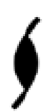
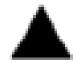
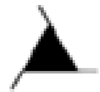
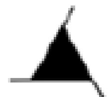
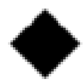
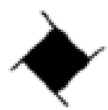
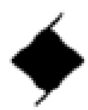
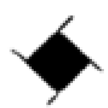
第八章 空间群图表的认识与使用

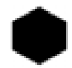
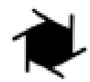
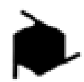
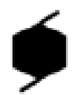
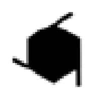
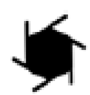
对称操作符号　必考！！　P 10-11页

SYMBOLS OF SYMMETRY AXES

Symmetry axes normal to the plane of projection (three dimensions) and symmetry points in the plane of the figure (two dimensions)

Symmetry axis or symmetry point	Graphical symbol	Screw vector of a right-handed screw rotation in units of the shortest lattice translation vector parallel to the axis	Printed symbol
Identity	None	None	1
Twofold rotation axis Twofold rotation point (two dimensions)		None	2
Twofold screw axis: '2 sub 1'		$^1/_2$	2_1

Threefold rotation axis Threefold rotation point (two dimensions)		None	3
Threefold screw axis: '3 sub 1'		$^1/_3$	3_1
Threefold screw axis: '3 sub 2'		$^2/_3$	3_2
Fourfold rotation axis Fourfold rotation point (two dimensions)		None	4
Fourfold screw axis: '4 sub 1'		$^1/_4$	4_1
Fourfold screw axis: '4 sub 2'		$^1/_2$	4_2
Fourfold screw axis: '4 sub 3'		$^3/_4$	4_3

Sixfold rotation axis Sixfold rotation point (two dimensions)		None	6
Sixfold screw axis: '6 sub 1'		$^{1}/_{6}$	6_1
Sixfold screw axis: '6 sub 2'		$^{1}/_{3}$	6_2
Sixfold screw axis: '6 sub 3'		$^{1}/_{2}$	6_3
Sixfold screw axis: '6 sub 4'		$^{2}/_{3}$	6_4
Sixfold screw axis: '6 sub 5'		$^{5}/_{6}$	6_5

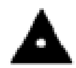
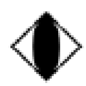
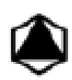
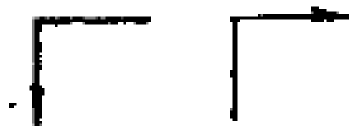
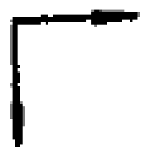
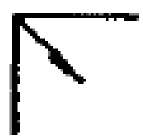
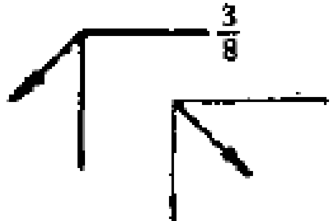
Centre of symmetry, inversion centre: ‘1 bar’ Reflection point, mirror point (one dimension)		None	$\bar{1}$
Inversion axis: ‘3 bar’		None	$\bar{3}$
Inversion axis: ‘4 bar’		None	$\bar{4}$
Inversion axis: ‘6 bar’		None	$\bar{6}$

表 1-3 对称面的符号

(a) 垂直于投影面的对称面

对称面	图示符号	滑移矢量(以平行于和垂直于投影面的点阵平移矢量为单位)	印刷符号
镜 面	——	无	m
轴 向 滑移面	- - - - -	平行于投影面某方向的 $\frac{1}{2}$	a, b 或 c
轴 向 滑移面	············	垂直于投影面方向的 $\frac{1}{2}$	a, b 或 c
对 角 滑移面	-·-·-·-	平行于投影面某方向的 $\frac{1}{2}$ 加上垂直于投影面方向的 $\frac{1}{2}$	n
金刚石 滑移面 (一对面，仅出现于有心晶胞中)	-·-·←·- -·-·→·-	平行于投影面某方向的 $\frac{1}{4}$ 加上垂直于投影面方向的 $\frac{1}{4}$(箭头指示平行于投影面的方向，此时垂直分量为正)	d

(b) 平行于投影面的对称面

对称面	图示符号[1]	滑移矢量(以平行于投影面的点阵平移矢量为单位)	印刷符号
镜　面	 $\frac{1}{4}$	无	m
轴向滑移面		箭头方向的 $\frac{1}{2}$	a, b 或 c
轴向滑移面		任一箭头方向的 $\frac{1}{2}$	a, b 或 c
对角滑移面		箭头方向的 $\frac{1}{2}$	n
金刚石滑移面(一对面，仅出现于有心晶胞中)	 $\frac{3}{8}$ $\frac{1}{8}$	箭头方向的 $\frac{1}{2}$。滑移矢量总是面心矢量或体心矢量之半，也就是惯用晶胞的对角线的 $\frac{1}{4}$	d

2

2_1

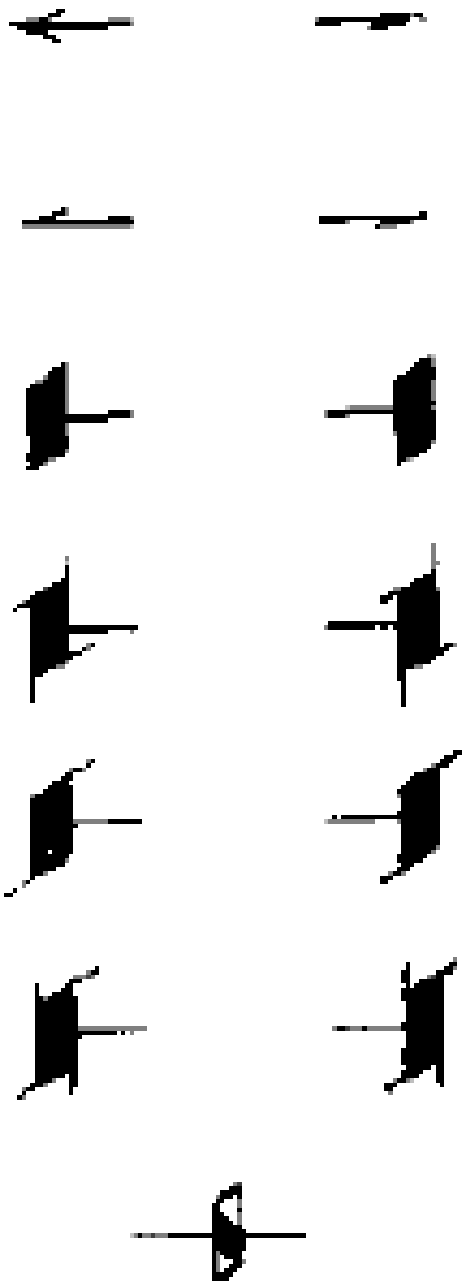
4

4_1

4_2

4_3

$\bar{4}$



平行于投影面的对称轴的图示符号

立方晶系特有的对称元素的图示符号

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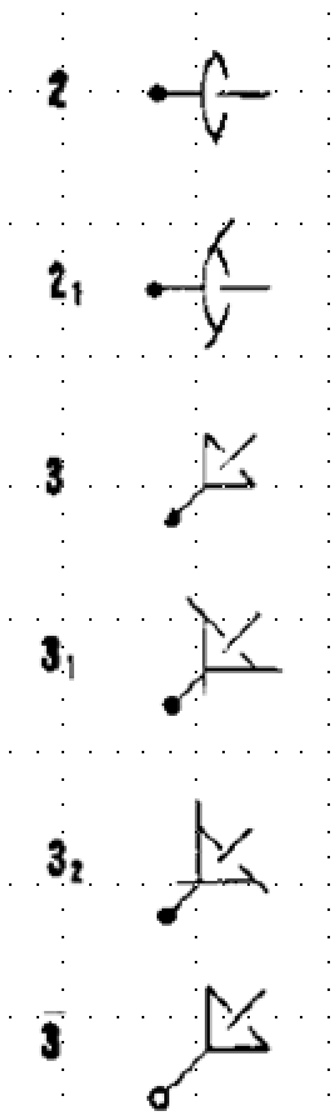
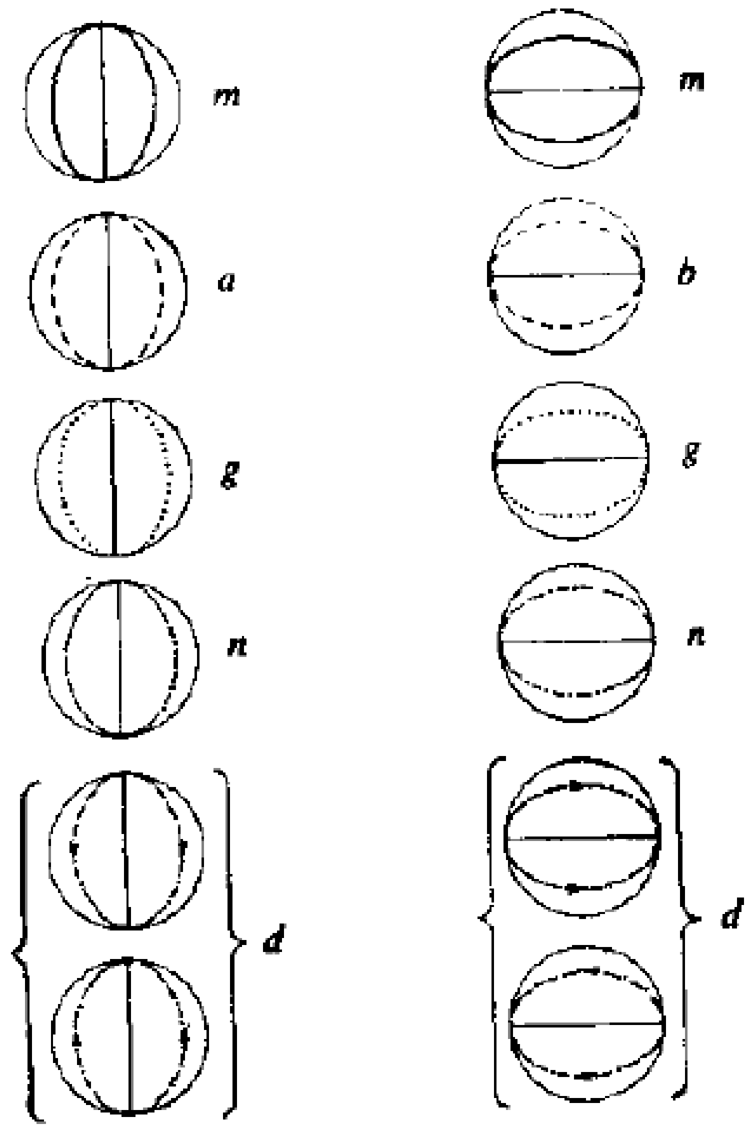




(a) (b)

第八章 空间群图表的认识与使用

P186-187， $Cmm2$ (35)

P188-189， $C2/c$ (15)

P190-191， $C2/c$ 三种不同的单胞选择

P192-194， $Fddd$ (70)

P196-198， $Fddd$ 不同的原点选择

P210， $P\bar{4}3m$ (218)

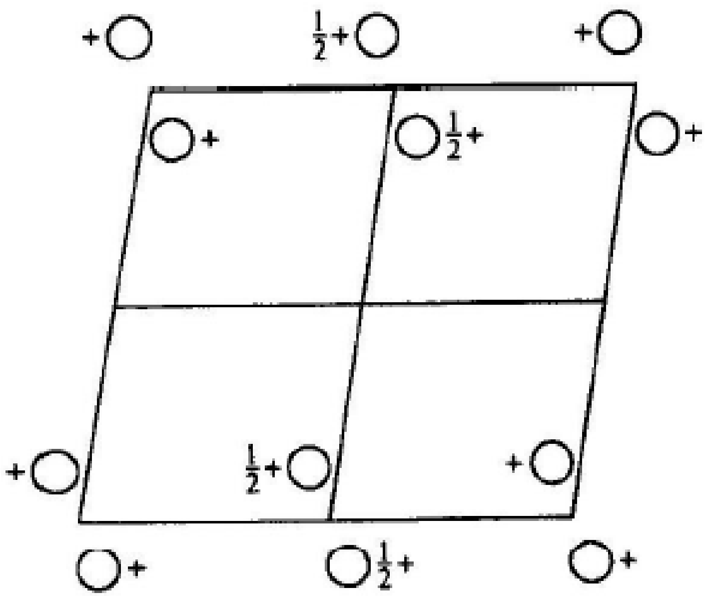
分发的 $Pbca$ (61)

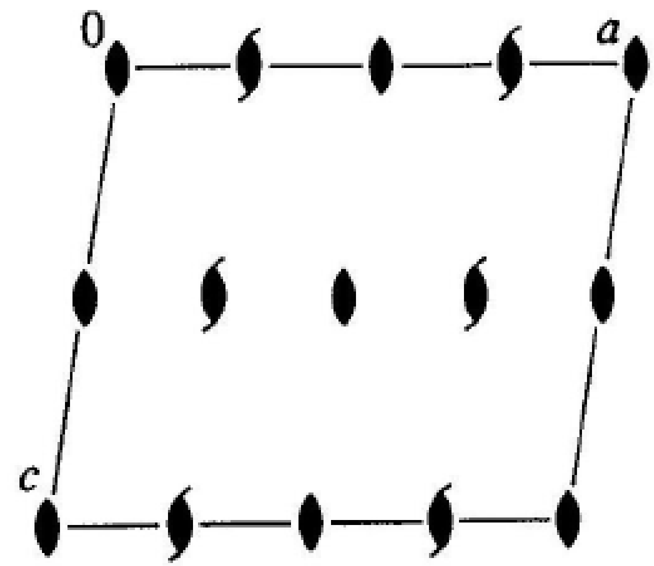
$C2$　　唯一性轴?　简略HM符号

完全HM符号:$C121$; $C211$;

$C2$	C_2^3	2	Monoclinic
No. 5	$C121$		Patterson symmetry $C12/m1$

UNIQUE AXIS b, CELL CHOICE 1



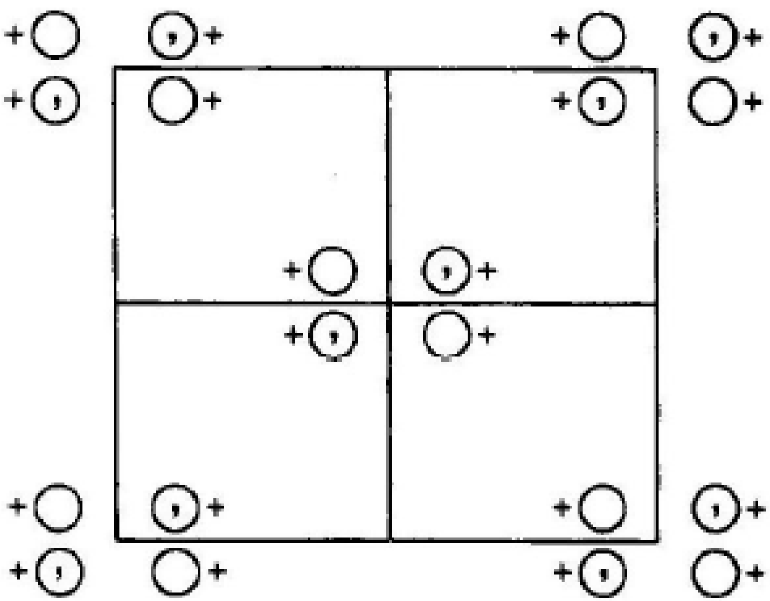


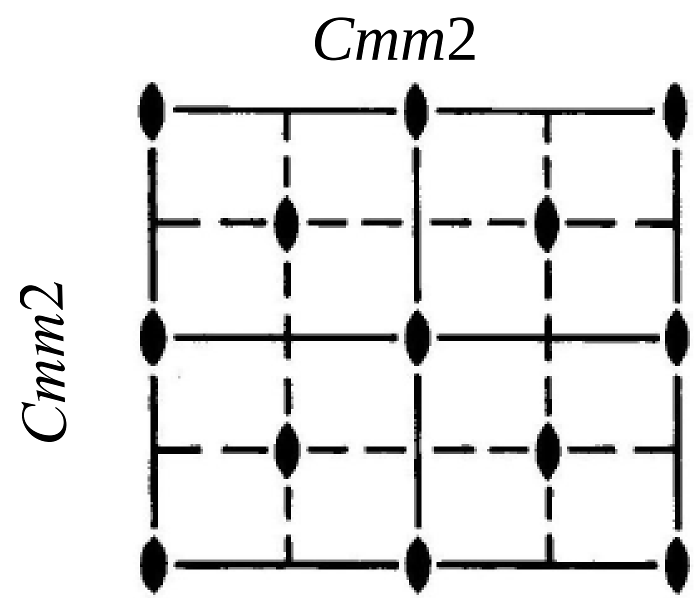
扩展HM符号：C 1 2 1; C 2 1 1

1 2_1 1　　2_1 1 1

*Cmm*2 C_{2v}^{11} *mm*2 Orthorhombic

No. 35 *Cmm*2 Patterson symmetry *Cmmm*

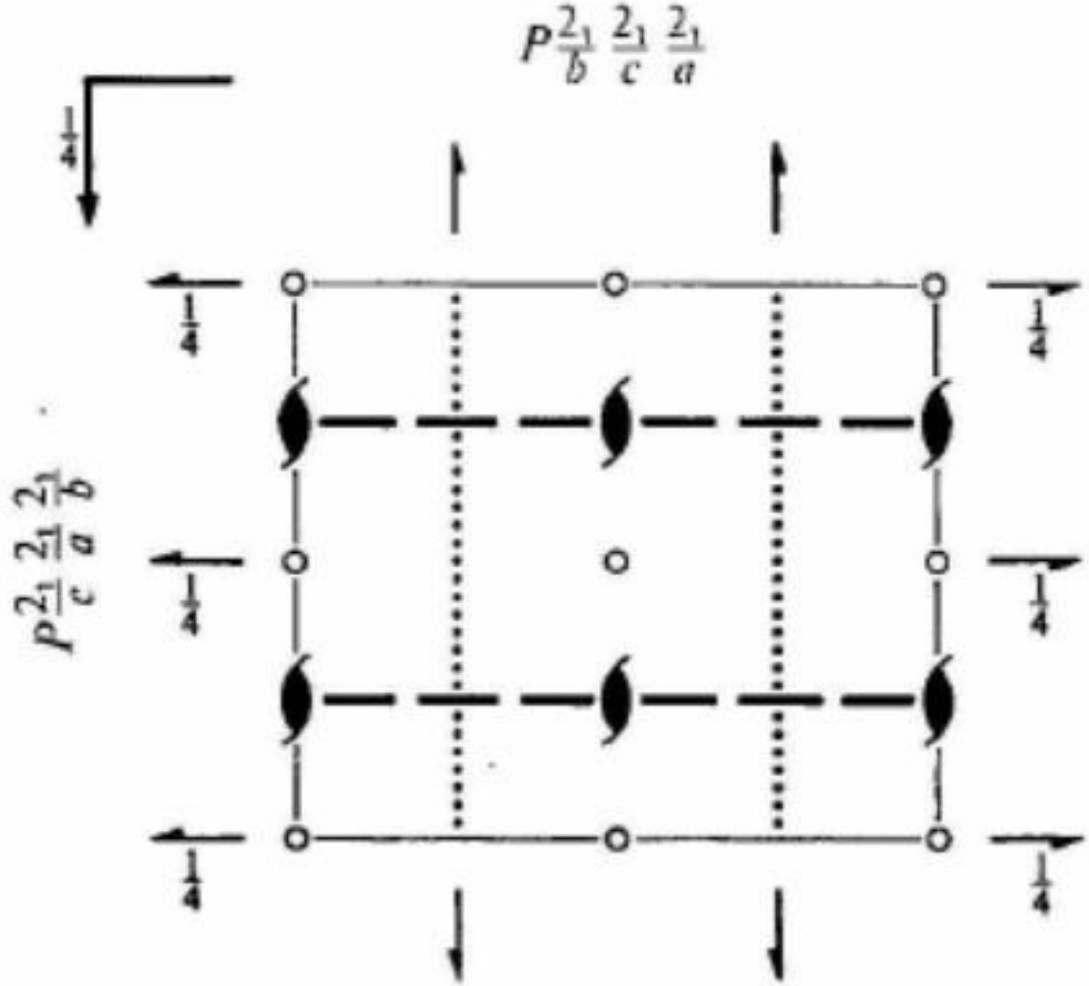




扩展HM符号：$\begin{matrix} C & m & m & 2 \\ & b & a & 2 \end{matrix}$

$Pbca$ D_{2h}^{15} mmm Orthorhombic

No. 61 $P\ 2_1/b\ 2_1/c\ 2_1/a$ Patterson symmetry $Pmmm$



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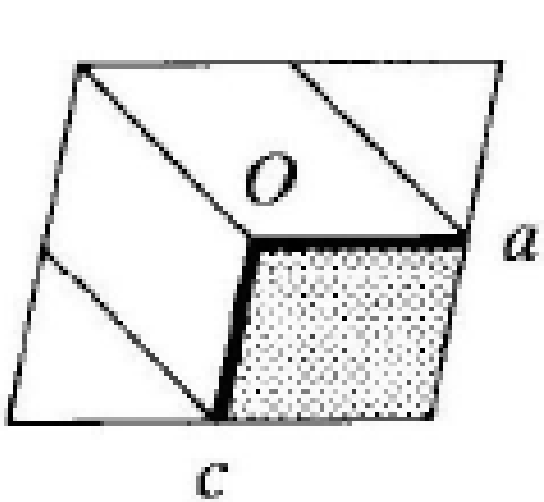
附表 7(b) 单斜晶系

