m.2m$	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x,0$	$x+\frac{1}{2},\bar{x},0$	no extra conditions
4	f	$2.mm$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	hkl : $h+k=2n$
4	e	$4..$	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hkl : $h+k=2n$
2	d	$m.mm$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl : $h+k=2n$
2	c	$m.mm$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h+k=2n$
2	b	$4/m..$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	a	$4/m..$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl : $h+k=2n$

Symmetry of special projections

NUANCE
Northwestern University Atomic and Nanoscale Characterization Experimental Center

Hu, et al, Scientific reports 4 (2014), 7367

Northwestern
EXPLORING INNER SPACE

For M_5B_2 phase:

$F_{M5B3} = F_{4h}^{M} + F_{4g}^{B} + F_{2a}^{M}$

$= 4(f_M * \cos\pi l + f_B) * \{\cos[2\pi(h+k)x + k\pi] + \cos[2\pi(k-h)x + h\pi]) +$

$e^{\pi i(h+k)}[\cos[2\pi(k-h)x + k\pi] + \cos[2\pi(h+k)x + h\pi]]\}$

$+ 4f_M * \{2 + 2e^{\pi i(h+k)}\}$

D5a-M_3B_2 boride: (M=Cr, Mo, Fe)
Space group: No. 127, P4/mbm
Lattice parameter: a=b=5.7 Å, c=3.0 Å

Atomic locations:
M: 4h, 0.173, 0.673, 0
M: 2a, 0, 0, 0
B: 4g, 0.388, 0.888, 0

- For (hkl) with special cases k=l=0, namely types of (h,0,0)

$F_{M5B3} = F_{4h}^{M} + F_{4g}^{B} + F_{2a}^{M}$

$= 4(f_M + f_B) * \{\cos 2\pi hx + \cos[2\pi(-h)x + h\pi]) +$

$e^{\pi i h}[\cos[2\pi(-h)x] + \cos[2\pi hx + h\pi]]\}$

$+ 4f_M * \{2 + 2e^{\pi i h}\}$

If h=even numbers, F=0; (reflection rule resulted from the screw axis 2^1 operation along [100] direction)

- For (hkl) with special cases h=0, namely types of (0,k,l)

$F_{M5B3} = F_{4h}^{M} + F_{4g}^{B} + F_{2a}^{M}$

$= 4(f_M * \cos\pi l + f_B) * \{\cos 2\pi(kx + k\pi) + \cos 2\pi kx +$

$e^{\pi i \boldsymbol{k}}[\cos 2\pi(kx + k\pi) + \cos 2\pi kx]\}$

$+ 4f_M * \{2 + 2e^{\pi i \boldsymbol{k}}\}$

If k=even numbers, F=0; (reflection rule resulted from the b glide reflection operation perpendicular to [100] direction)

Extinction rule for space group of P4/mbm:

D5a-M_3B_2 boride: (M=Cr, Mo, Fe)
Space group: No. 127, P4/mbm
Lattice parameter: a=b=5.7 Å, c=3.0 Å

Extinction rule at general positions:

- For (hkl) with special cases k=l=0, namely types of (h,0,0)

If h=even numbers, F=0; (reflection rule resulted from the screw axis 2^1 operation along [100] direction)

- For (hkl) with special cases h=0, namely types of (0,k,l)

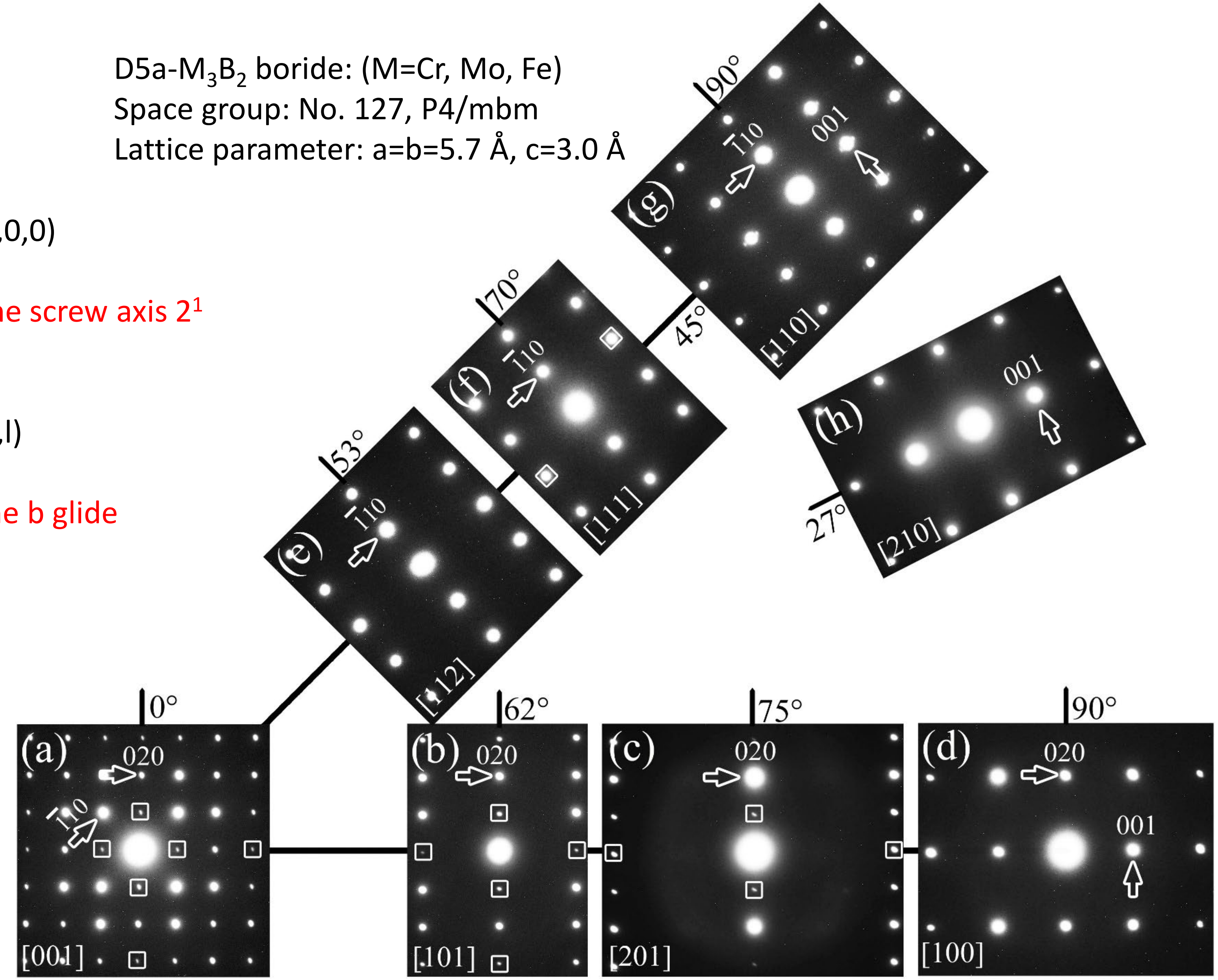
If k=even numbers, F=0; (reflection rule resulted from the b glide reflection operation perpendicular to [100] direction)