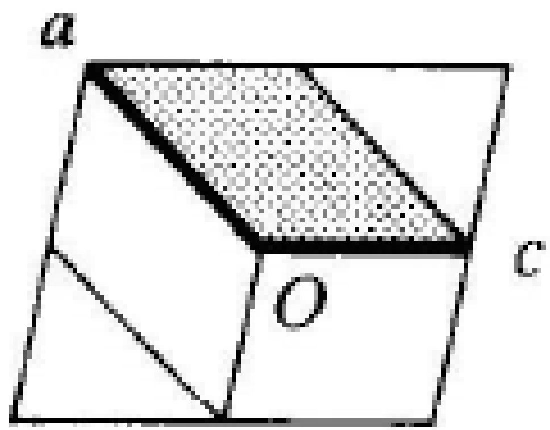
空间群序号	Schoenflies 符号	标准的简略 Hermann-Mauguin 符号	各种定向和单胞选择的扩展 Hermann-Mauguin 符号						
			$a\underline{b}c$	$c\bar{b}a$					唯一性轴 b
					$ab\underline{c}$	$ba\bar{c}$			唯一性轴 c
							$\underline{a}bc$	$\bar{a}cb$	唯一性轴 a
3	C_2^1	$P2$	$P1\ 2\ 1$	$P1\ 2\ 1$	$P1\ 1\ 2$	$P1\ 1\ 2$	$P\ 2\ 1\ 1$	$P\ 2\ 1\ 1$	
4	C_2^2	$P2_1$	$P1\ 2_1\ 1$	$P1\ 2_1\ 1$	$P1\ 1\ 2_1$	$P1\ 1\ 2_1$	$P\ 2_1\ 1\ 1$	$P\ 2_1\ 1\ 1$	
5	C_2^3	$C2$	$C1\ 2\ 1$ 2_1	$A1\ 2\ 1$ 2_1	$A1\ 1\ 2$ 2_1	$B1\ 1\ 2$ 2_1	$B\ 2\ 1\ 1$ 2_1	$C\ 2\ 1\ 1$ 2_1	单胞选择 1
			$A1\ 2\ 1$ 2_1	$C1\ 2\ 1$ 2_1	$B1\ 1\ 2$ 2_1	$A1\ 1\ 2$ 2_1	$C\ 2\ 1\ 1$ 2_1	$B\ 2\ 1\ 1$ 2_1	单胞选择 2
			$I1\ 2\ 1$ 2_1	$I1\ 2\ 1$ 2_1	$I1\ 1\ 2$ 2_1	$I1\ 1\ 2$ 2_1	$I\ 2\ 1\ 1$ 2_1	$I\ 2\ 1\ 1$ 2_1	单胞选择 3

单斜晶系中不同的单胞选择



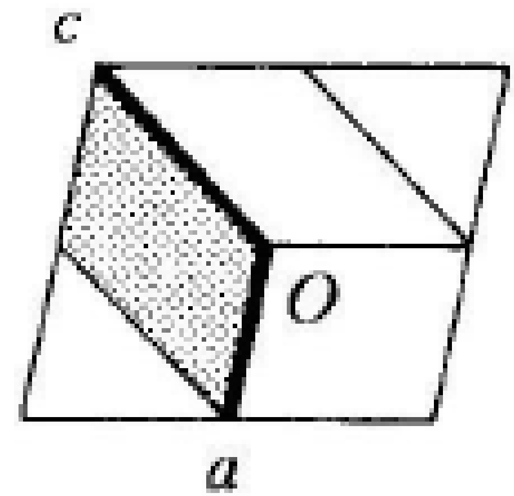
单胞选择1

C121



单胞选择2

A121

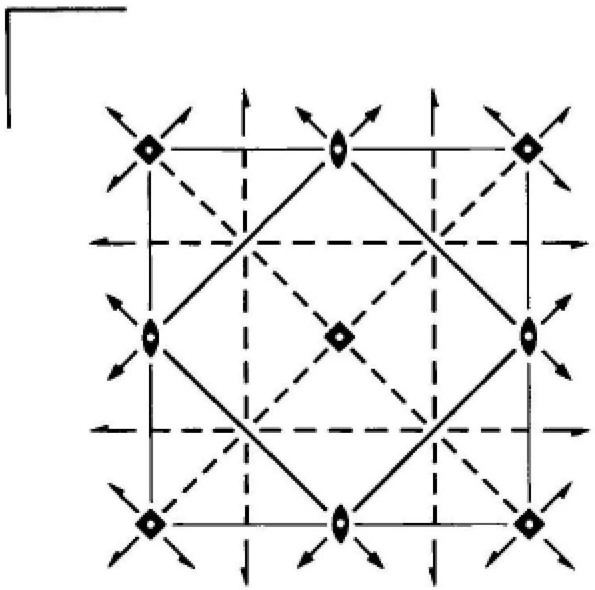


单胞选择3

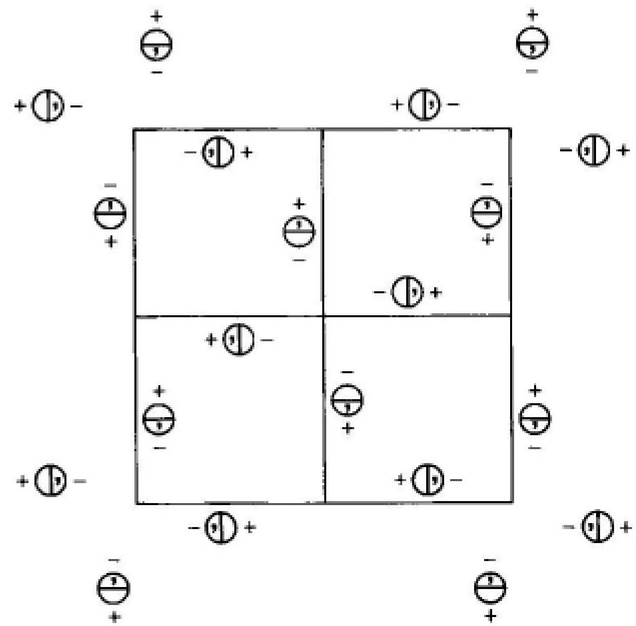
I121

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

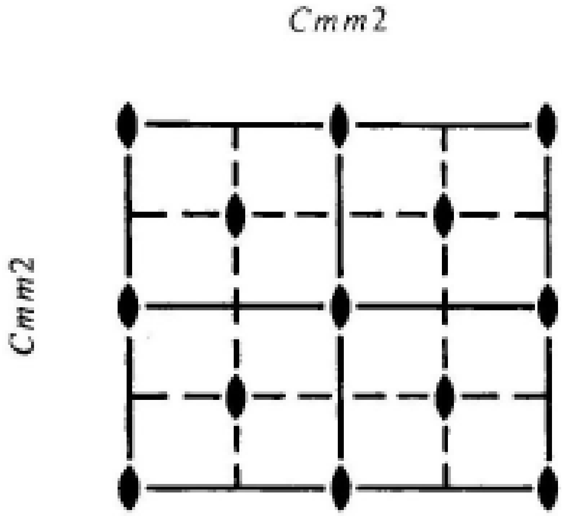
No. 127 $P\ 4/m\ 2_1/b\ 2/m$ Patterson symmetry $P4/mmm$

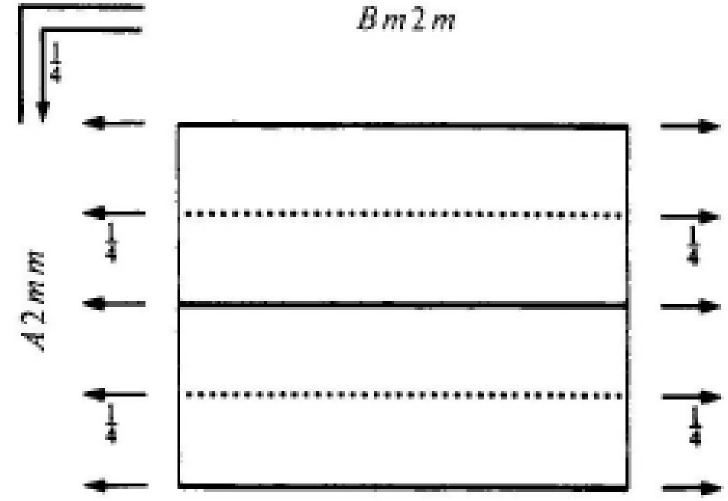


对称元素配置图

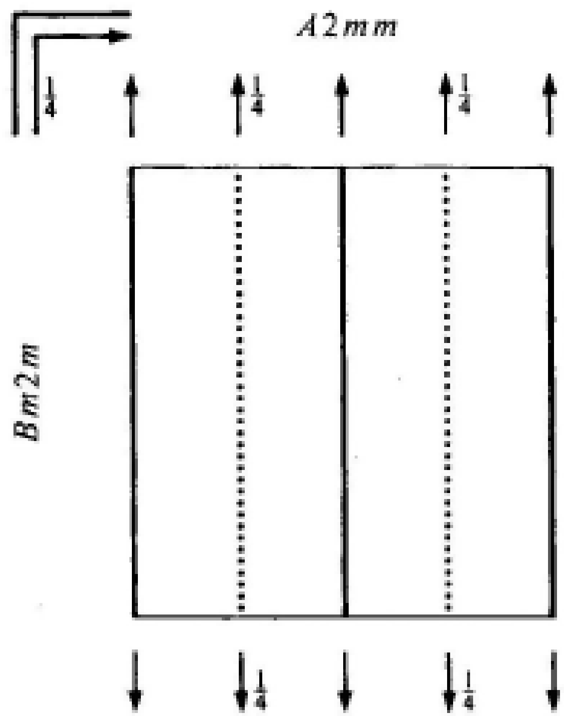


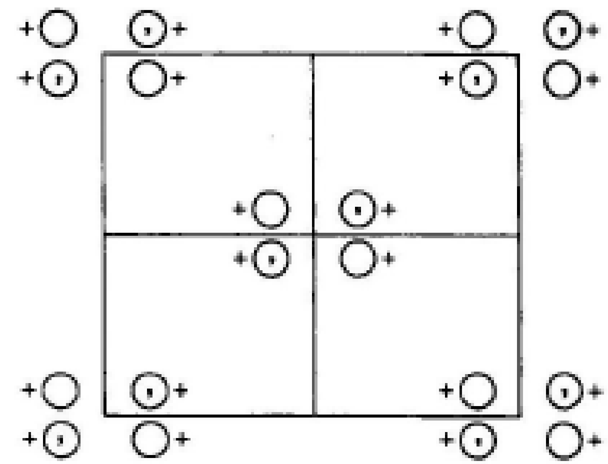
一般等效位置配置图

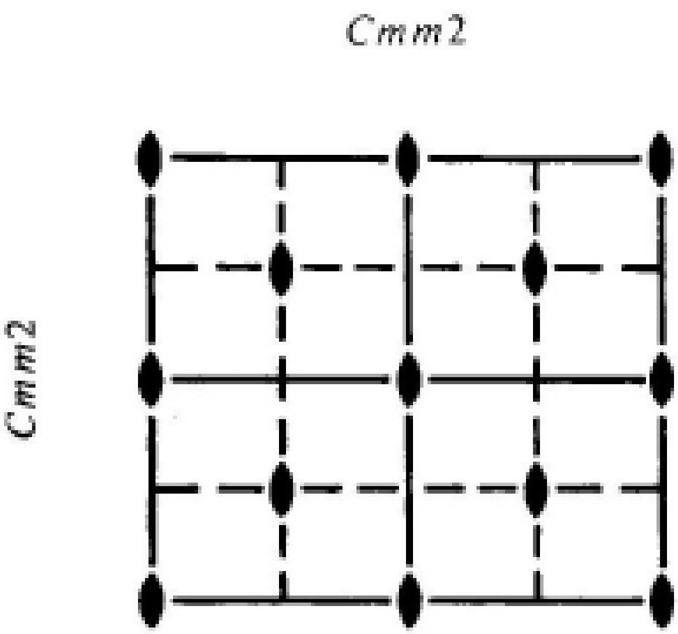


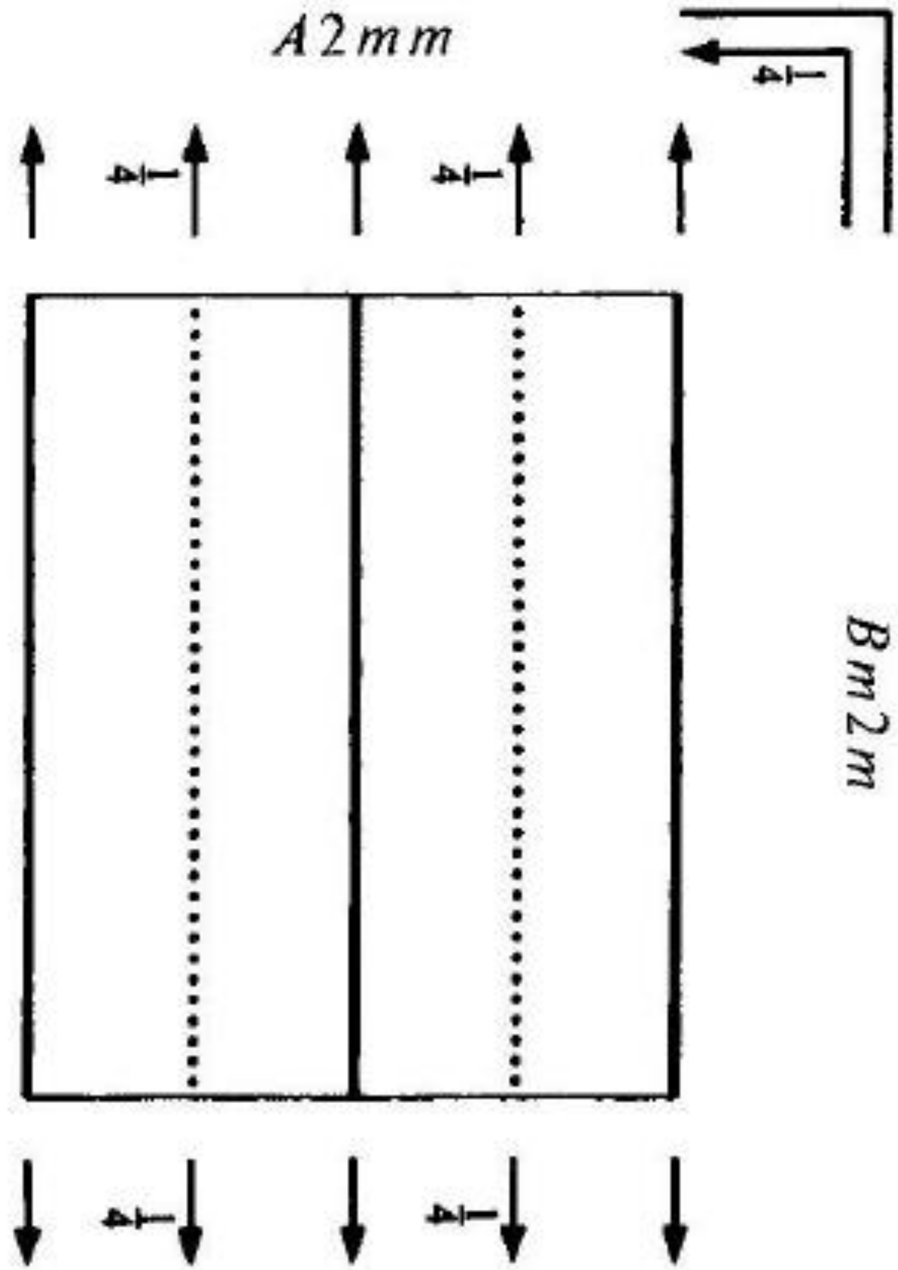


P186-187， *Cmm*2 (35)

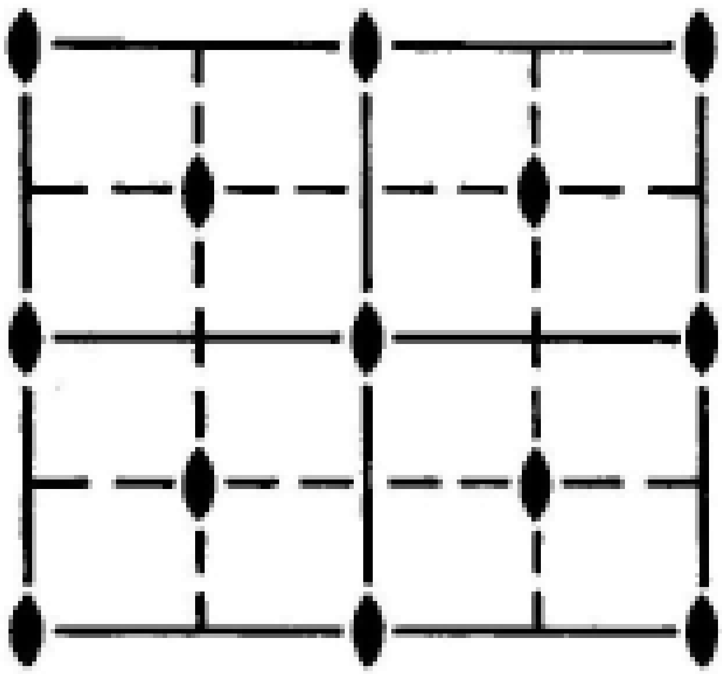





Cmm2
Cmm2

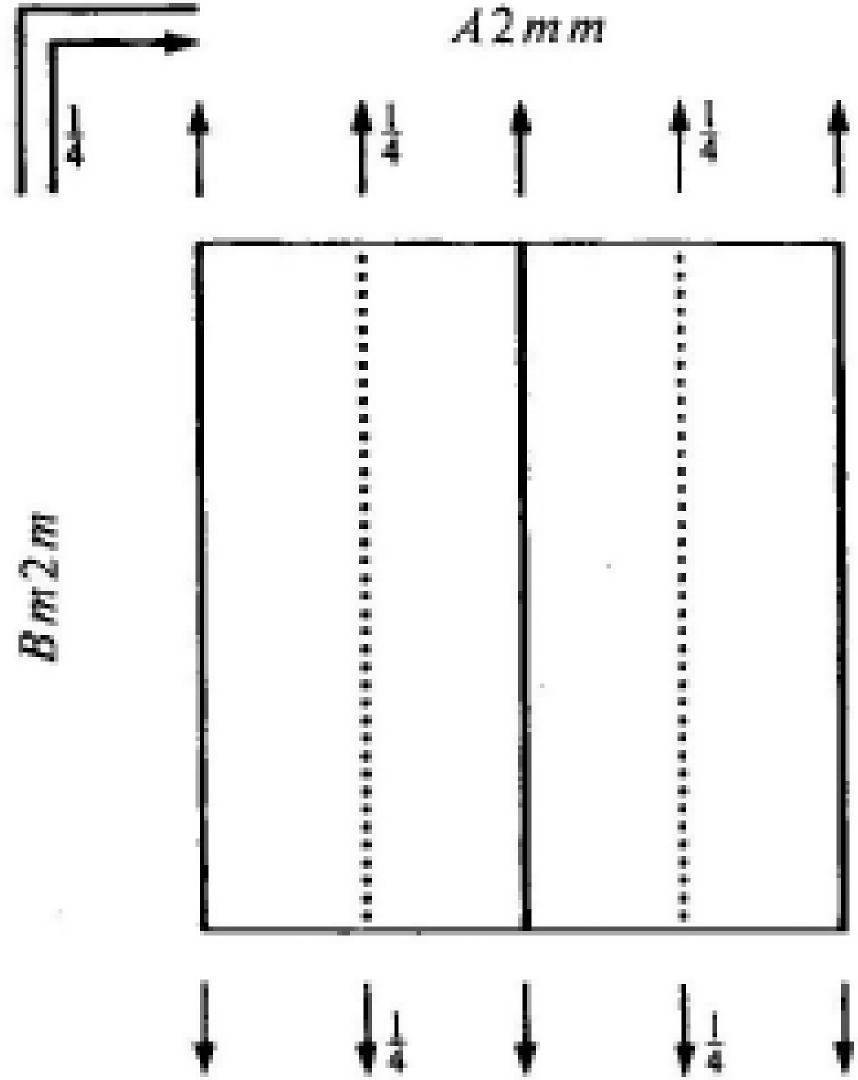

A2mm
Bm2m

*Cmm*2



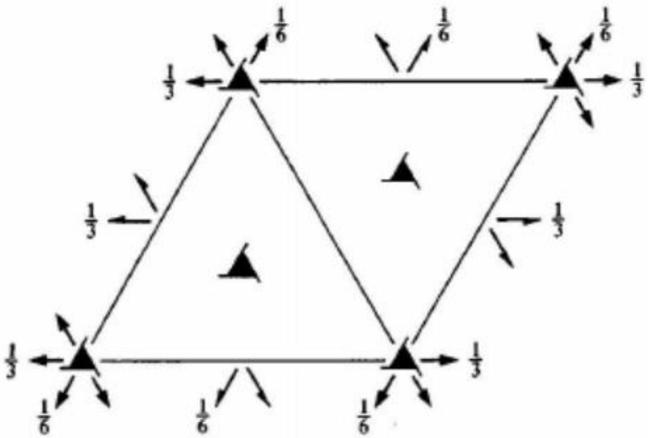
*A*2*mm*

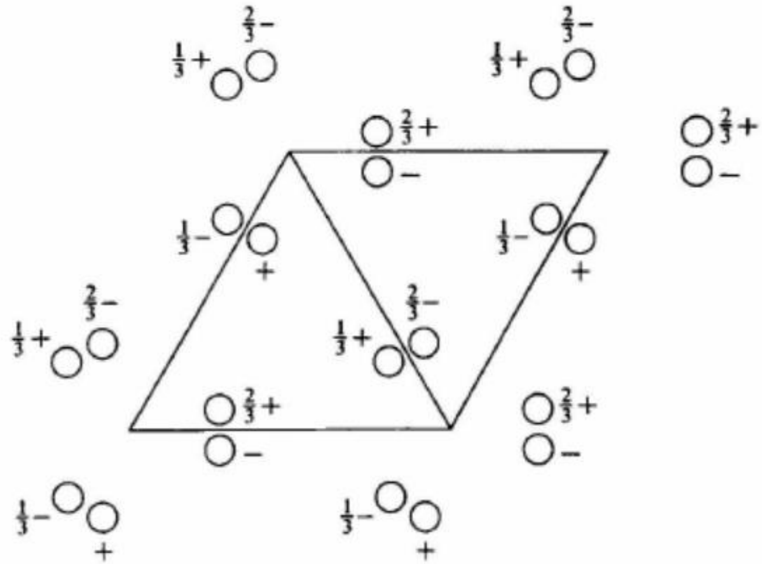
*Bm*2*m*



$P\,3_2\,2\,1$ D_3^6 $3\,2\,1$ Trigonal

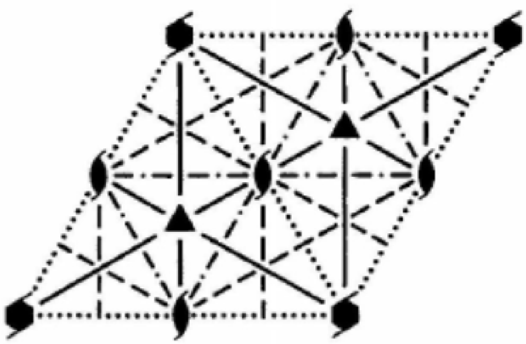
No. 154 $P\,3_2\,2\,1$ Patterson symmetry $P\,\bar{3}\,m\,1$

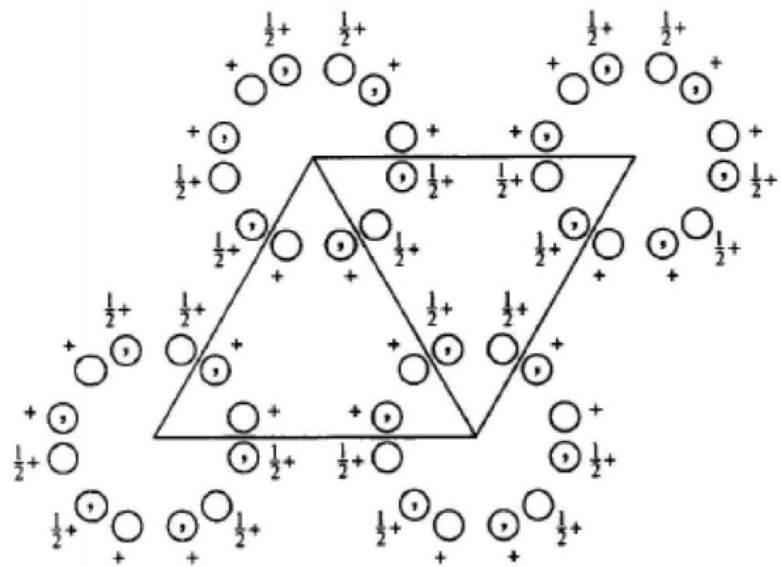




$P6_3mc$ C_{6v}^4 $6mm$ Hexagonal

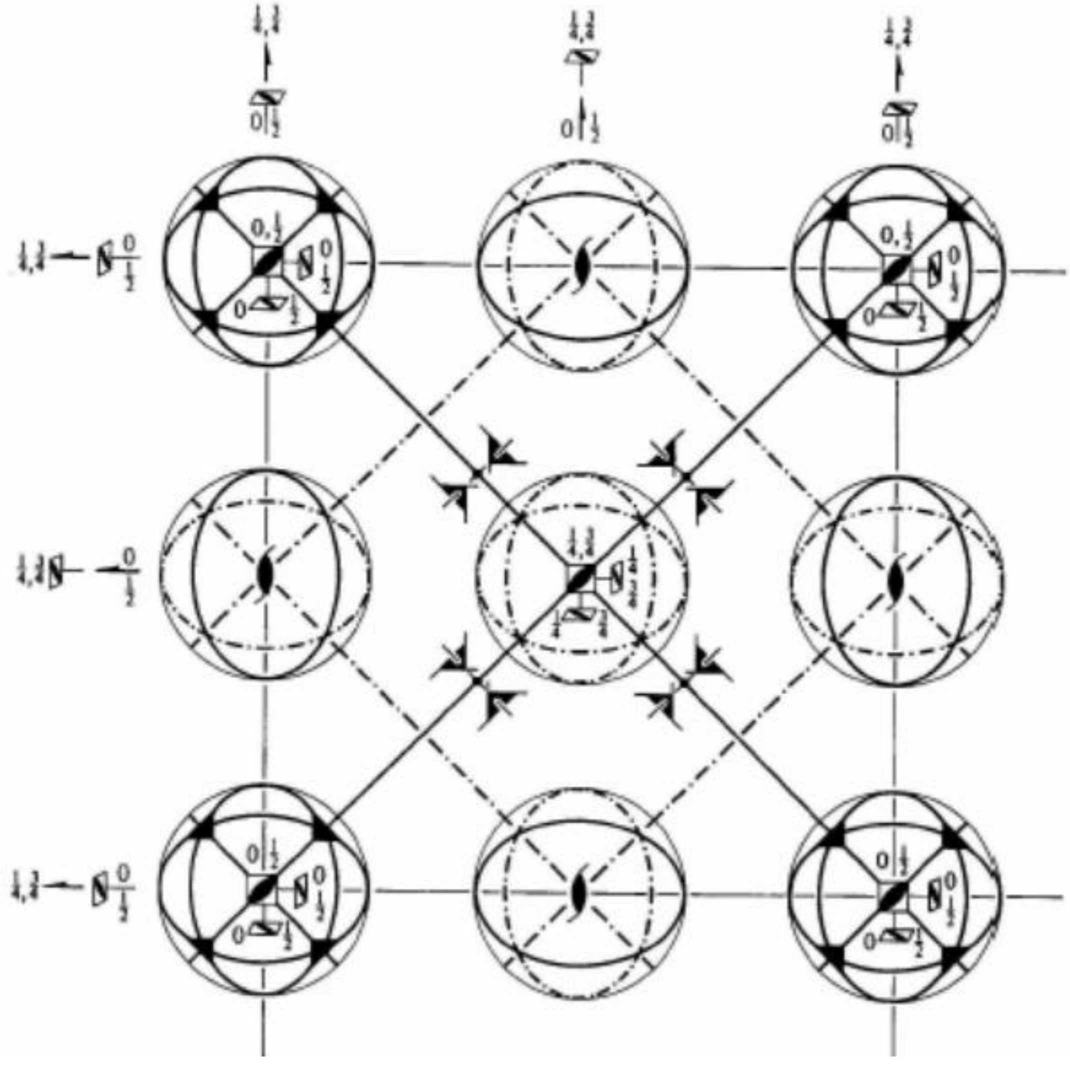
No. 186 $P6_3mc$ Patterson symmetry $P6/mmm$





$F\bar{4}3m$ T_d^2 $\bar{4}3m$ Cubic

No. 216 $F\bar{4}3m$ Patterson symmetry $Fm\bar{3}m$



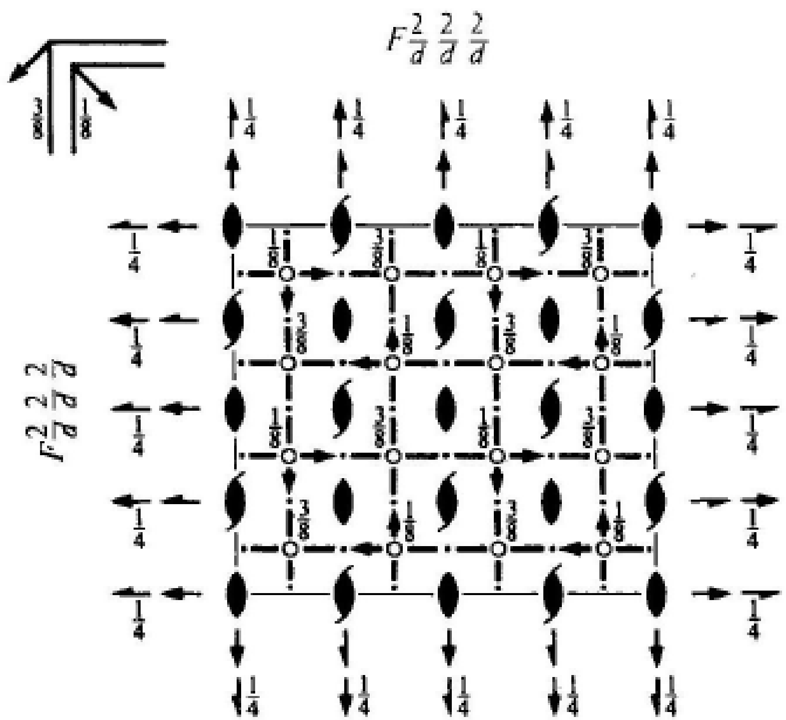
不同原点的选择

P192-194， *Fddd* （70）

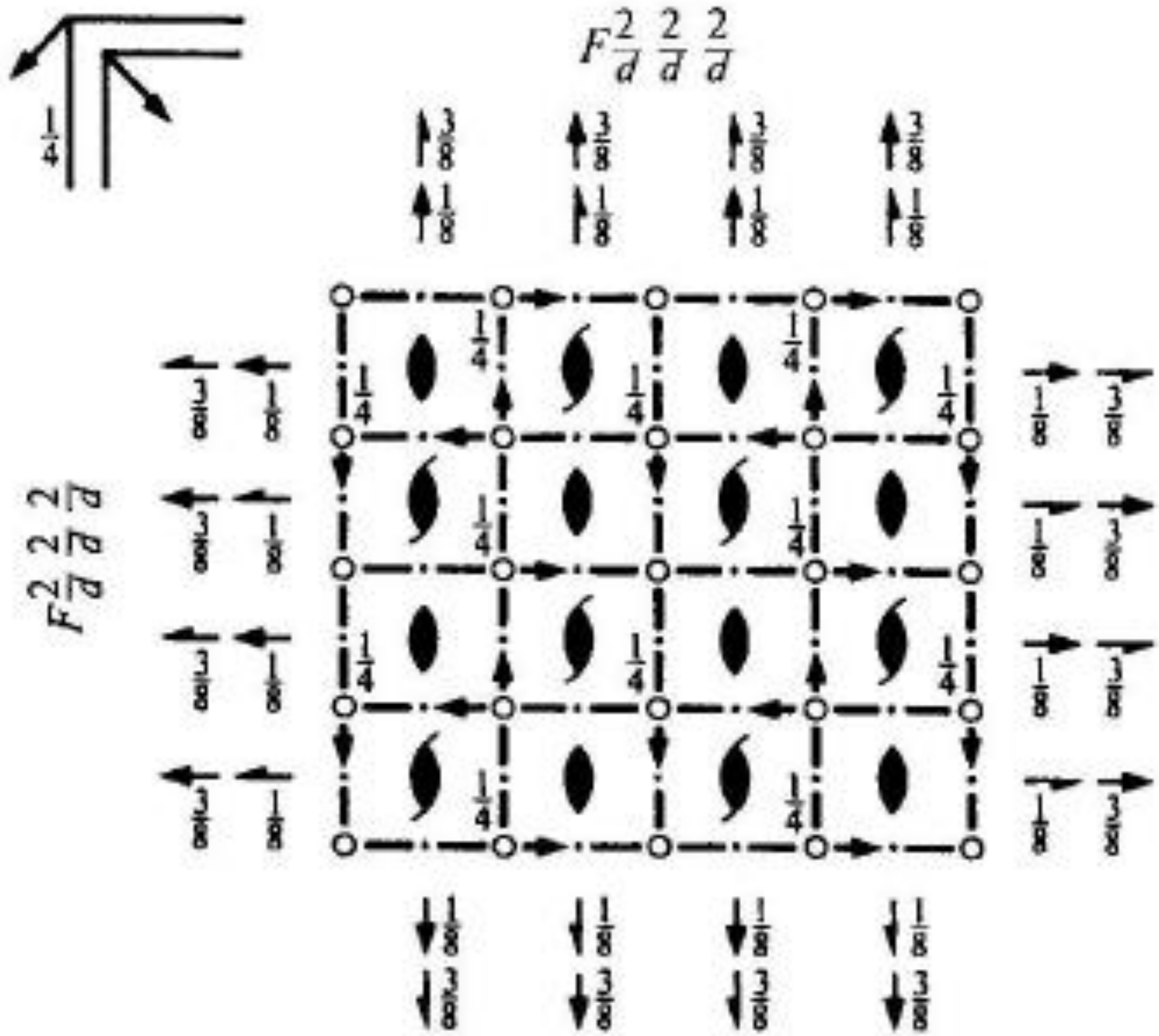
$F\,d\,d\,d$ $\quad$ D_{2h}^{24}

No. 70 $\quad$ $F\ 2/d\ 2/d\ 2/d$

ORIGIN CHOICE 1 $\quad$ **Origin** at 222, at $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}$ from $\bar{1}$



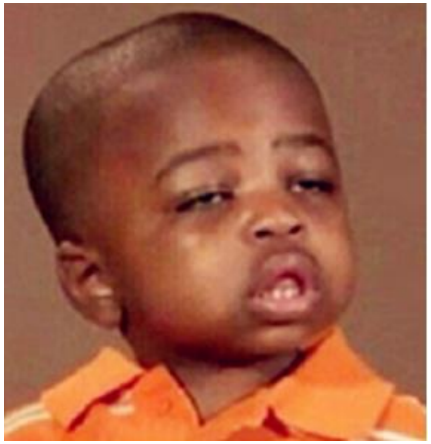
ORIGIN CHOICE 2 **Origin** at $\bar{1}$ at ddd, at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ from 222

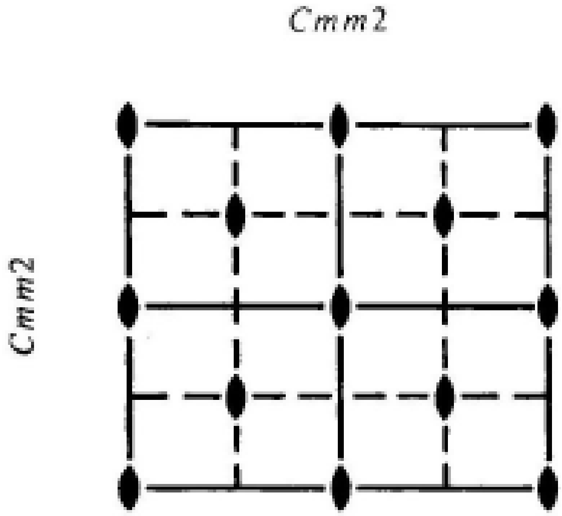


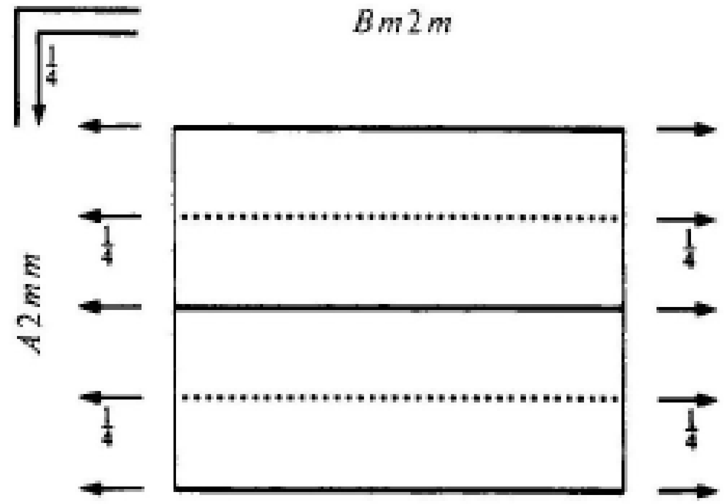
P196-198， *Fddd* 不同的原点选择

8-2-3 无对称单元

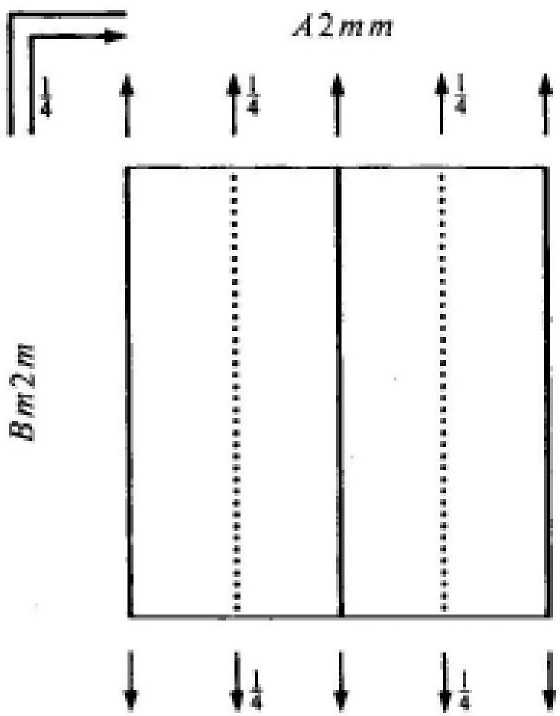
空间群的无对称单元是空间中的一部分区域，由它出发施以该空间群的对称操作，就恰好填满了整个空间。因此，无对称单元包含了为充分描述晶体结构所必需的一切信息，是基本的区域。

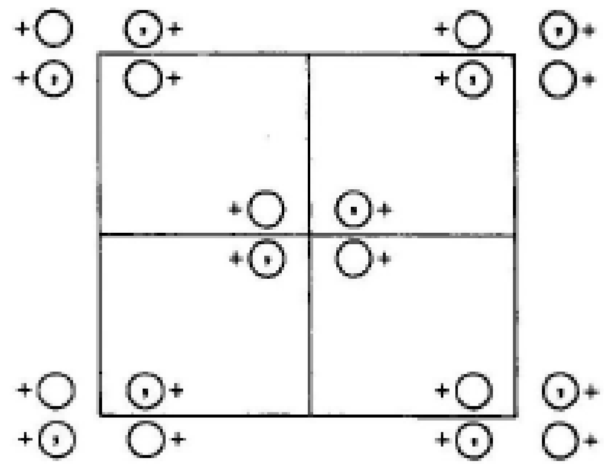






P186-187， *Cmm*2 (35)





8-3-1 对称操作与一般位置坐标

$$G = T + T(W_2, w_2) + T(W_3, w_3) + \ldots + T(W_h, w_h)$$
$$= T + (W_2, w_2)T + (W_3, w_3)T + \ldots + (W_h, w_h)T$$

点群：$P = \{I, W_2, \ldots\ldots W_h\}$，点阵平移群$: T$

$t_j = u_j\vec{a} + v_j\vec{b} + w_j\vec{c}$，$\vec{a}, \vec{b}, \vec{c}$为惯用胞基矢， u_j，v_j，w_j是整数。

适合简单点阵，不适用于有心点阵。

$U = \{(I, t_j)\}$ $\quad t_j = u_j\vec{a} + v_j\vec{b} + w_j\vec{c}$

(1) 简单点阵P: $\quad T_p = U$

(2) C心点阵C: $\quad T_C = U + U(I, \tfrac{1}{2}\ \tfrac{1}{2}\ 0)$

(3) 体心点阵I: $\quad T_I = U + U(I, \tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2})$

8-3-1 对称操作与一般位置坐标

τ 表示有心平移

点阵	n_c	τ_i
体心	2	$0;\quad \frac{1}{2}\frac{1}{2}\frac{1}{2}$
面心	4	$0;\quad 0\frac{1}{2}\frac{1}{2};\quad \frac{1}{2}0\frac{1}{2};\quad \frac{1}{2}\frac{1}{2}0$
C心	2	$0;\quad \frac{1}{2}\frac{1}{2}0$
R	3	$0;\quad \frac{2}{3}\frac{1}{3}\frac{1}{3};\quad \frac{1}{3}\frac{2}{3}\frac{2}{3}$

8-3-2 生成操作

Generators selected

例：Cmm2 $\underbrace{\underbrace{(1);\quad t(1,0,0);\quad t(0,1,0);\quad t(0,0,1);}_{\text{惯用胞平移群U}}\quad \underbrace{t\left(\tfrac{1}{2},\tfrac{1}{2},0\right);}_{\text{有心平移}}}_{\text{平移群T}}\quad \underbrace{\underbrace{(2);\quad (3)}_{(2)(3)=(4)}}_{\text{全部}(W_i,\,w_i)}$

选生成操作的原则：

（1)同晶类的空间群尽可能选同类型的生成操作

（2）按子群链选

（3）仅出现二次幂

(4) 有$\bar{1}$时必选$\bar{1}$

8-4-3 Wyckoff位置

Wyckoff字母（Wyckoff letter)
位置对称性（Site symmetry)
位置的坐标(Coordinates)
反射条件（Reflection conditions)

晶体结构中的原子团必具有它所在Wyckoff位置的位置对称性

8-4-2 位置对称性符号

每个Wyckoff位置的对称性可用一个点群来描述

用 • 标明没有对称元素的方 向；

去掉 • 之后即简略HM点群符号

分发的 *Pbca* （61）

Positions

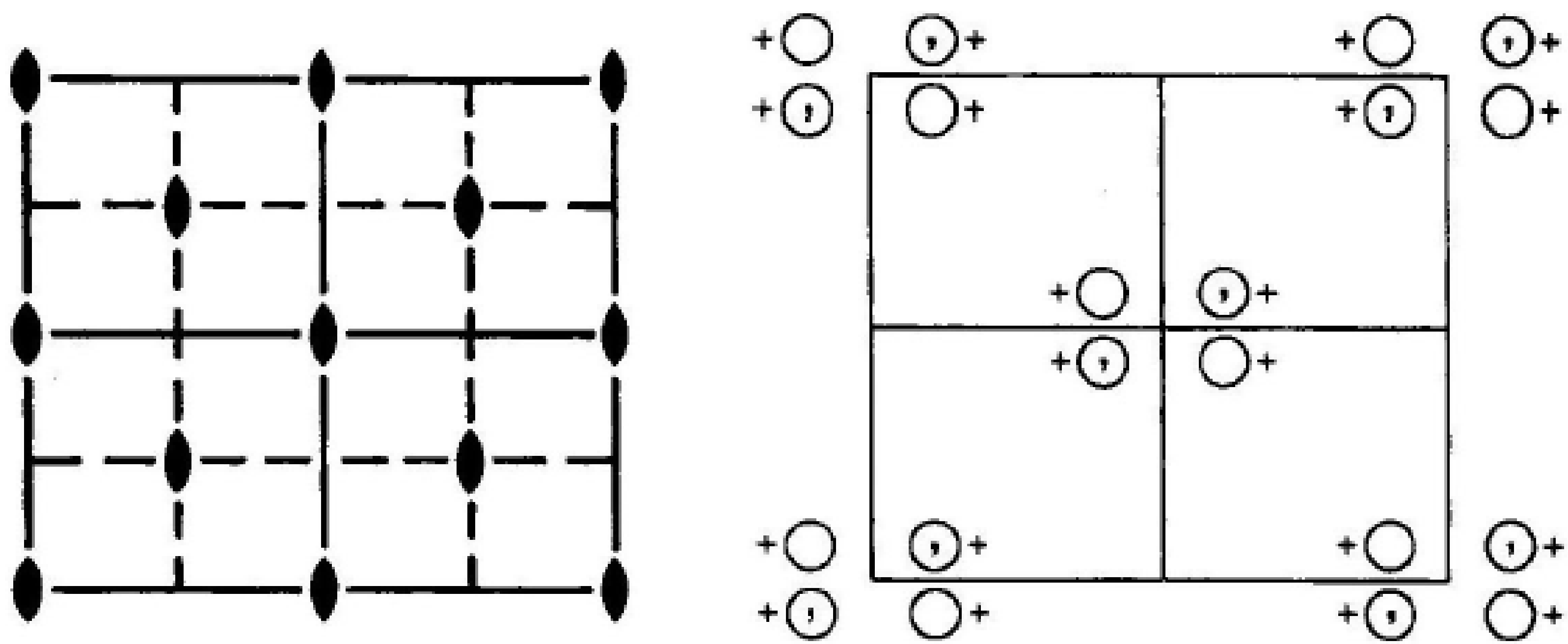
Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	c	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$0kl$: $k=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$h0l$: $l=2n$
							$hk0$: $h=2n$
							$h00$: $h=2n$
							$0k0$: $k=2n$
							$00l$: $l=2n$
							Special: as above, plus
4	b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h+k,h+l,k+l=2n$
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl : $h+k,h+l,k+l=2n$

例：Cmm2(35)