Extincted reflection: (100),(300), (010), (030)
Existed reflection: (200),(110), (120), (210)

(110) + (010) = (120)

(110) + (100) = (210)

Kinematics forbidden but occurred due to dynamically effect



Hu, et al, Scientific reports 4 (2014), 7367

Reflection rules for structure with various operation elements

Operation elements		Translation vector (t)	Reflection rule
Inversion	$\bar{1}$	Not Appliable	Not Appliable
Reflection	m		
Rotation axis	2, $\bar{2}$		
	3, $\bar{3}$		
	4, $\bar{4}$, 6, $\bar{6}$		

Operation element			Symmetry direction/plane	Translation vector (t)	Reflection rule
Pure translation	Face centered	F	N.A.	$\frac{a+b}{2}, \frac{a+c}{2}, \frac{b+c}{2}$	(h, k, l) with h + k, k + l, and h + l = 2n
	Body centered	I		$\frac{a+b+c}{2}$	(h, k, l) with h + k + l = 2n
	rhombohedral centered	R		$\frac{2a+b+c}{3}, \frac{a+2b+2c}{3}$	(h, k, l) with -h + k + l = 3n
	Side centered	A		$\frac{b+c}{2}$	(0, k, l) with k + l = 2n
		B		$\frac{a+c}{2}$	(h, 0, l) with h + l = 2n
		C		$\frac{a+b}{2}$	(h, k, 0) with h + k = 2n
Screw axis (rotation + translation)	3-fold basis	3_1, 3_2	[001]	$\pm\frac{c}{3}$	(0, 0, l) with l = 3n
	4-fold basis	4_1, 4_3	[100]; [010]; [001]	$\pm\frac{a}{4}; \pm\frac{b}{4}; \pm\frac{c}{4}$	(h, 0, 0) with h = 4n; (0, k, 0) with k = 4n; (0, 0, l) with l = 4n
		4_2	[100]; [010]; [001]	$\pm\frac{a}{2}; \pm\frac{b}{2}; \pm\frac{c}{2}$	(h, 0, 0) with h = 2n; (0, k, 0) with k = 2n; (0, 0, l) with l = 2n
	6-fold basis	6_1, 6_5	[001]	$\pm\frac{c}{6}$	(0, 0, l) with l= 6n
		6_2, 6_4		$\pm\frac{c}{3}$	(0, 0, l) with l= 3n
		6_3		$\frac{c}{2}$	(0, 0, l) with l= 2n
Glide reflection (reflection + translation)	Simple glide	a	(010); (001)	$\frac{a}{2}$	(h, 0, l) with h= 2n; (h, k, 0) with h= 2n
		b	(100); (001)	$\frac{b}{2}$	(0, k, l) with k= 2n; (h, k, 0) with k= 2n
		c	(100); (010)	$\frac{c}{2}$	(0, k, l) with l= 2n; (h, 0, l) with l= 2n
	Diagonal glide	n	(100); (010); (001)	$\frac{b+c}{2}; \frac{a+c}{2}; \frac{a+b}{2}$	(0, k, l) with k + l= 2n; (h, 0, l) with h + l= 2n; (h, k, 0) with h + k= 2n
			(110)	$\frac{a+b+c}{2}$	(h, h, l) with l= 2n
		d	(100); (010); (001)	$\frac{b+c}{4}; \frac{a+c}{4}; \frac{a+b}{4}$	(0, k, l) with k + l= 4n; (h, 0, l) with h + l= 4n; (h, k, 0) with h + k= 4n
			(110)	$\frac{a+b+c}{4}$	(h, h, l) with 2h + l=4n

Thank you for your attention!

Contact Information:
Email: xbhu@northwestern.edu
Office: Tech Building Ground Floor JG14
Phone: 847-467-4992

Q.&A.