4	e	$m..$	$0, y, z$	$0, \bar{y}, z$
4	d	$.m.$	$x, 0, z$	$\bar{x}, 0, z$
4	c	$..2$	$1/4, 1/4, z$	$1/4, 3/4, z$

Cmm2

Cmm2



Cmm2(35)：

对称操作			矩阵	一般位置坐标	
$For\,(0,0,0)+set$				（0，0，0）+	
(1)	1		$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	(1)	x,y,z
(2)	2	$0,0,z$	$\begin{pmatrix}\bar{1}&0&0\\0&\bar{1}&0\\0&0&1\end{pmatrix}$	(2)	$\bar{x},\bar{y},z$
(3)	m	$x,0,z$	$\begin{pmatrix}1&0&0\\0&\bar{1}&0\\0&0&1\end{pmatrix}$	(3)	$x,\bar{y},z$
(4)	m	$0,y,z$	$\begin{pmatrix}\bar{1}&0&0\\0&1&0\\0&0&1\end{pmatrix}$	(4)	$\bar{x},y,z$

$$For(\tfrac{1}{2},\tfrac{1}{2},0)+set$$

$(1)'\quad t(\tfrac{1}{2},\tfrac{1}{2},0)$

$(2)'\ 2\quad \tfrac{1}{4},\tfrac{1}{4},z$

$(3)'a\quad x,\tfrac{1}{4},z$

$(4)'b\quad \tfrac{1}{4},y,z$

$$\begin{pmatrix} 1 & 0 & 0 & \frac{1}{2} \\ 0 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\begin{pmatrix} \bar{1} & 0 & 0 & \frac{1}{2} \\ 0 & \bar{1} & 0 & \frac{1}{2} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 0 & \frac{1}{2} \\ 0 & \bar{1} & 0 & \frac{1}{2} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\begin{pmatrix} \bar{1} & 0 & 0 & \frac{1}{2} \\ 0 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$(\tfrac{1}{2},\tfrac{1}{2},0)+$$

$(1)'x+\frac{1}{2},y+\frac{1}{2},z$

$(2)'-x+\frac{1}{2},-y+\frac{1}{2},z$

$(3)'x+\frac{1}{2},-y+\frac{1}{2},z$

$(4)'-x+\frac{1}{2},y+\frac{1}{2},z$

对称操作矩阵的缩写

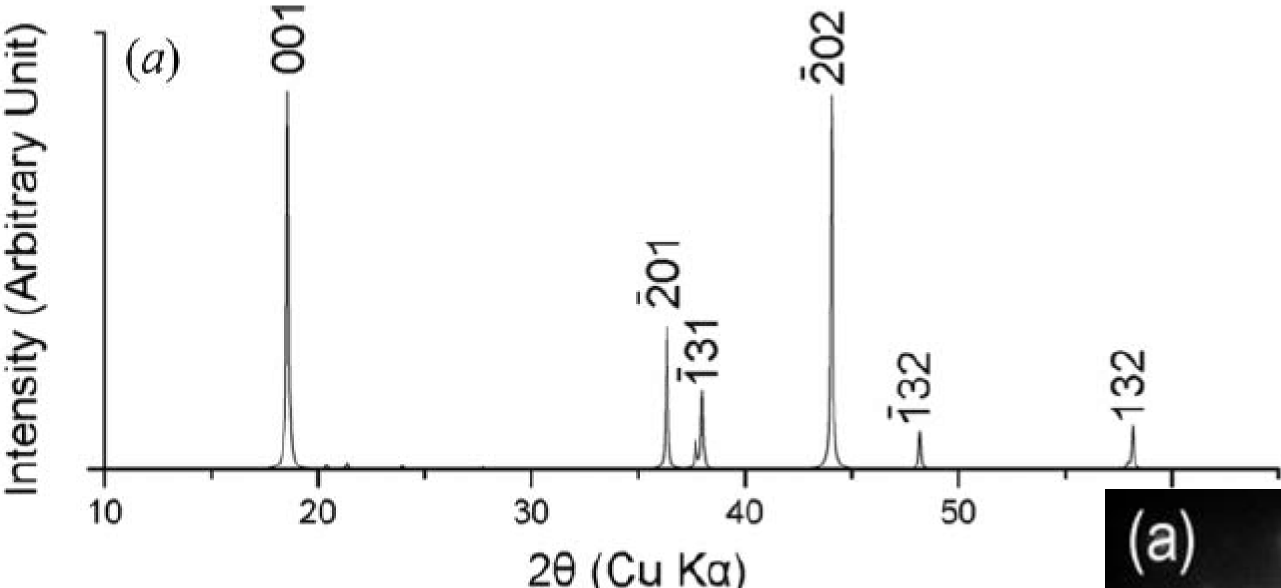
8-3-3 由简略HM符号求对称操作

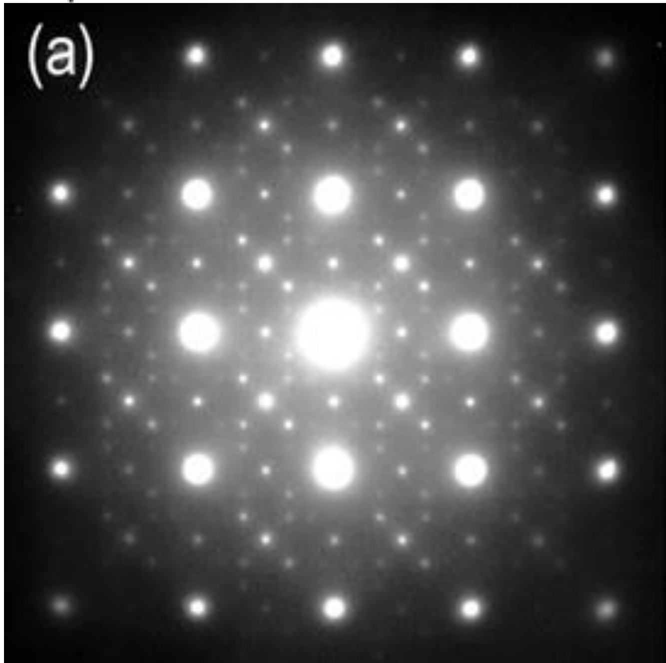
8-3-4 空间群对称元素配置图的推导

8-3-5 立方空间群的对称元素配置图

8-3-6 原点移动，对称操作的点对称操作无变化

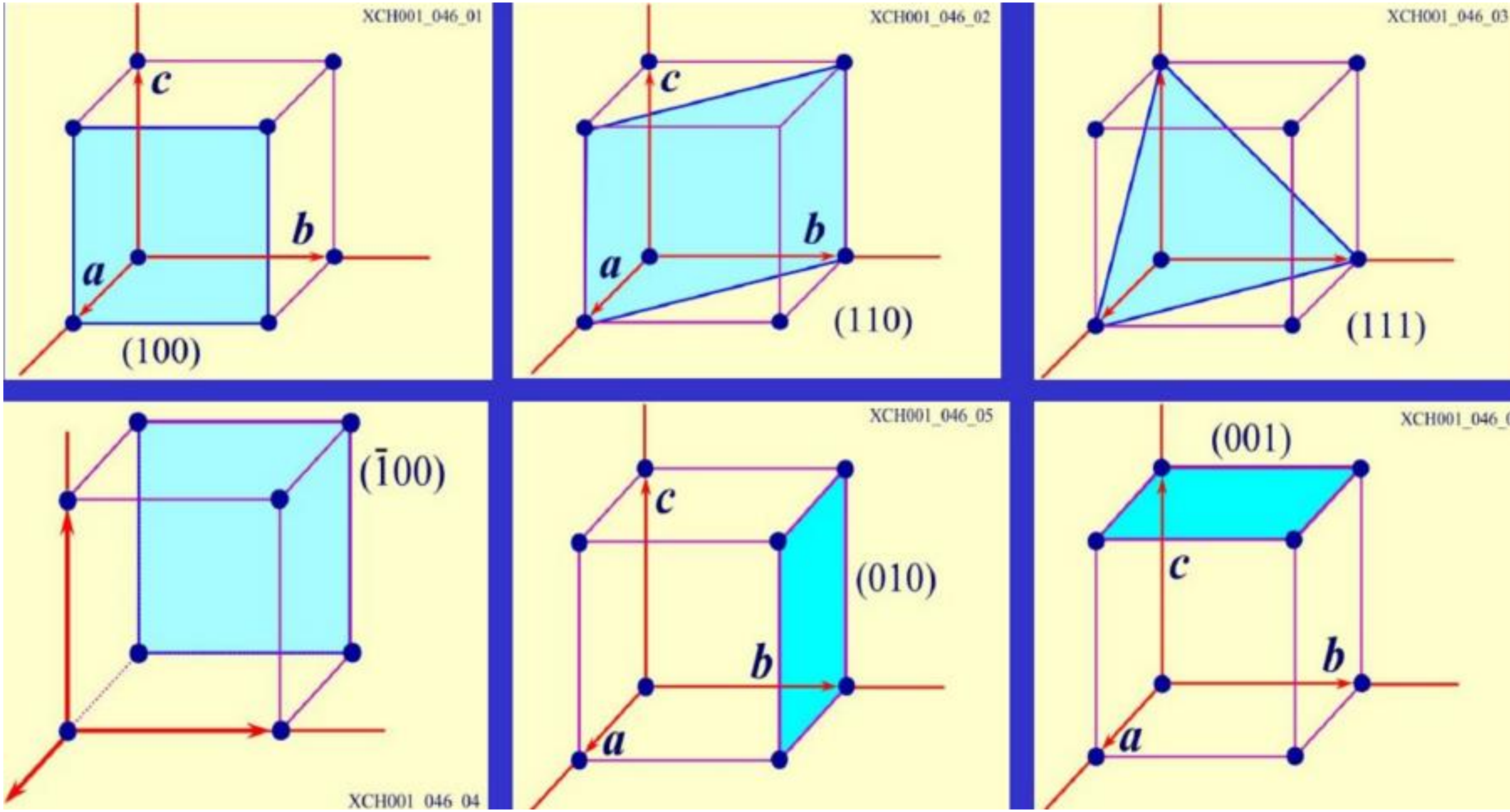
§ 8-5 x射线反射可能出现的条件





5-3 倒空间（倒易点阵）

晶向与晶面



XCH001_046_01
c
b
a
(100)
XCH001_046_02
c
b
a
(110)
XCH001_046_03
(111)
(1̄00)
XCH001_046_04
XCH001_046_05
c
(010)
b
a
XCH001_046_06
(001)
c
b
a

§5-3 倒易点阵

5-3-1 定义

$$a^* = \frac{b \times c}{V} \qquad b^* = \frac{c \times a}{V} \qquad c^* = \frac{a \times b}{V}$$

单胞体积 $V = a \cdot (b \times c) = \begin{vmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{vmatrix}$

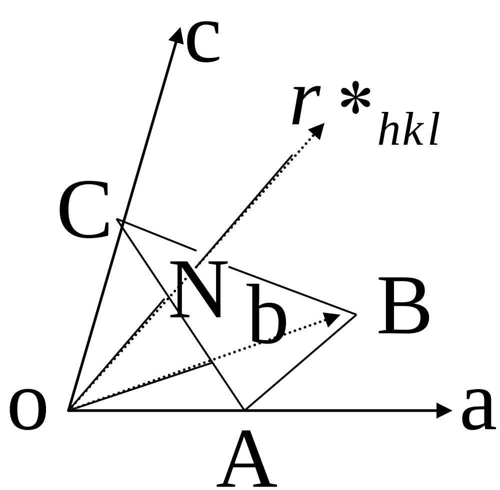
$a^* = kb \times c$ $\qquad a \cdot a^* = ka \cdot b \times c = 1 \quad \therefore k = 1/V$

5-3-2 倒易关系

(1)

$$\begin{pmatrix} a^* \\ b^* \\ c^* \end{pmatrix}(abc) = \begin{pmatrix} a^* \bullet a & a^* \bullet b & a^* \bullet c \\ b^* \bullet a & b^* \bullet b & b^* \bullet c \\ c^* \bullet a & c^* \bullet b & c^* \bullet c \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = I = \begin{pmatrix} a \\ b \\ c \end{pmatrix}(a^* b^* c^*)$$

(2) $\vec{r}*_{hkl} = h\vec{a}* + k\vec{b}* + l\vec{c}* \perp (hkl)$面， $r*_{hkl} = \dfrac{1}{d_{hkl}}$



(hkl)平面族中最靠近原点O但不通过原点的平面ABC

$$\overrightarrow{OA} = \frac{\vec{a}}{h}, \overrightarrow{OB} = \frac{\vec{b}}{k}, \overrightarrow{OC} = \frac{\vec{c}}{l}$$

$$\vec{r}*_{hkl} \bullet \begin{Bmatrix} \overrightarrow{AB} \\ \overrightarrow{AC} \end{Bmatrix} = 0, \therefore \vec{r}*_{hkl} \perp (hkl)$$

$$d_{hkl} = ON = OA \bullet \frac{\vec{r}^*_{hkl}}{\left|\vec{r}^*_{hkl}\right|} = \frac{1}{r^*_{hkl}}$$

(3) v= $\dfrac{1}{v^*}$,倒易点阵单胞体积 $V^* = a^* \bullet b^* \times c^*$

$$(a\bullet b\times c)(A\bullet B\times C)=\begin{vmatrix}a_x & a_y & a_z\\ b_x & b_y & b_z\\ c_x & c_y & c_z\end{vmatrix}\begin{vmatrix}A_x & A_y & A_z\\ B_x & B_y & B_z\\ C_x & C_y & C_z\end{vmatrix}$$

行列式与它的转置行列式相等

$$=\begin{vmatrix}a_x & a_y & a_z\\ b_x & b_y & b_z\\ c_x & c_y & c_z\end{vmatrix}\begin{vmatrix}A_x & B_x & C_x\\ A_y & B_y & C_y\\ A_z & B_z & C_z\end{vmatrix}$$

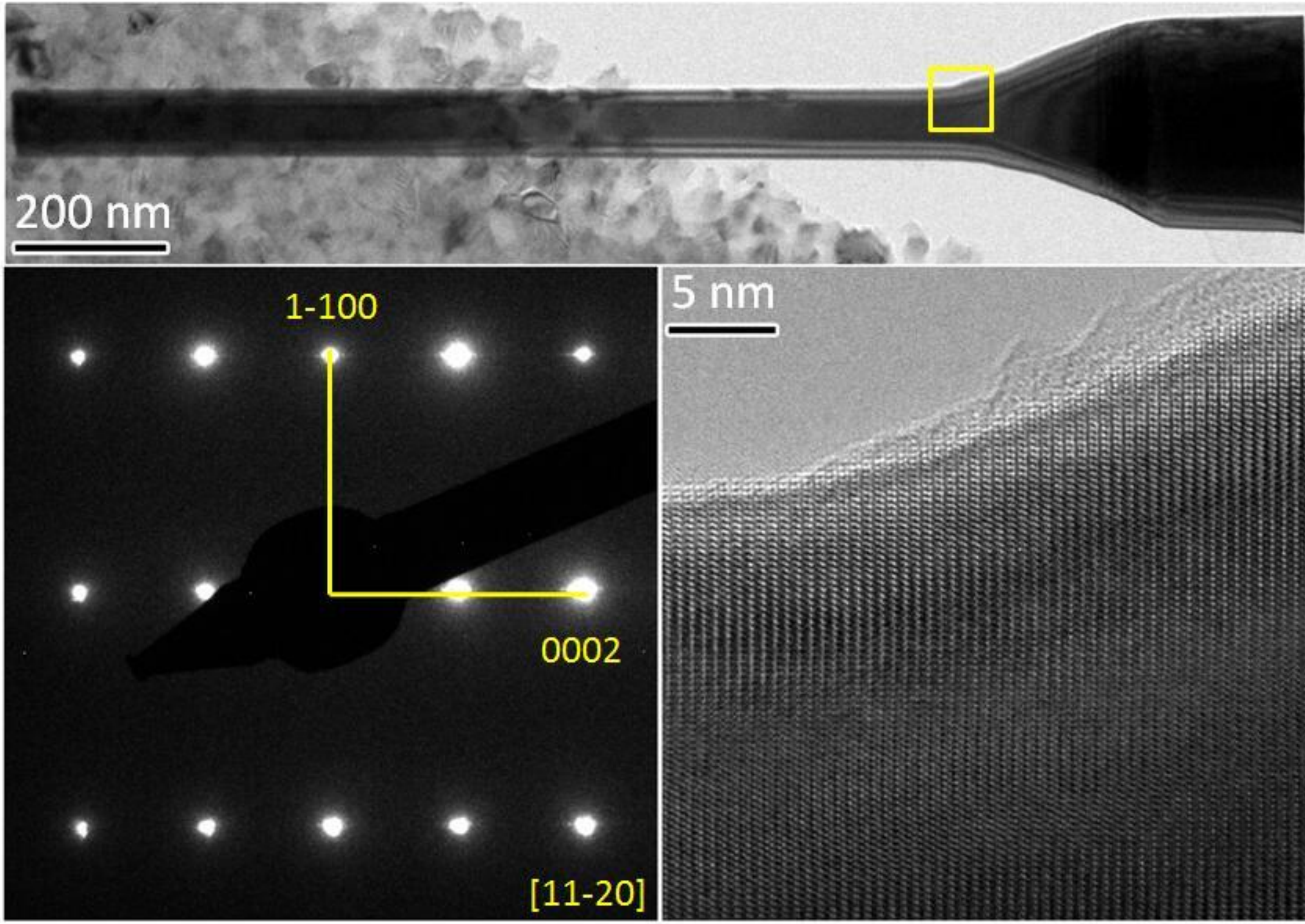
矩阵的行列式的积等于矩阵乘积的行列式

$$=\left|\begin{pmatrix}a_x & a_y & a_z\\ b_x & b_y & b_z\\ c_x & c_y & c_z\end{pmatrix}\begin{pmatrix}A_x & B_x & C_x\\ A_y & B_y & C_y\\ A_z & B_z & C_z\end{pmatrix}\right|$$

$$=\begin{vmatrix}a\bullet A & a\bullet B & a\bullet C\\ b\bullet A & b\bullet B & b\bullet C\\ c\bullet A & c\bullet B & c\bullet C\end{vmatrix}\Rightarrow(a\bullet b\times c)(a^*\bullet b^*\times c^*)=1\text{即}VV^*=1$$

$$V^2=(a\bullet b\times c)(a\bullet b\times c)=\begin{vmatrix}a\bullet a & a\bullet b & a\bullet c\\ b\bullet a & b\bullet b & b\bullet c\\ c\bullet a & c\bullet b & c\bullet c\end{vmatrix}$$

$$\therefore V=abc\sqrt{1+2\cos\alpha\cos\beta\cos\gamma-\cos^2\alpha-\cos^2\beta-\cos^2\gamma}$$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5-3-3 度量张量

$$G=\begin{pmatrix}a\\b\\c\end{pmatrix}\begin{pmatrix}a & b & c\end{pmatrix}=\begin{pmatrix}a\bullet a & a\bullet b & a\bullet c\\ b\bullet a & b\bullet b & b\bullet c\\ c\bullet a & c\bullet b & c\bullet c\end{pmatrix}=\begin{pmatrix}a^2 & ab\cos\gamma & ac\cos\beta\\ ab\cos\gamma & b^2 & bc\cos\alpha\\ ac\cos\beta & bc\cos\alpha & c^2\end{pmatrix}$$

倒易度量张量

$$G^{-1}=\frac{a^2b^2c^2}{V^2}\begin{pmatrix}\dfrac{\sin^2\alpha}{a^2} & \dfrac{\cos\alpha\cos\beta-\cos\gamma}{ab} & \dfrac{\cos\alpha\cos\gamma-\cos\beta}{ac}\\ \dfrac{\cos\alpha\cos\beta-\cos\gamma}{ab} & \dfrac{\sin^2\beta}{b^2} & \dfrac{\cos\beta\cos\gamma-\cos\alpha}{bc}\\ \dfrac{\cos\alpha\cos\gamma-\cos\beta}{ac} & \dfrac{\cos\beta\cos\gamma-\cos\alpha}{bc} & \dfrac{\sin^2\gamma}{c^2}\end{pmatrix}$$

表5-5（p.114)作出

$$\begin{pmatrix}A\\B\\C\end{pmatrix}=G^{-1}\begin{pmatrix}a\\b\\c\end{pmatrix}, \text{则}\begin{pmatrix}A\\B\\C\end{pmatrix}\begin{pmatrix}a & b & c\end{pmatrix}=G^{-1}G=I, \text{可见}\begin{pmatrix}a^*\\b^*\\c^*\end{pmatrix}=G^{-1}\begin{pmatrix}a\\b\\c\end{pmatrix}$$

$$倒易点阵的度量张量G^* = \begin{pmatrix} a^* \\ b^* \\ c^* \end{pmatrix}(a^* b^* c^*) = G^{-1} \begin{pmatrix} a \\ b \\ c \end{pmatrix}\begin{pmatrix} a^* & b^* & c^* \end{pmatrix} = G^{-1}$$

$$\therefore G^{-1} = G^* = \begin{pmatrix} a^* \bullet a^* & a^* \bullet b^* & a^* \bullet c^* \\ b^* \bullet a^* & b^* \bullet b^* & b^* \bullet c^* \\ c^* \bullet a^* & c^* \bullet b^* & c^* \bullet c^* \end{pmatrix}$$

$$\therefore a^* = \frac{bc\sin\alpha}{V}, b^* = \frac{ca\sin\beta}{V}, c^* = \frac{ab\sin\gamma}{V}$$

$$\cos\alpha^* = \frac{\vec{b}^* \bullet \vec{c}^*}{b^* c^*} = \frac{\cos\beta\cos\gamma - \cos\alpha}{\sin\beta\sin\gamma}, \cos\beta^* = \frac{\cos\gamma\cos\alpha - \cos\beta}{\sin\gamma\sin\alpha}, \cos\gamma^* = \frac{\cos\alpha\cos\beta - \cos\gamma}{\sin\alpha\sin\beta}$$

直接求G^{-1}的表达式：

由$\vec{a}^{*}=\dfrac{\vec{b}\times\vec{c}}{V}$直接可得$a^{*}=\dfrac{bc\sin\alpha}{V}$

由（$(\vec{A}\times\vec{B})\bullet(\vec{C}\times\vec{D})=\vec{A}\bullet\left[\vec{B}\times\left(\vec{C}\times\vec{D}\right)\right]$

$=\vec{A}\bullet\left[\vec{C}\left(\vec{B}\bullet\vec{D}\right)-\vec{D}\left(\vec{B}\bullet\vec{C}\right)\right]=\left(\vec{A}\bullet\vec{C}\right)\left(\vec{B}\bullet\vec{D}\right)-\left(\vec{A}\bullet\vec{D}\right)\left(\vec{B}\bullet\vec{C}\right)$

可得$\vec{b}^{*}\bullet\vec{c}^{*}=\dfrac{\left(\vec{c}\times\vec{a}\right)}{V}\bullet\dfrac{\left(\vec{a}\times\vec{b}\right)}{V}=\dfrac{\left(\vec{c}\bullet\vec{a}\right)\left(\vec{a}\bullet\vec{b}\right)-\left(\vec{c}\bullet\vec{b}\right)\left(\vec{a}\bullet\vec{a}\right)}{V^{2}}$

$=\dfrac{a^{2}bc}{V^{2}}\left(\cos\beta\cos\gamma-\cos\alpha\right)$

表5－6（$p.116)\Rightarrow$ 倒易点阵与相应的正点 阵属同一*Bravais*系，

以六角*Bravais*系为例

5-3-4 **晶体几何学中的计算公式**

(1)

$$\frac{1}{d_{hkl}^{\ 2}}=\overrightarrow{r_{hkl}}^{*}\bullet\overrightarrow{r_{hkl}}^{*}=\begin{pmatrix}h & k & l\end{pmatrix}\begin{pmatrix}a^{*}\\ b^{*}\\ c^{*}\end{pmatrix}\begin{pmatrix}a^{*} & b^{*} & c^{*}\end{pmatrix}\begin{pmatrix}h\\ k\\ l\end{pmatrix}=\begin{pmatrix}h & k & l\end{pmatrix}G^{-1}\begin{pmatrix}h\\ k\\ l\end{pmatrix}$$

(2) 点阵平面($h_1k_1l_1$) 与($h_2k_2l_2$)的夹角φ

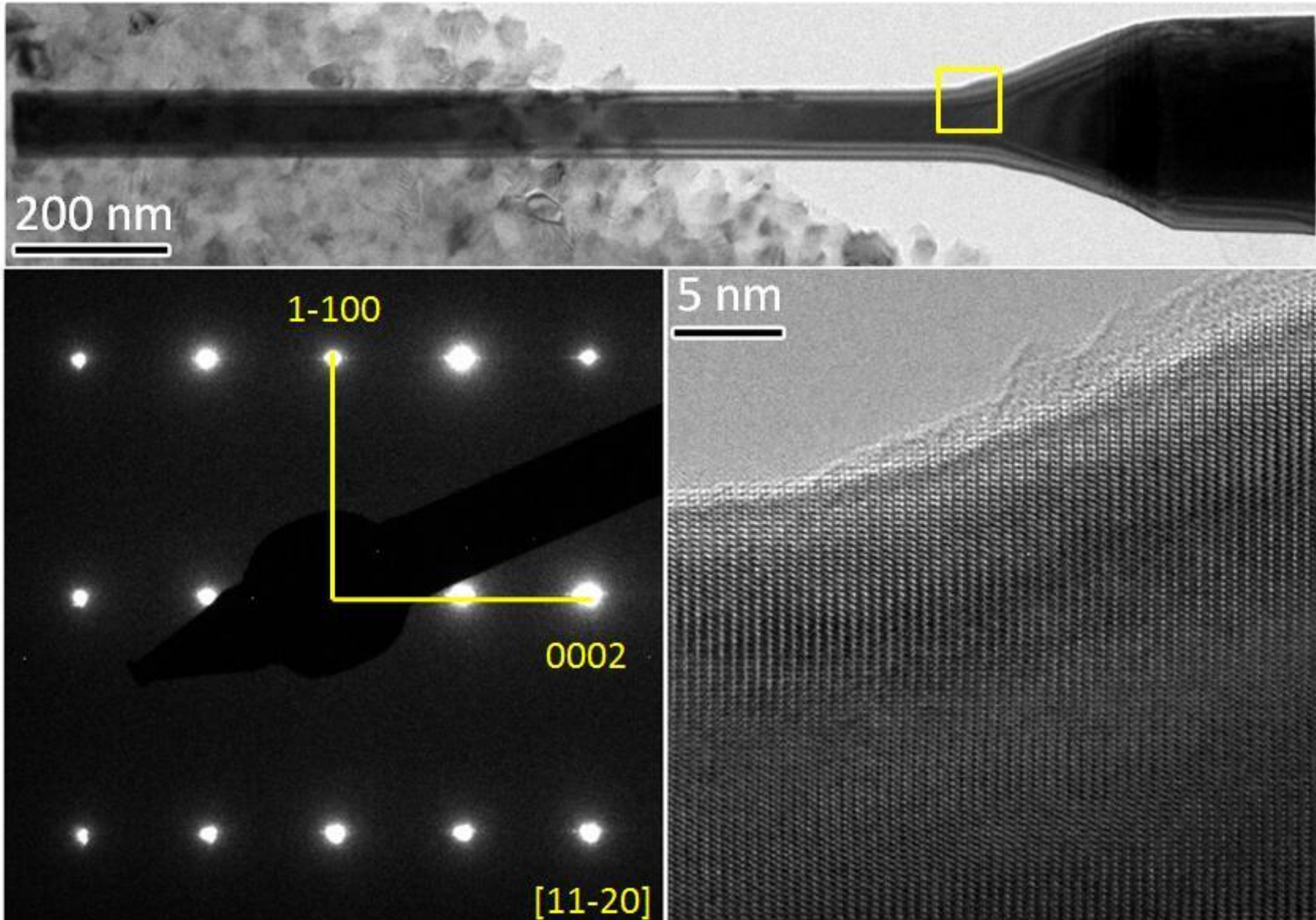
$$\cos\varphi=\frac{\overrightarrow{r_{h_1k_1l_1}}^{*}\bullet\overrightarrow{r_{h_2k_2l_2}}^{*}}{r_{h_1k_1l1}^{\ \ *}r_{h_2k_2l_{\ 2}}^{\ \ *}}=\frac{1}{r_{h_1k_1l_1}^{\ \ *}r_{h_2k_2l_2}^{\ \ *}}\begin{pmatrix}h_1 & k_1 & l_1\end{pmatrix}G^{-1}\begin{pmatrix}h_2\\ k_2\\ l_2\end{pmatrix}$$

$$(3)r_{uvw}^{\ \ 2}=(uvw)\begin{pmatrix}a\\ b\\ c\end{pmatrix}\begin{pmatrix}a & b & c\end{pmatrix}\begin{pmatrix}u\\ v\\ w\end{pmatrix}=\begin{pmatrix}u & v & w\end{pmatrix}G\begin{pmatrix}u\\ v\\ w\end{pmatrix}$$

(4)点阵矢量$\begin{bmatrix}u_1 & v_1 & w_1\end{bmatrix}$与$\begin{bmatrix}u_2 & v_2 & w_2\end{bmatrix}$的夹角$\phi$

$$\cos\phi=\frac{1}{r_{u_1v_1w1}r_{u_2v_2w2}}\begin{pmatrix}u_1 & v_1 & w_1\end{pmatrix}G\begin{pmatrix}u_2\\ v_2\\ w_2\end{pmatrix}$$

表5－7（p.117)　　　　　　习题:2、9、13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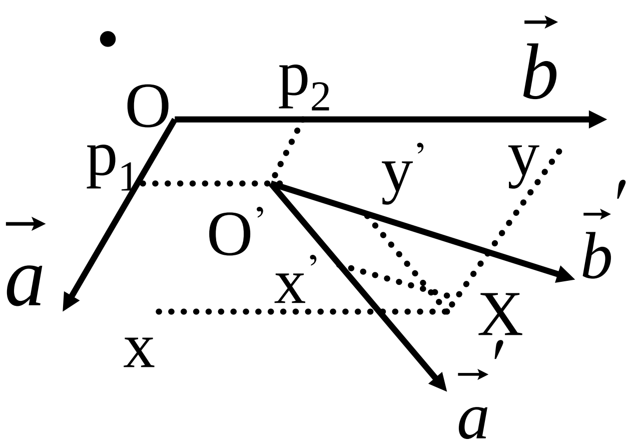
坐标系与单胞变化

- 正交变换：仅基矢方向变。基矢间夹角、基矢长度不变。P为正交矩阵：$PP^t=I$
- 线性变换：基矢改变，但坐标原点不变。$\vec{p}=0$
- 仿射变换：坐标原点也可移动。

$$\left(\vec{a}',\ \vec{b}',\ \vec{c}'\right)=\left(\vec{a},\ \vec{b},\ \vec{c}\right)P$$

- 

坐标原点位移

$$\vec{p}=\left(\vec{a}\quad \vec{b}\quad \vec{c}\right)\begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}=\left(\vec{a}'\quad \vec{b}'\quad \vec{c}'\right)\begin{pmatrix} p_1' \\ p_2' \\ p_3' \end{pmatrix}$$

5-4-2　　线性变换

$$\begin{pmatrix} a' & b' & c' \end{pmatrix} = \begin{pmatrix} a & b & c \end{pmatrix} P$$

$$\begin{pmatrix} a & b & c \end{pmatrix} = \begin{pmatrix} a' & b' & c' \end{pmatrix} Q$$

$$Q = P^{-1}$$

$$\begin{pmatrix} a' \\ b' \\ c' \end{pmatrix} = P^{t} \begin{pmatrix} a \\ b \\ c \end{pmatrix}$$

转置逆

1.倒易点阵基矢

$$\begin{pmatrix} a^* \\ b^* \\ c^* \end{pmatrix} \begin{pmatrix} a & b & c \end{pmatrix} = I = \begin{pmatrix} a^{*\prime} \\ b^{*\prime} \\ c^{*\prime} \end{pmatrix} \begin{pmatrix} a' & b' & c' \end{pmatrix}$$

↑ 左乘Q　　　↑ 右乘P

$$\therefore \begin{pmatrix} a^{*\prime} \\ b^{*\prime} \\ c^{*\prime} \end{pmatrix} = Q \begin{pmatrix} a^* \\ b^* \\ c^* \end{pmatrix}$$

因为是单位矩阵，等式左边乘，右边可不乘。

2.点X的坐标x, y, z和正点阵方向指数$\left[u \quad v \quad w\right]$

$$\begin{pmatrix} a & b & c \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \vec{r} = \begin{pmatrix} a' & b' & c' \end{pmatrix}\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}$$

$$\downarrow$$

$$\begin{pmatrix} a' & b' & c' \end{pmatrix} Q \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$\therefore \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = Q \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$\begin{pmatrix} u' \\ v' \\ w' \end{pmatrix} = Q \begin{pmatrix} u \\ v \\ w \end{pmatrix}$$

[uvw]与$a^* \ b^* \ c^*$
一样变换

3.点阵平面指数(hkl)

$$(h \quad k \quad l)\begin{pmatrix} a^* \\ b^* \\ c^* \end{pmatrix} = \vec{r}^{\,*} = (h' \quad k' \quad l')\begin{pmatrix} a^{*\prime} \\ b^{*\prime} \\ c^{*\prime} \end{pmatrix}$$

$$\downarrow$$

$$(h \quad k \quad l)P\begin{pmatrix} a^{*\prime} \\ b^{*\prime} \\ c^{*\prime} \end{pmatrix}$$

$$\therefore (h' \quad k' \quad l') = (h \quad k \quad l)P$$

$$\begin{pmatrix} h' \\ k' \\ l' \end{pmatrix} = P^t \begin{pmatrix} h \\ k \\ l \end{pmatrix}$$

（hkl)与(abc)一样变换

总结：线性变换 $\begin{pmatrix} a' \\ b' \\ c' \end{pmatrix} = P^t \begin{pmatrix} a \\ b \\ c \end{pmatrix}, \begin{pmatrix} h' \\ k' \\ l' \end{pmatrix} = P^t \begin{pmatrix} h \\ k \\ l \end{pmatrix}; \begin{pmatrix} a^{*\prime} \\ b^{*\prime} \\ c^{*\prime} \end{pmatrix} = Q\begin{pmatrix} a^* \\ b^* \\ c^* \end{pmatrix}, \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = Q\begin{pmatrix} x \\ y \\ z \end{pmatrix}$

4、正交矩阵：当P为正交矩阵时，$PP^t=I$, ∴$P^t=Q$ 四者都按Q变换。

5. 度量张量G和倒易度量张量$G^{-1}=G^*$

$$G'=\begin{pmatrix} a' \\ b' \\ c' \end{pmatrix}\begin{pmatrix} a' & b' & c' \end{pmatrix}=P^t\begin{pmatrix} a \\ b \\ c \end{pmatrix}\begin{pmatrix} a & b & c \end{pmatrix}P=P^tGP$$

$$G^{*'}=\begin{pmatrix} a^{*'} \\ b^{*'} \\ c^{*'} \end{pmatrix}\begin{pmatrix} a^{*'} & b^{*'} & c^{*'} \end{pmatrix}=Q\begin{pmatrix} a^* \\ b^* \\ c^* \end{pmatrix}\begin{pmatrix} a^* & b^* & c^* \end{pmatrix}Q^t=QG^*Q^t$$

7.点对称操作矩阵W

$$\begin{pmatrix}\tilde{x}\\ \tilde{y}\\ \tilde{z}\end{pmatrix}=W\begin{pmatrix}x\\ y\\ z\end{pmatrix},\begin{pmatrix}\tilde{x}'\\ \tilde{y}'\\ \tilde{z}'\end{pmatrix}=W'\begin{pmatrix}x'\\ y'\\ z'\end{pmatrix}$$

$$Q\begin{pmatrix}\tilde{x}\\ \tilde{y}\\ \tilde{z}\end{pmatrix}=W'Q\begin{pmatrix}x\\ y\\ z\end{pmatrix}$$

$$QW\begin{pmatrix}x\\ y\\ z\end{pmatrix}=W'Q\begin{pmatrix}x\\ y\\ z\end{pmatrix}$$

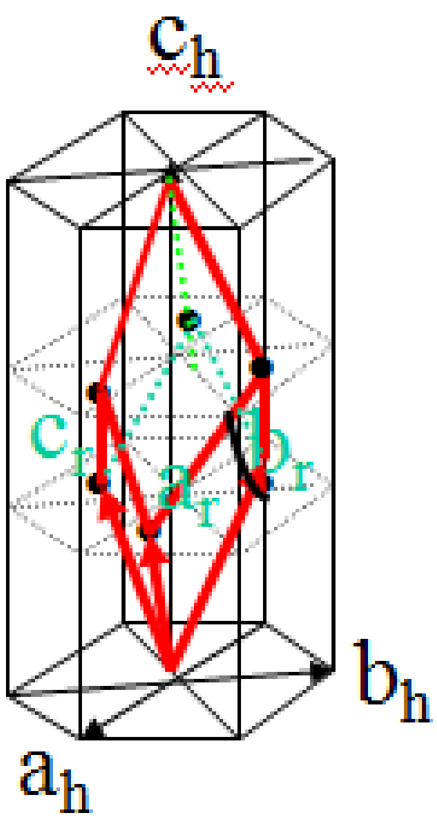
$$\therefore QW=W'Q$$

$$W'=QWP$$

$$trW'=trW$$

$$\det W'=\det W$$

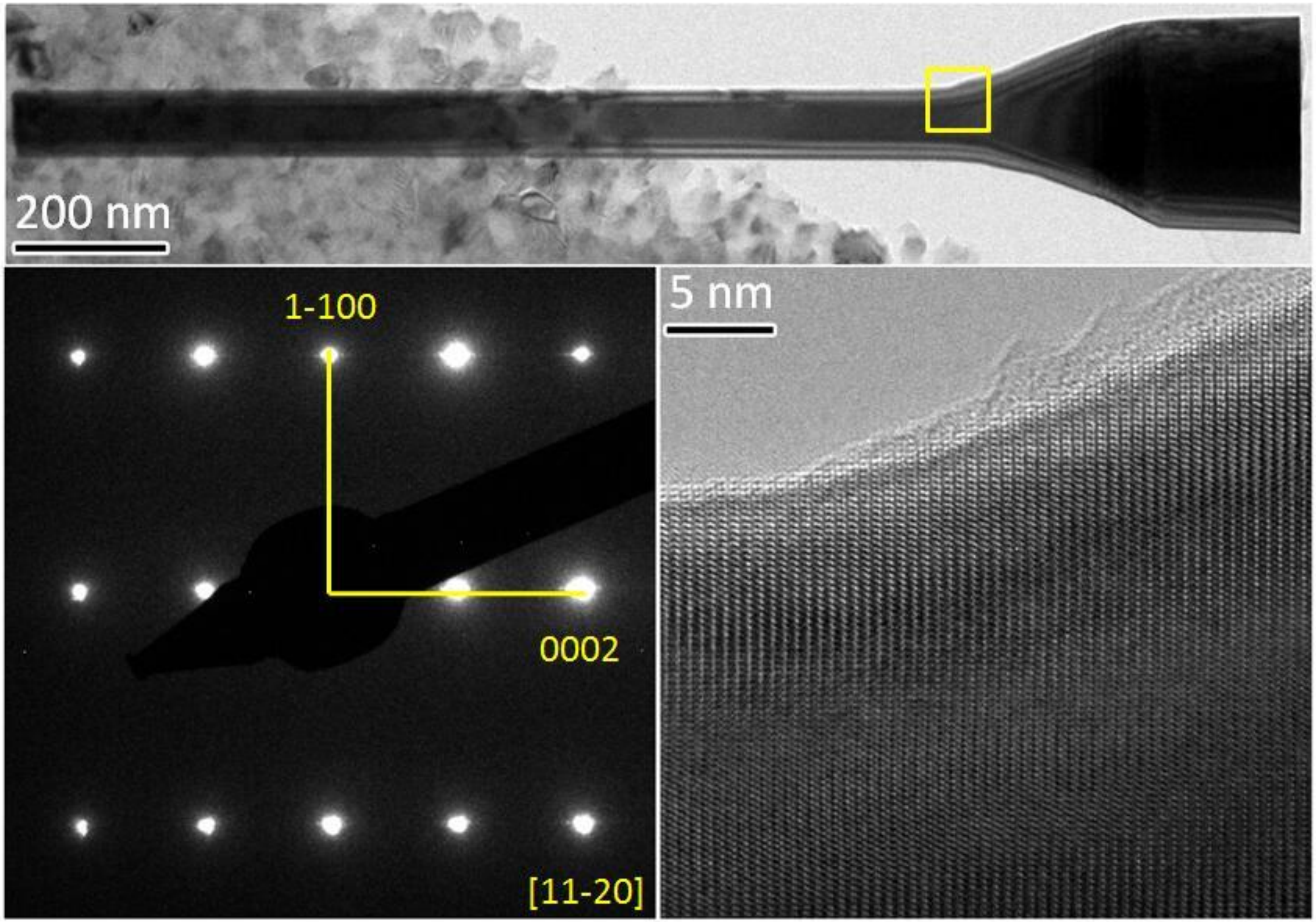
§5-2-2 六角坐标系与菱面体坐标系的关系(P106页)



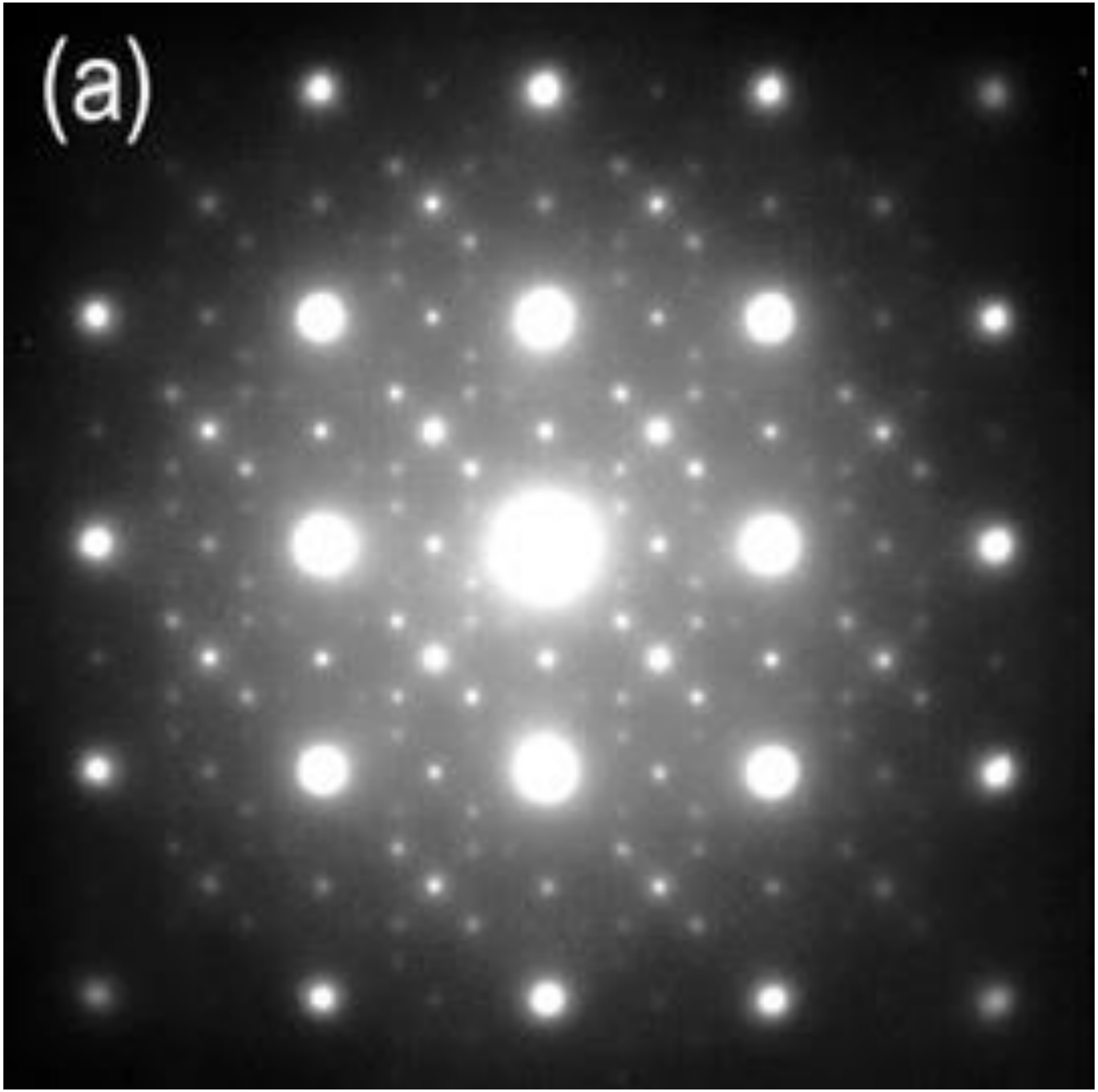
$$(a_h\ \ b_h\ \ c_h)=(a_r\ \ b_r\ \ c_r)\begin{pmatrix}1 & 0 & 1\\ -1 & 1 & 1\\ 0 & -1 & 1\end{pmatrix}$$

$$(a_r\ \ b_r\ \ c_r)=(a_h\ \ b_h\ \ c_h)\begin{pmatrix}2/3 & -1/3 & -1/3\\ 1/3 & 1/3 & -2/3\\ 1/3 & 1/3 & 1/3\end{pmatrix}$$

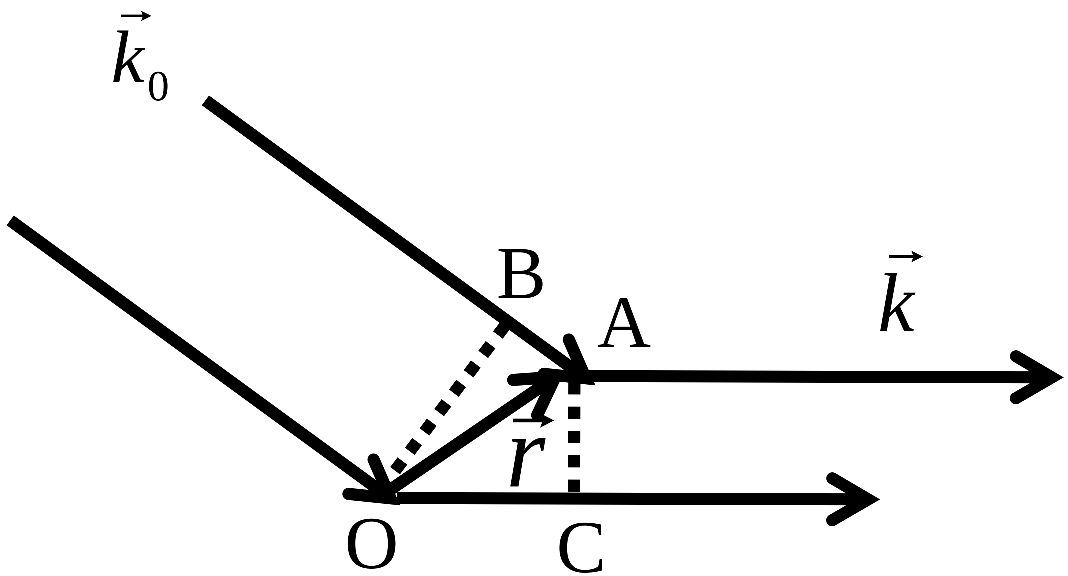
[100]r	[111]r	(111)r	(110)r
[2/3 1/3 1/3]h	[001]h	(003)h	(012)h



200 nm
1-100
0002
[11-20]
5 nm


(a)

§ 8-5 x射线反射可能出现的条件



一个电子产生的散射波的振幅：A_e；$\vec{r}$处的电子密度 $\rho(\vec{r})=\rho(X,Y,Z)$

$\vec{r}=X\vec{a}+Y\vec{b}+Z\vec{c}$；$\vec{r}$处$dV$体积对散射波振幅的贡献：$A_e\cdot\rho(\vec{r})dV$

$\vec{r}$处散射波向对于原点的程差

$$\Delta=AB-OC=\vec{r}\cdot\frac{\vec{k}_0-\vec{k}}{|k_0|}=-\vec{s}\cdot\vec{r}\lambda$$

相位因子$\exp(-\frac{2\pi i\Delta}{\lambda})=\exp(2\pi i\vec{s}\cdot\vec{r})$

衍射矢量$\vec{S}=\vec{k}-\vec{k}_0$

$$=h\vec{a}^*+k\vec{b}^*+l\vec{c}^*$$

$$|\vec{k}|=|\vec{k}_0|=1/\lambda$$

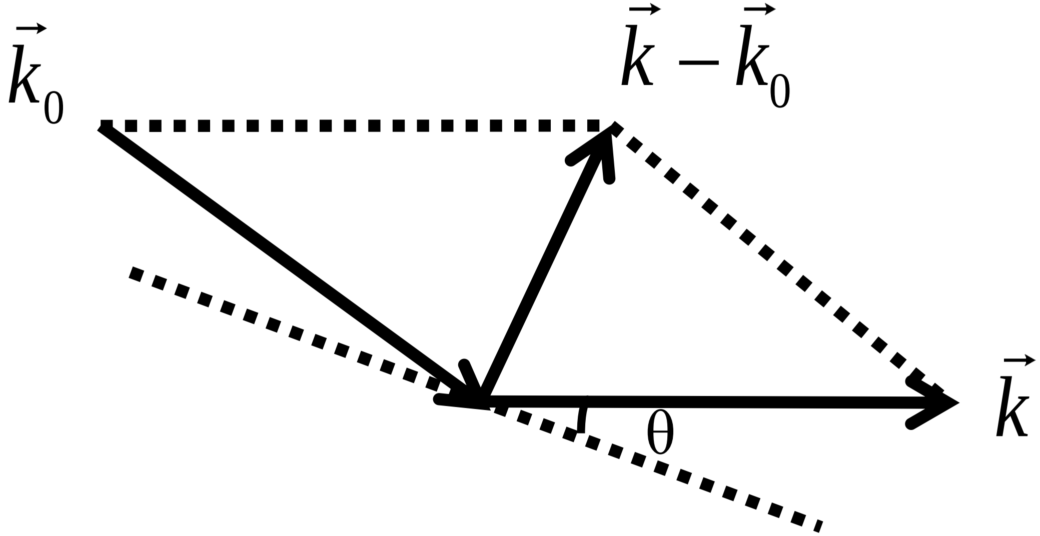
$$\text{结构因子F}(hkl)=\frac{\text{一个晶胞的散射波振幅}}{\text{一个电子的散射波振幅}}$$

$$=\int_{v_c}\rho(\vec{r})\exp(2\pi i\vec{s}\cdot\vec{r})dV$$

把一个单胞内的电子密度$\rho(\vec{r})$分解成该单胞内N个原子的电子密度函数$\rho_n(\vec{r})$之和： $\rho(\vec{r})=\sum_{n=1}^{N}\rho_n(\vec{r})$

定义原子散射因子 $\mathrm{f_n}=\int\rho_n(\vec{r})\exp[2\pi i\vec{s}\cdot(\vec{r}-\vec{r}_n)]dV$

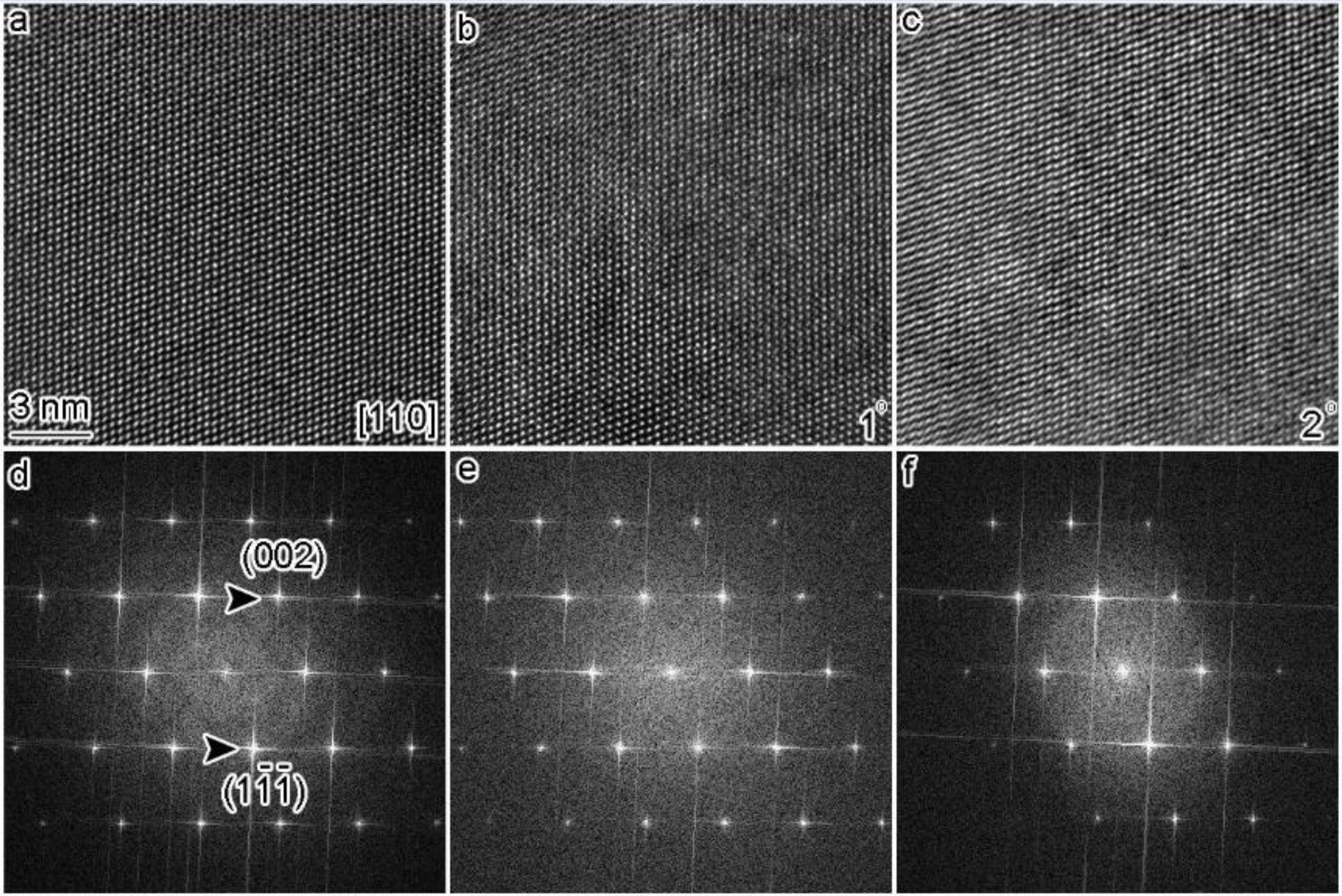
则$\mathrm{F}(hkl)=\sum_{n=1}^{N}f_n\exp(2\pi i\vec{s}\cdot\vec{r}_n)=\sum_{n=1}^{N}f_n\exp[2\pi i(hX_n+kY_n+lZ_n)]$



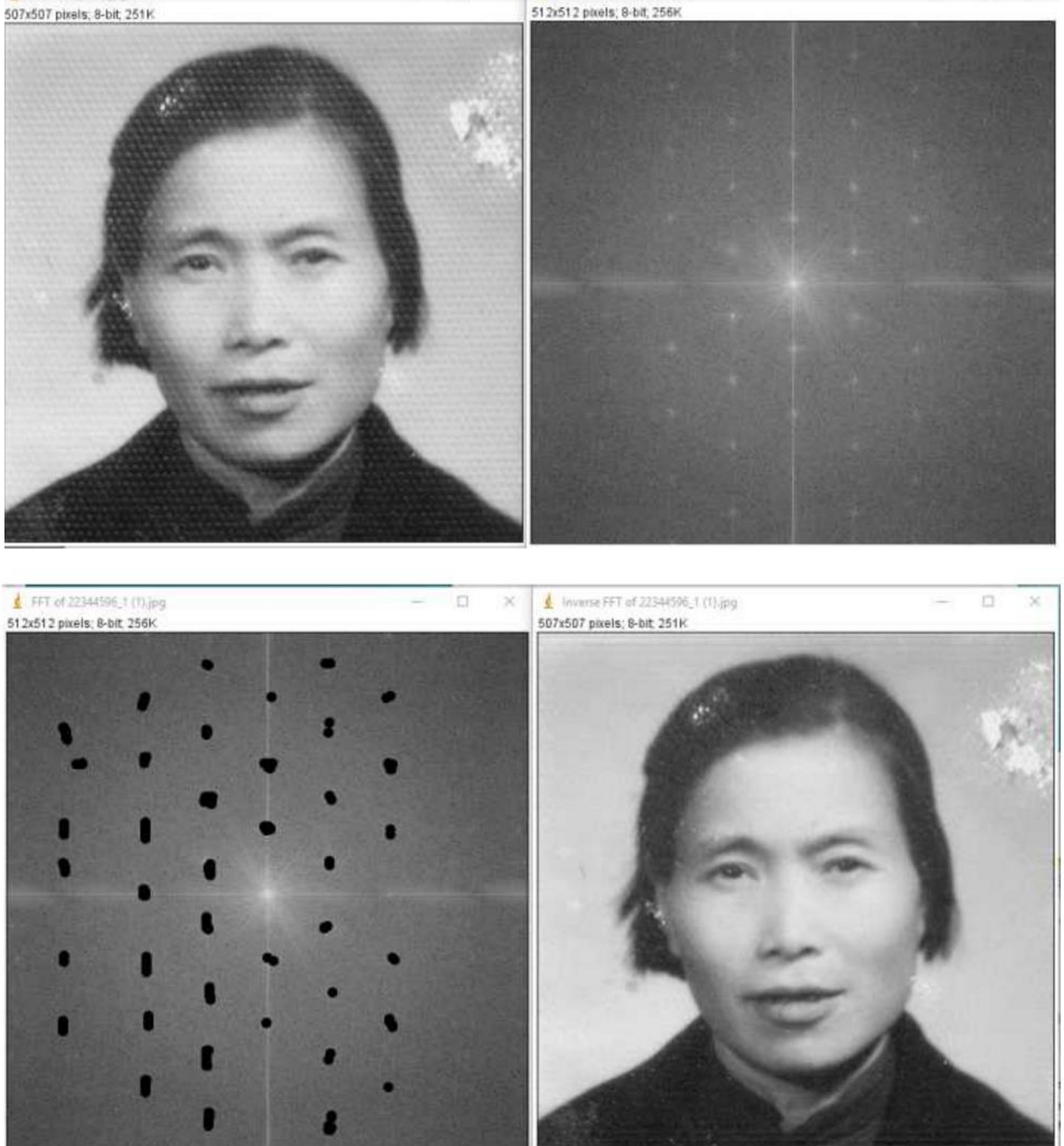
$$\left|\vec{k}-\vec{k}_0\right| = 2\left|\vec{k}_0\right|\sin\theta = 2\sin\theta/\lambda$$

Bragg散射：$\vec{k}-\vec{k}_0 = \vec{g}$ （倒格矢） ➡ $2d\sin\theta = \lambda$

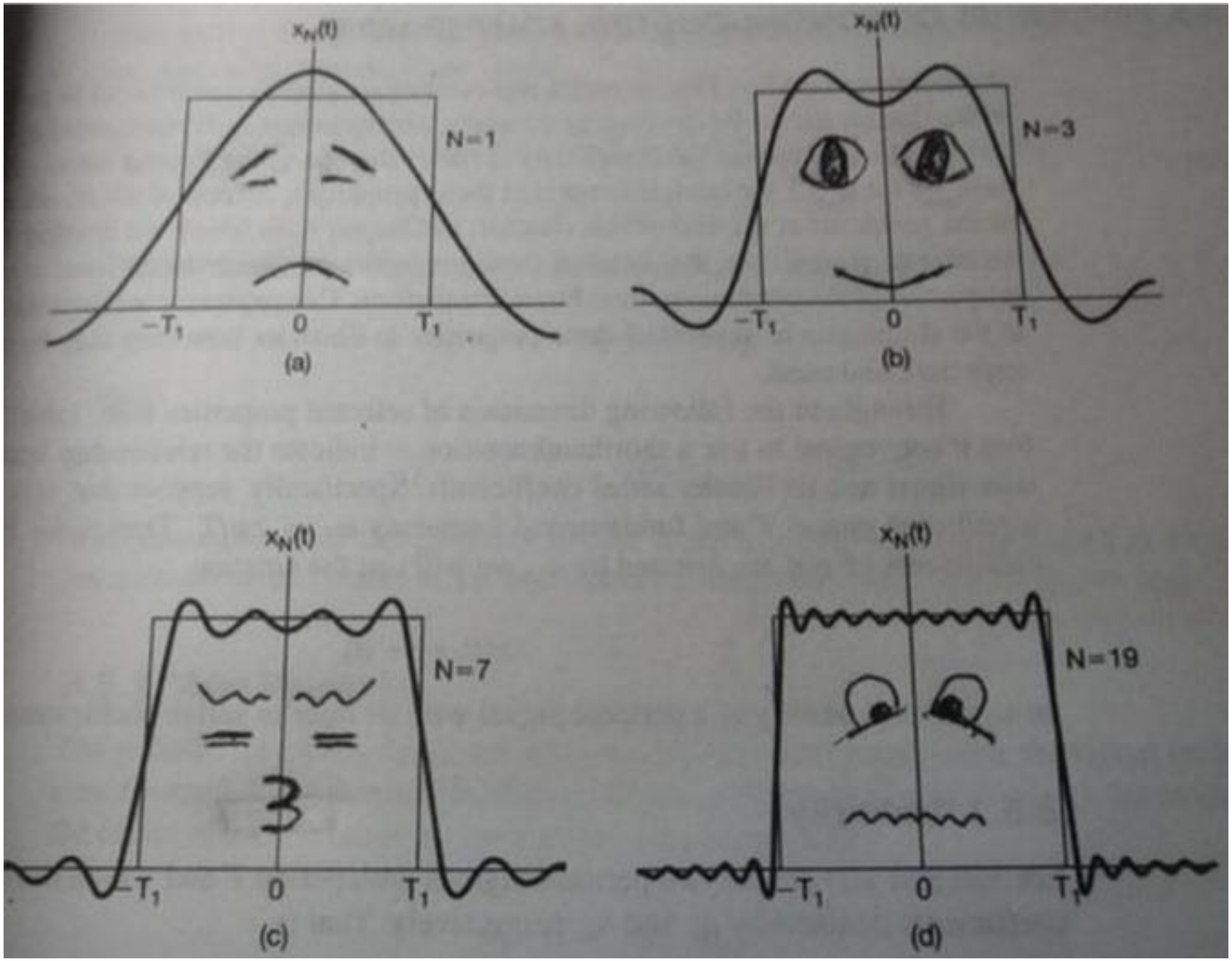
$$\mathrm{F}(hkl) = \sum_{n=1}^{N} f_n \exp(2\pi i\vec{s}\cdot\vec{r}_n) = \sum_{n=1}^{N} f_n \exp\left[2\pi i(hX_n + kY_n + lZ_n)\right]$$

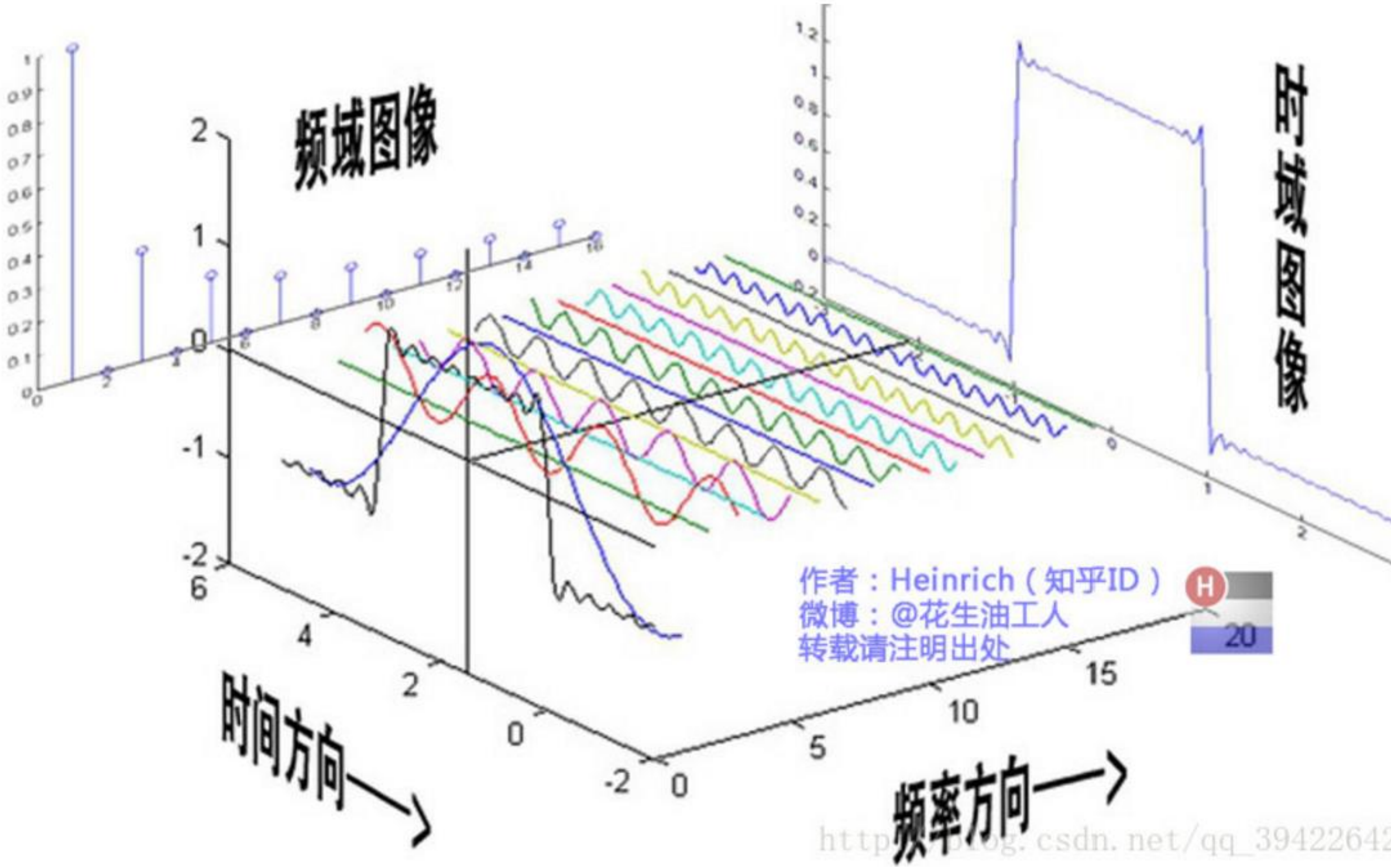


a
b
c
3 nm
[110]
1°
2°
d
e
f
(002)
(1$\bar{1}\bar{1}$)


507x507 pixels; 8-bit; 251K
512x512 pixels; 8-bit; 256K
FFT of 22344596_1 (1).jpg
512x512 pixels; 8-bit; 256K
Inverse FFT of 22344596_1 (1).jpg
507x507 pixels; 8-bit; 251K

时域和频域




频域图像
时域图像
时间方向
频率方向
作者：Heinrich（知乎ID）
微博：@花生油工人
转载请注明出处
http://blog.csdn.net/qq_39422642

考试时间：12月7号，19:00—20:00

考试地点：同上课地点

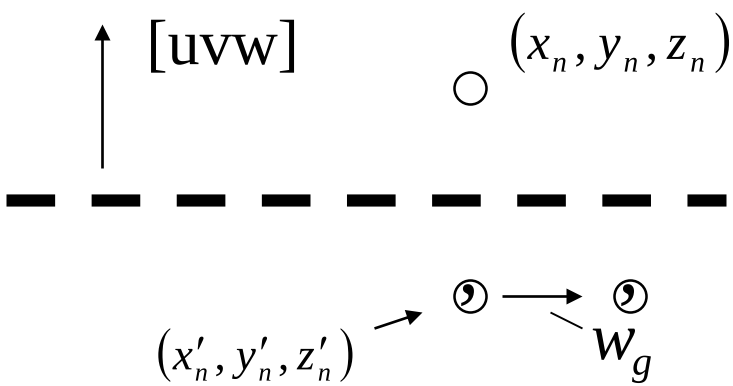
8-5-2 滑移面 ⟶ 晶带反射条件 (P221页）

设: 滑移面 $\perp [u \quad v \quad w]$, 滑移量为 $\vec{w}_g$

则：属于 $[u \quad v \quad w]$ 晶带的 hkl 反射 $(\vec{g}_{hkl} \perp [u \quad v \quad w])$

可能出现的条件是 $\vec{g}_{hkl} \cdot \vec{w}_g = n$

证：
$$F(hkl)=\sum_{n=1}^{N/2} f_n[\exp 2\pi i(hx_n+ky_n+lz_n)+\exp 2\pi i(hx'_n+ky'_n+lz'_n+\vec{g}_{hkl}\cdot\vec{w}_g)]$$
$$=\sum_{n=1}^{N/2} f_n \exp 2\pi i(hx_n+ky_n+lz_n)$$
$$[1+\exp 2\pi i\{h(x'_n-x_n)+k(y'_n-y_n)+l(z'_n-z_n)+\vec{g}_{hkl}\cdot\vec{w}_g\}]$$



由于$\left[x_n' - x_n, y_n' - y_n, z_n' - z_n\right] // \left[uvw\right]$,

$$F\left(hkl\right) = \sum_{n=1}^{N/2} f_n [\exp 2\pi i\left(hx_n + ky_n + lz_n\right)\left[1 + \exp 2\pi i \vec{g}_{hkl} \cdot \vec{w}_g\right]$$

8-5-3　螺旋轴 $\longrightarrow$ 系列反射条件（P223页）

8-5-4 空间群图表所载反射条件

按　整体 → 晶带 → 系列反射条件的顺序

例：　$p.\ 188$　$C12/c1\,(15)$　一般

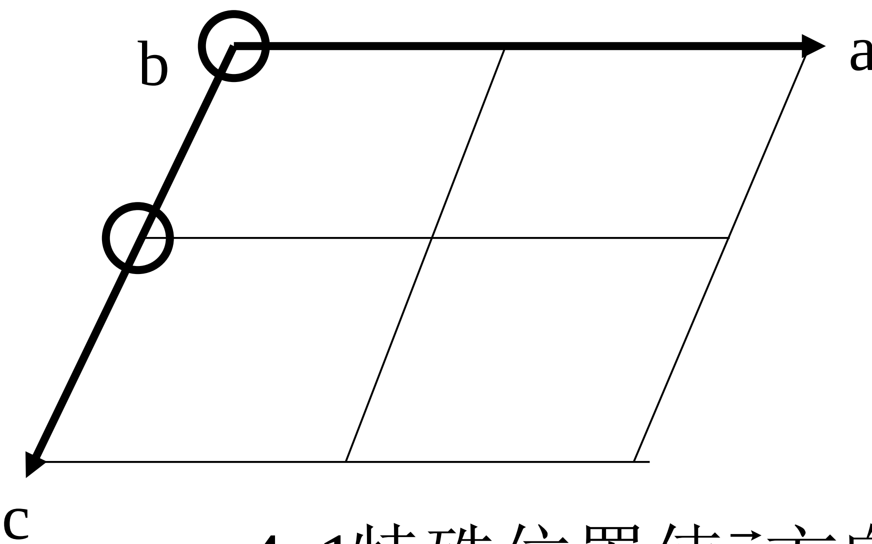
整体：　hkl :　$h + k = 2n \Leftarrow C$心

晶带：
- $h0l$:　$h, l = 2n \Leftarrow c$
- $0kl$:　$k = 2n$
- $hk0$:　$h + k = 2n$

系列：
- $0k0$:　$k = 2n$
- $h00$:　$h = 2n$
- $00l$:　$l = 2n$

特殊

$4a$　1　$0, 0, 0$　$0, 0, \frac{1}{2}$　hkl : $l = 2n$



$4a1$特殊位置使$\vec{c}$方向周期减半，故$l = 2n$

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$			General:
8	f	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	hkl : $h+k=2n$ $0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	e	$m\,.\,.$	$0,y,z$	$0,\bar{y},z$			no extra conditions
4	d	$.\,m\,.$	$x,0,z$	$\bar{x},0,z$			no extra conditions
4	c	$.\,.\,2$	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z$			hkl : $h=2n$
2	b	$m\,m\,2$	$0,\frac{1}{2},z$				no extra conditions
2	a	$m\,m\,2$	$0,0,z$				no extra conditions

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				h,k,l cyclically permutable General:
48	h	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	hkl : $h+k+l=2n$
			(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 : $l=2n$
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $x,y,\bar{z}$	(15) $x,\bar{y},z$	(16) $\bar{x},y,z$	$h00$: $h=2n$
			(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z},x,y$	(19) $z,x,\bar{y}$	(20) $z,\bar{x},y$	
			(21) $\bar{y},\bar{z},\bar{x}$	(22) $y,\bar{z},x$	(23) $\bar{y},z,x$	(24) $y,z,\bar{x}$	

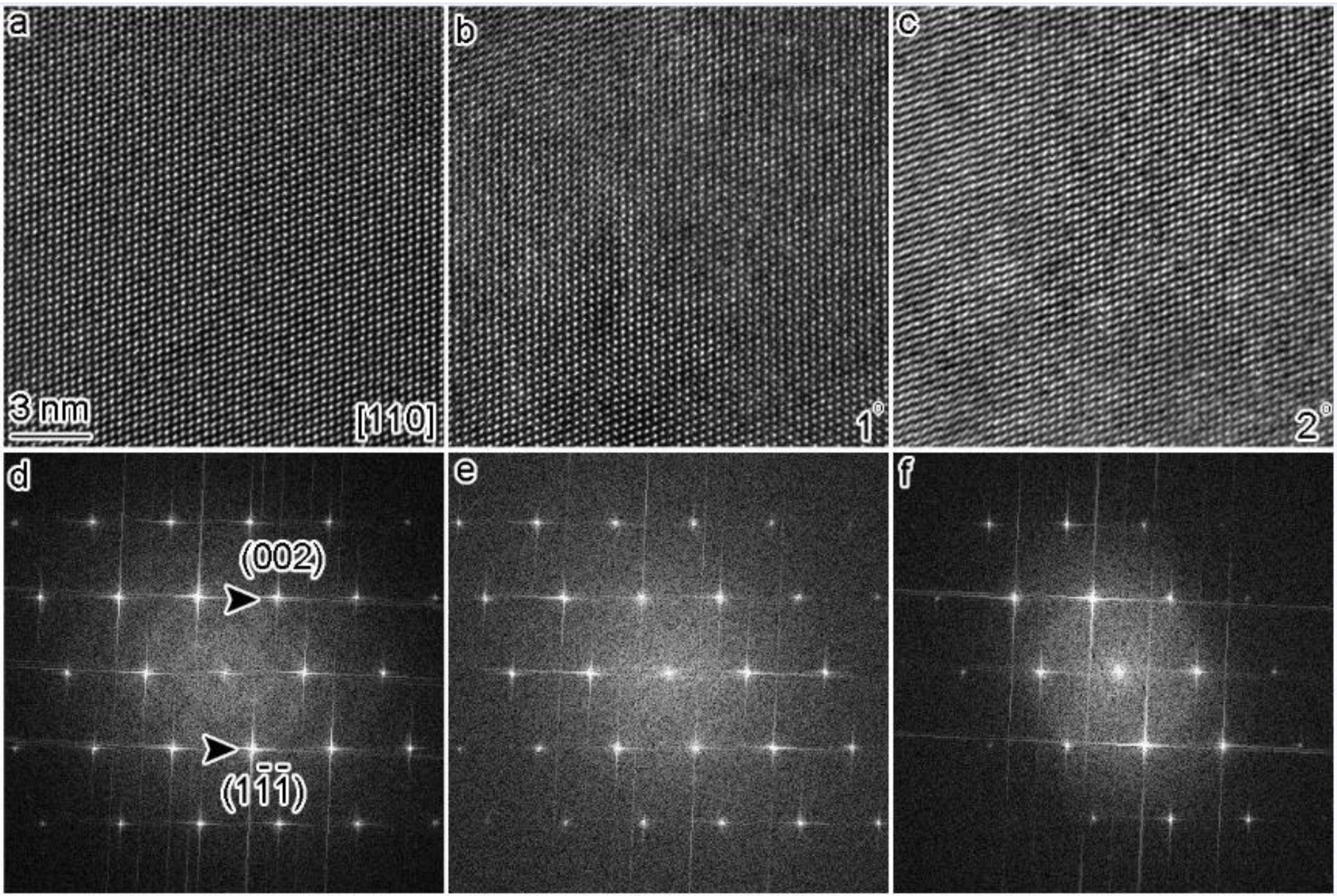
Special: as above, plus

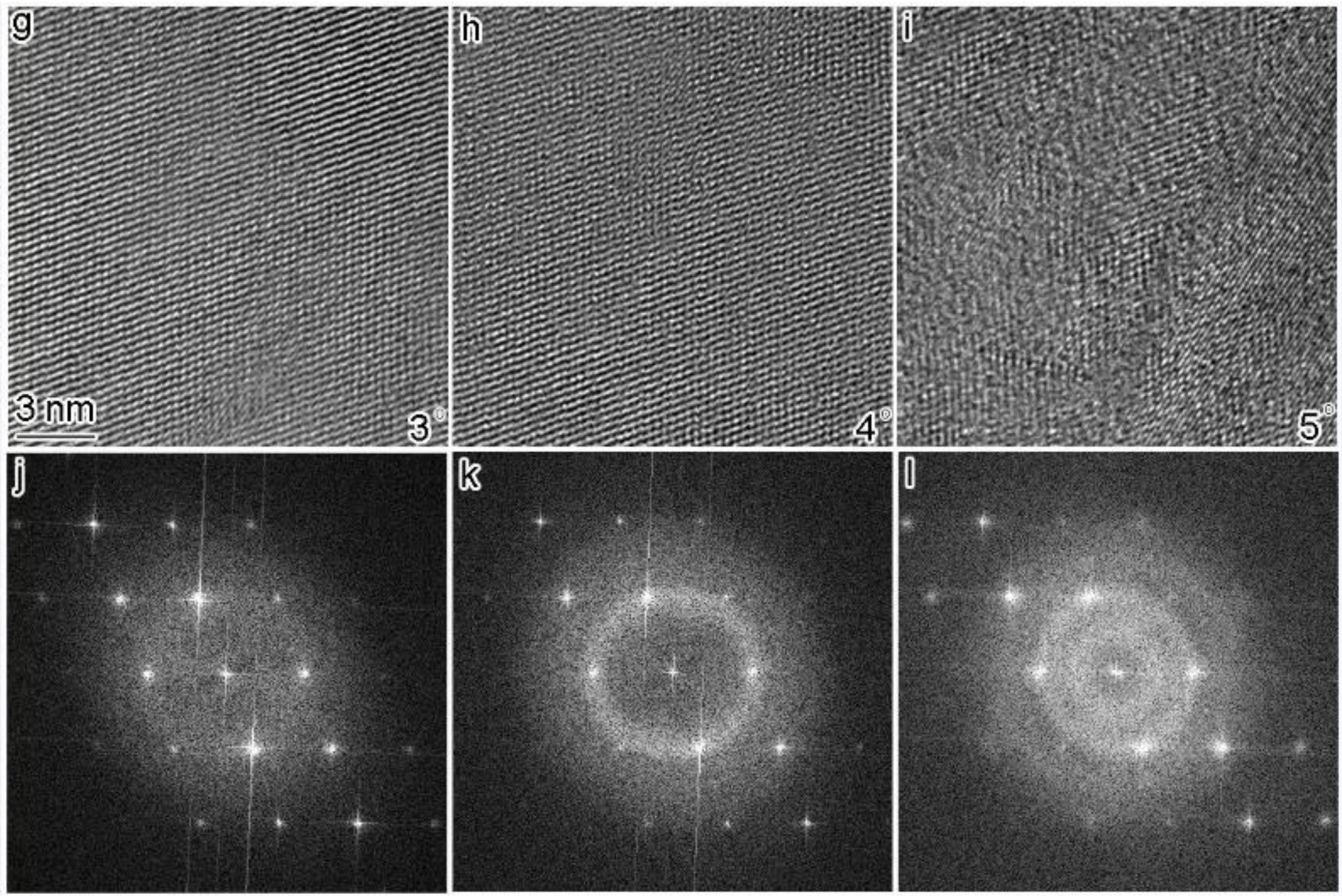
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+\quad(0,\frac{1}{2},\frac{1}{2})+$				General:
8	f	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y,\bar{z}$	hkl : $k+l=2n$ $hk0$: $h,k=2n$ $0kl$: $k+l=2n$ $h0l$: $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	e	2	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}$			no extra conditions
4	d	$\bar{1}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$			hkl : $h+k=2n$
4	c	$\bar{1}$	$0,\frac{1}{4},\frac{1}{4}$	$\frac{1}{2},\frac{3}{4},\frac{1}{4}$			hkl : $h+k=2n$
4	b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl : $h=2n$
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$			hkl : $h=2n$

§8—7　特殊投影的对称性

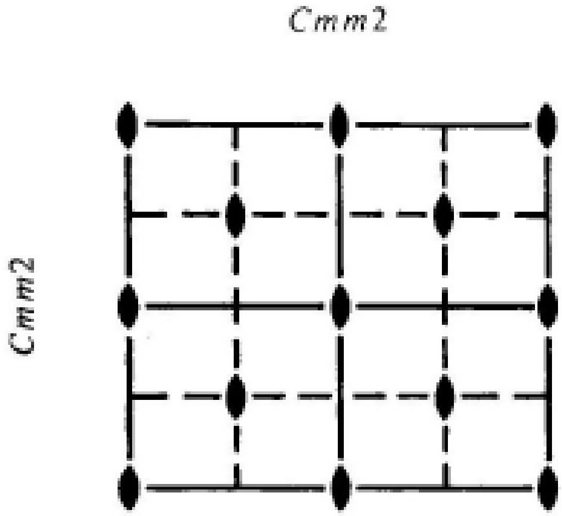


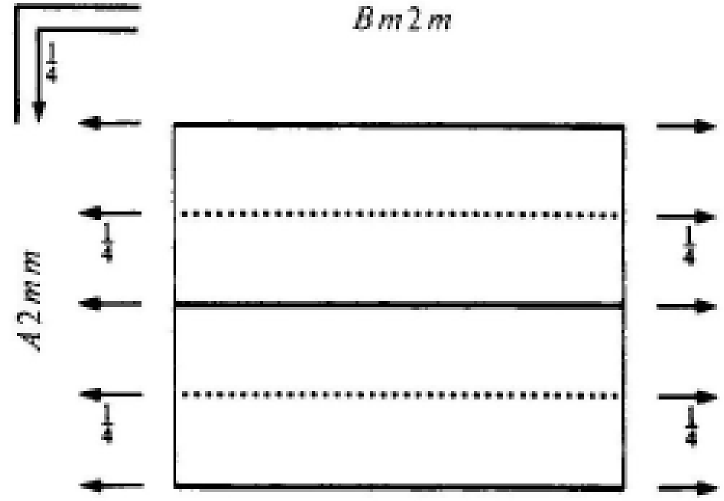


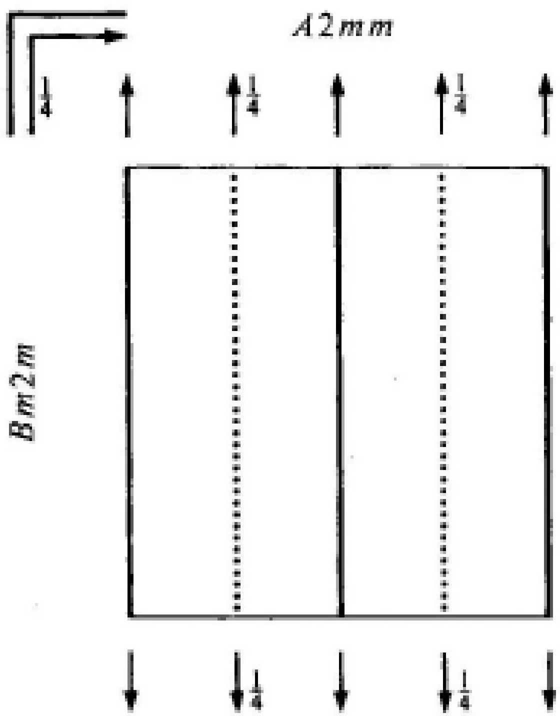
g
h
i
3 nm
3°
4°
5°
j
k
l

8-7-2 有心单胞和对称元素的投影（P233页）

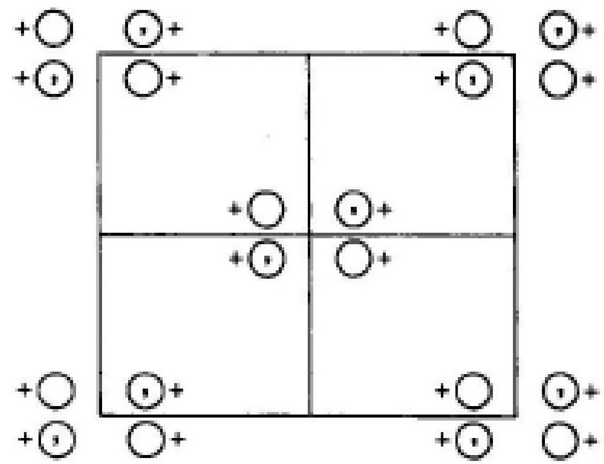
对称元素及投影方向	投影中的对称元素
$\bar{1}$	2
n：沿轴方向	n
n：$\perp$ 轴向，$n=2,4,6$	m
n：$\perp$ 轴向，$n=3$	1
n_m：沿轴方向	m
n_m：$\perp$ 轴向，含有$2(4_2,6_2,6_4)$	n
n_m：$\perp$ 轴向，含有$2(2_1,4_1,4_3,6_1,6_3,6_5)$	g
$\bar{4}$：沿轴方向	4
$\bar{4}$：$\perp$ 轴向	m
$\bar{3}$：沿轴方向	6
$\bar{3}$：$\perp$ 轴向	2
m：$// m$	m
m：$\perp m$	1
g：$// g$，$// w_g$	m
g：$// g$，不 $// w_g$	g
g：$\perp g$	平移t







P186-187， *Cmm*2 (35)



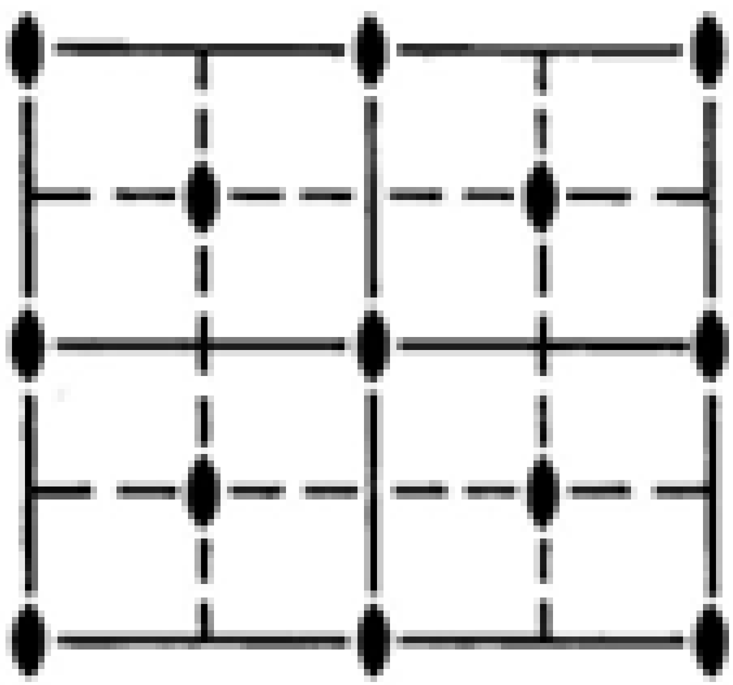
Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

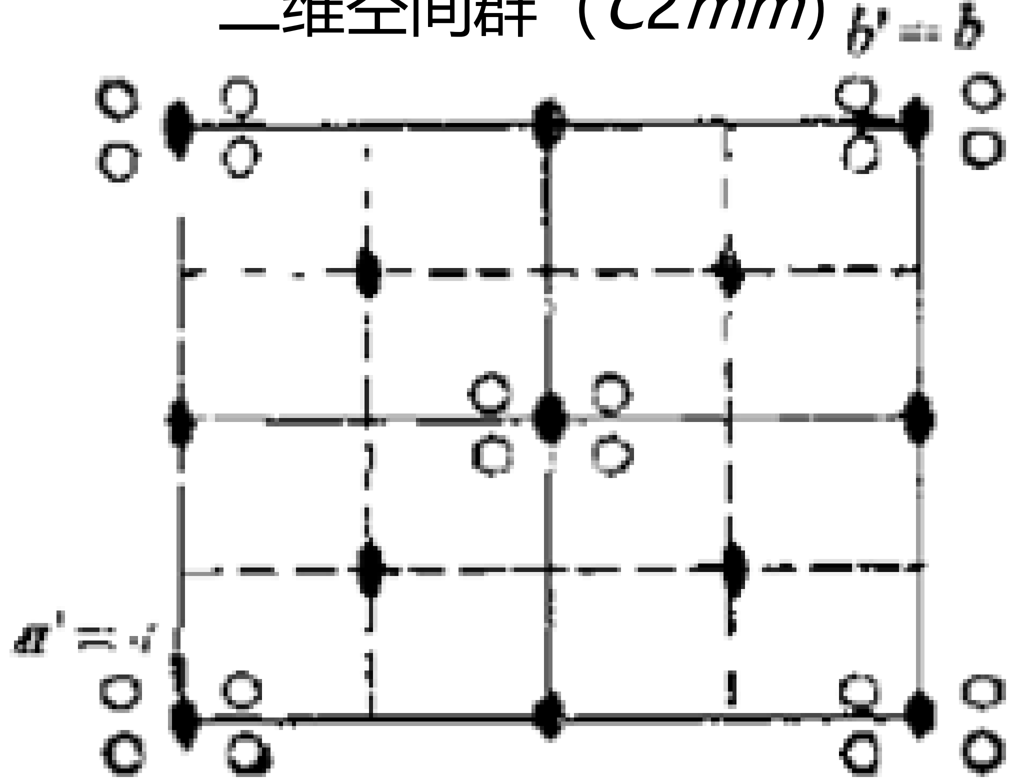
Along [100] $p1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along [010] $p11m$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0, y, 0$

三维空间群（*Cmm*2）



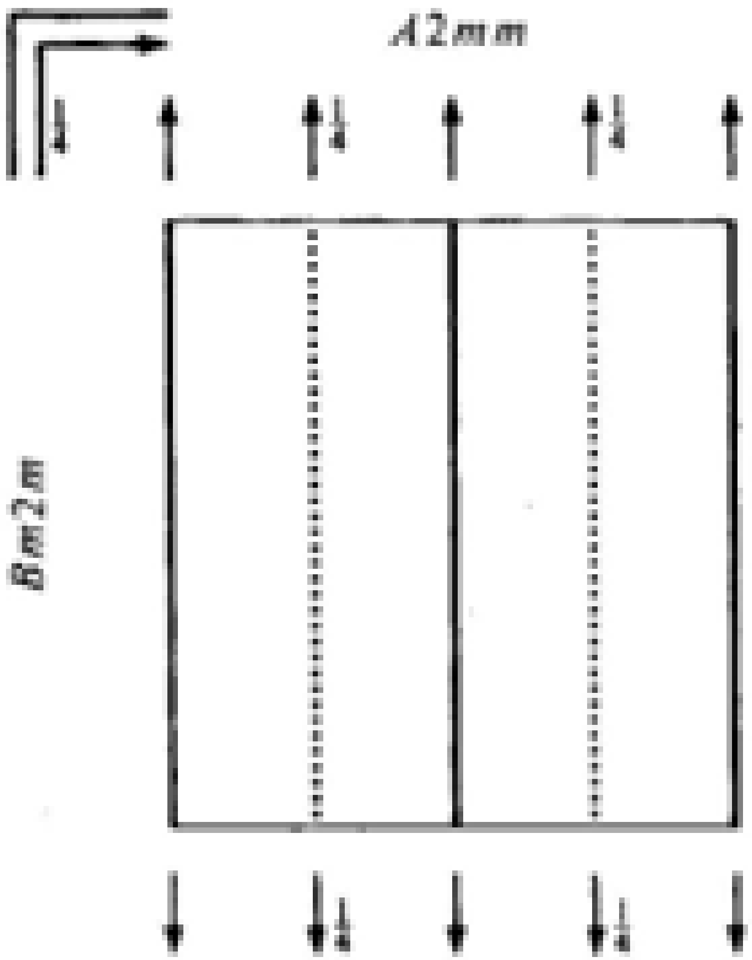
二维空间群（*C*2*mm*）



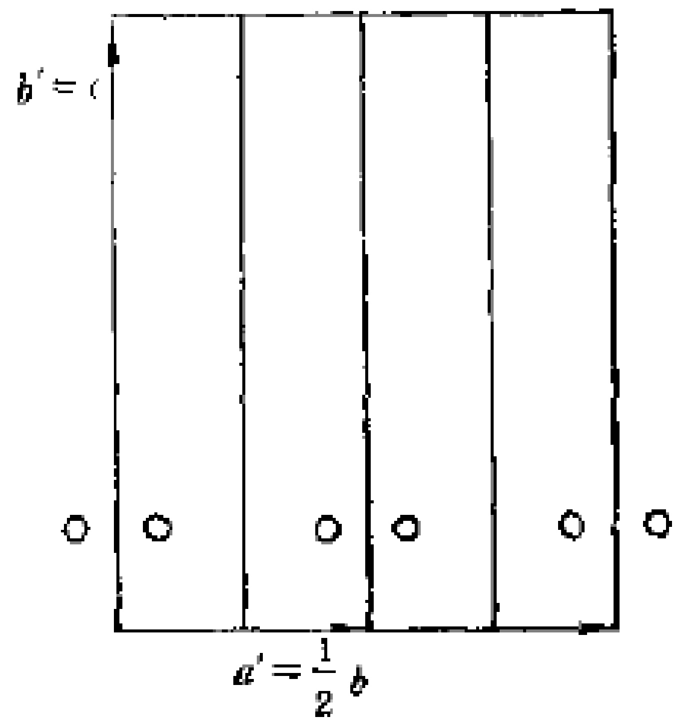
沿[001]方向投影

Symmetry of special projections

Along [001] $c2mm$	Along [100] $p1m1$	Along [010] $p11m$
$\mathbf{a}' = \mathbf{a}$ $\quad \mathbf{b}' = \mathbf{b}$	$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\quad \mathbf{b}' = \mathbf{c}$	$\mathbf{a}' = \mathbf{c}$ $\quad \mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0, 0, z$	Origin at $x, 0, 0$	Origin at $0, y, 0$



二维空间群（$P1m1$）



沿[100]方向投影

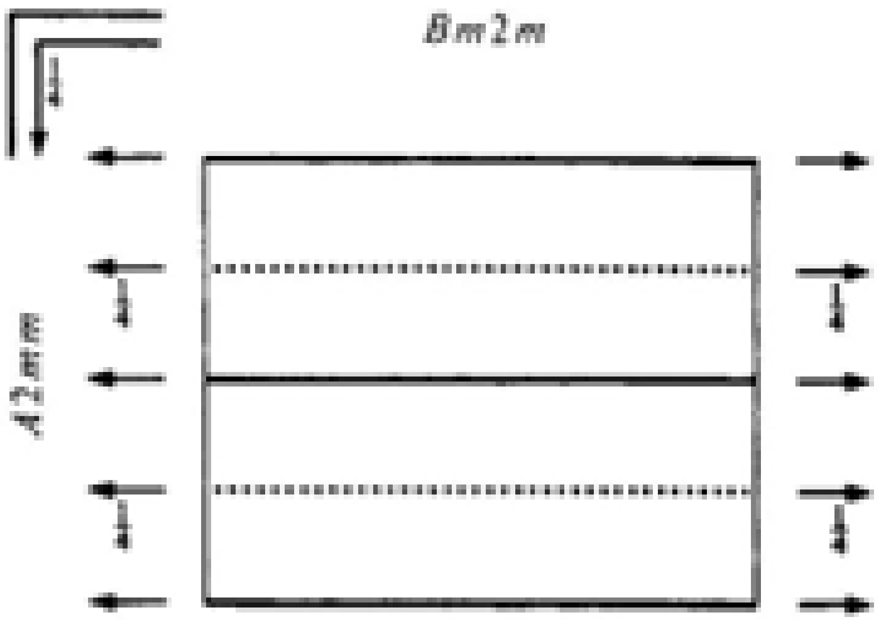
Symmetry of special projections

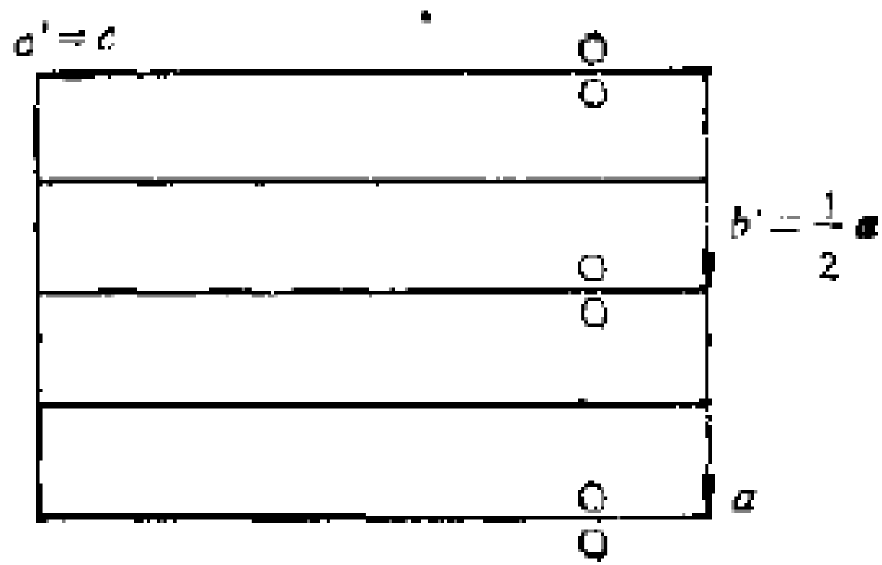
Along [001] $c2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

二维空间群（$P11m$)





沿[010]方向投影

8-8-2 空间群的最大子群　　　　8-8-3 空间群的最大母群

$G \supset H$ ： G是H的母群，H是G的子群

不存在满足条件$G \supset M \supset H$的M :G是H的最小母群

H是G的最大子群

空间群的子群有三种类型：

(I)t子群(同平移子群)： $Cmm2 \supset \begin{matrix} C112 \\ C1m1 \\ Cm11 \end{matrix}$

(II)k子群(同晶类子群)：

(IIa)母子群的惯用胞相同， $\mathrm{Cmm2} \supset \begin{matrix} \mathrm{Pmm2} \\ \mathrm{Pba2} \\ \mathrm{Pbm2} \\ \mathrm{Pma2} \end{matrix}$

子群H失去了G的有心平移

最大不同构子群的个数是有限的

(IIb) H的惯用晶胞比 G大，但H与G不同构

$$Ccc2;\ Cmc2_1;\ Imm2;\ Ibm2;\ Ccm2_1;\ Iba2;\ Ima2$$

$(\mathrm{II}c)$ H的惯用胞比G大，且H与G同构（同一种空间群或互相对映的空间群）

$$\underbrace{\mathrm{Cmm2}(\mathrm{abc}) \supset Cmm2\begin{pmatrix} a' = 3a \\ \text{或}\mathrm{b}' = 3b \\ \text{或}\mathrm{c}' = 2c \end{pmatrix}}_{\text{最低指数的最大同构子群}} \qquad \left.\begin{matrix} \mathrm{a}' = (2\mathrm{n}+1)a \\ \text{或}\mathrm{b}' = (2n+1)b \\ \text{或}\mathrm{c}' = nc \end{matrix}\right\}\text{最大同构子群无限多}$$

素数

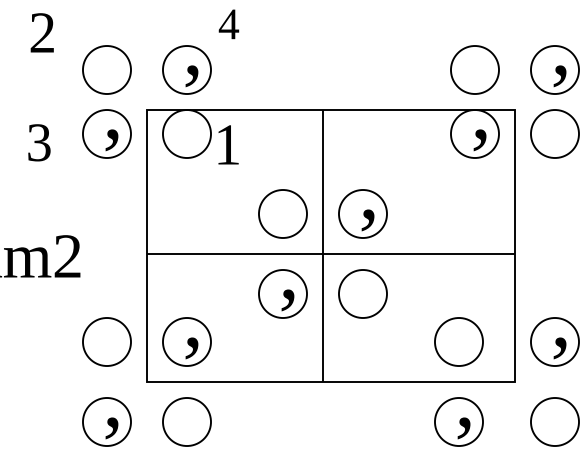
$$P23(a,b,c) \supset P23(a' = 3a, b' = 3b, c' = 3c)$$

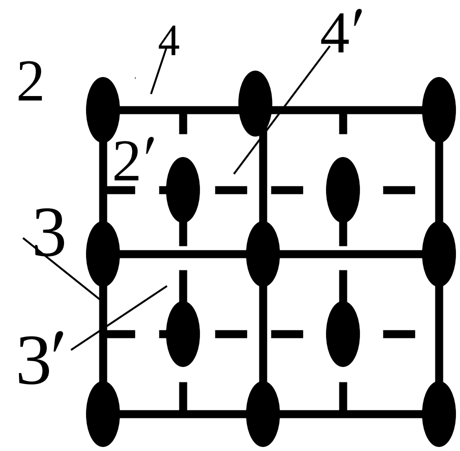
$$\text{但}P23(a,b,c) \supset I23(a' = 2a, b' = 2b, c' = 2c) \supset \underline{P23(a' = 2a, \cdots)}$$

不是最大子群

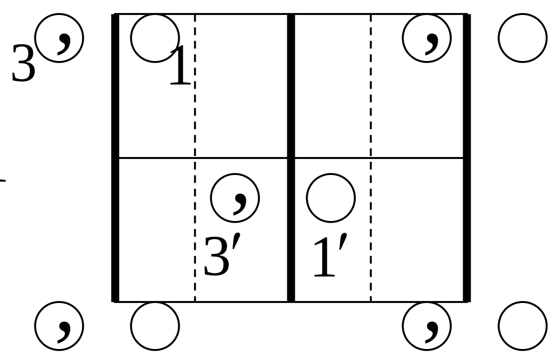
8-8-1 空间群的子群

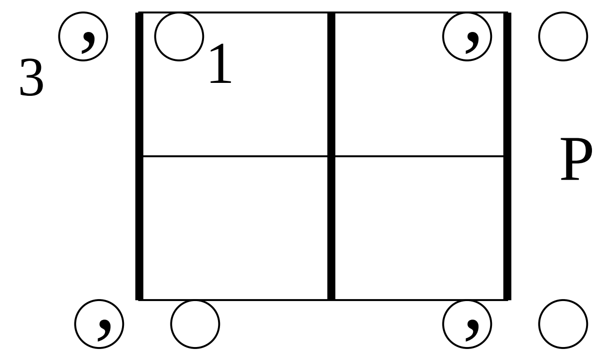
Cmm2



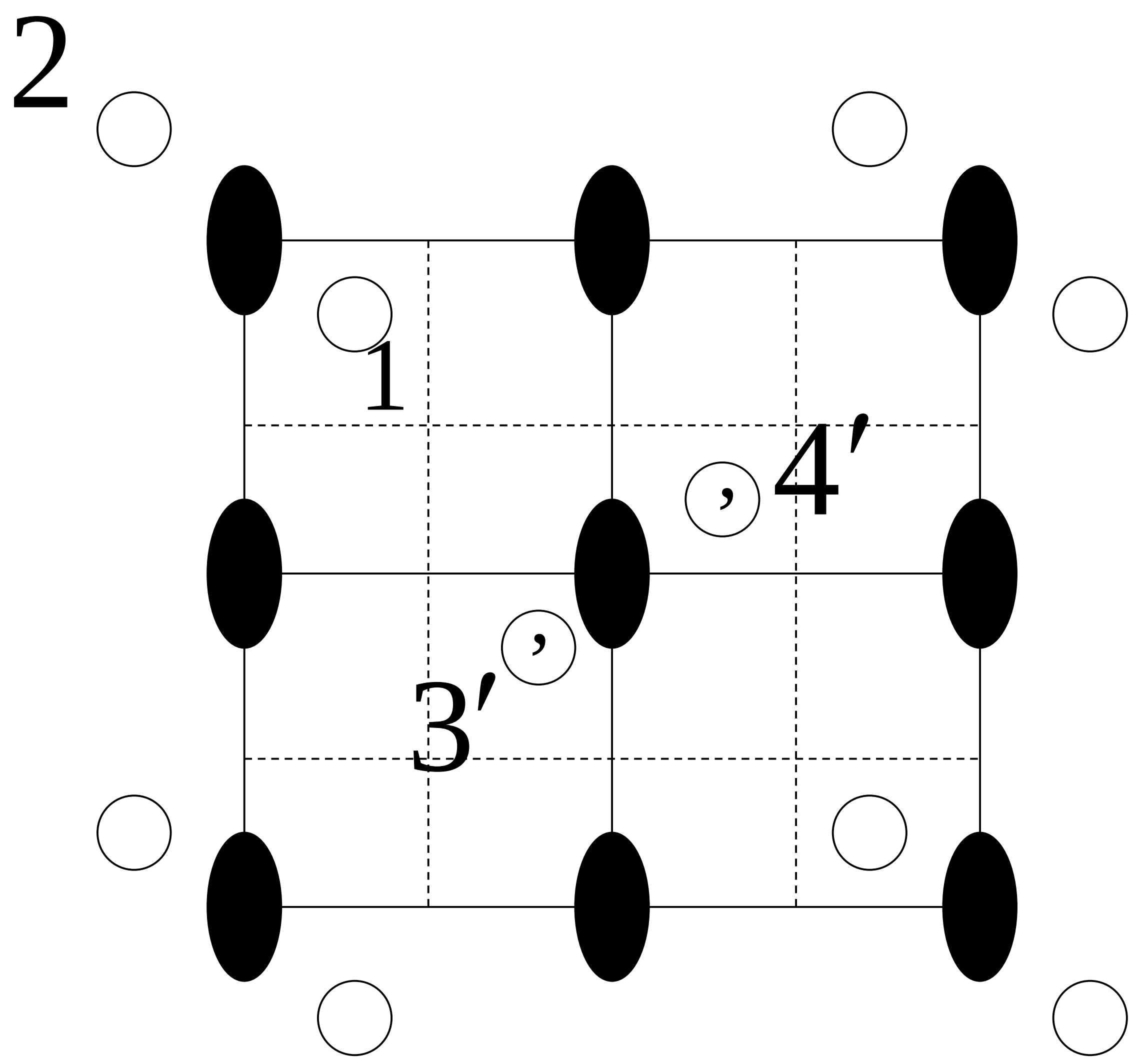


C1m1

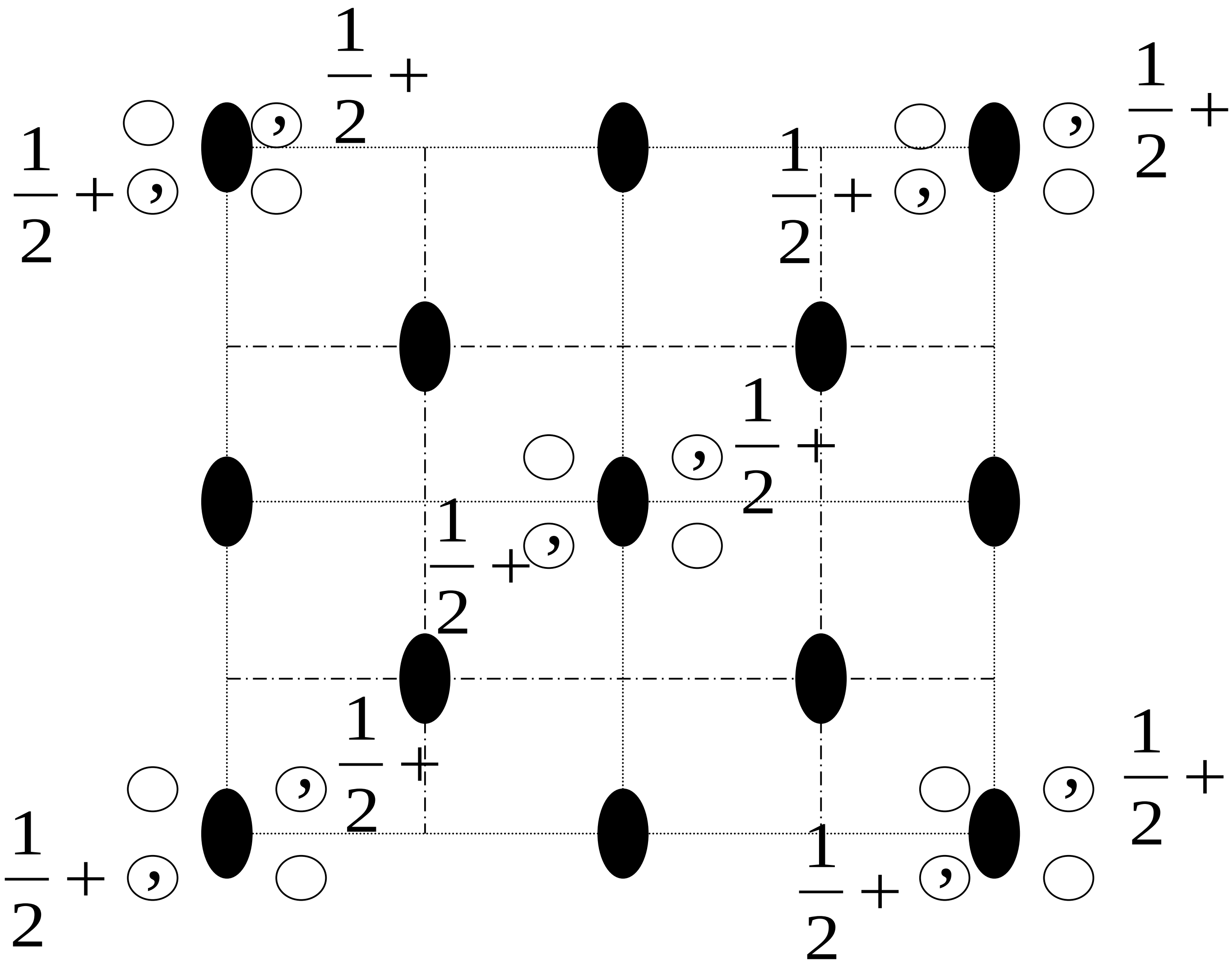




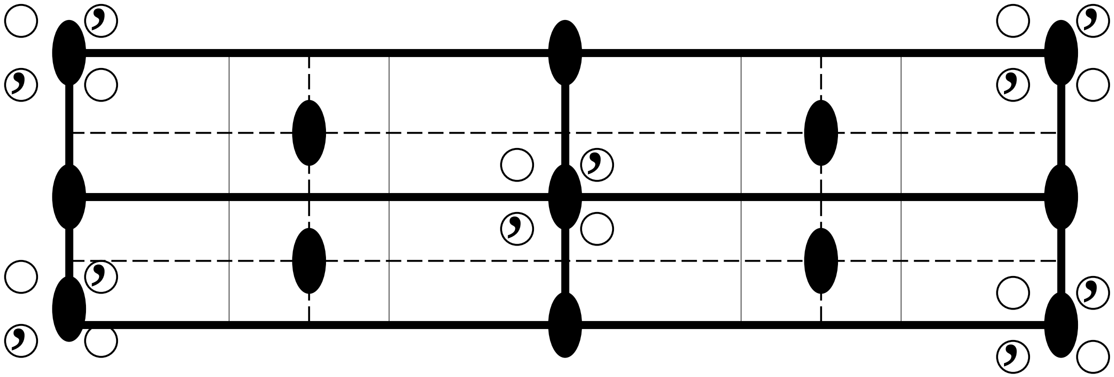
P1m1



Pba2



Ccc2
C’=2c



Cmm2 $\quad b' = 3b$

$Cmm2$ C_{2v}^{11} $mm2$ Orthorhombic

No. 35 $Cmm2$ Patterson symmetry $Cmmm$

Maximal non-isomorphic subgroups

I	[2] $C1m1$ (Cm, 8)	(1; 3)+
	[2] $Cm11$ (Cm, 8)	(1; 4)+
	[2] $C112$ ($P2$, 3)	(1; 2)+
IIa	[2] $Pba2$ (32)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbm2$ ($Pma2$, 28)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pma2$ (28)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmm2$ (25)	1; 2; 3; 4

IIb [2] $Ima2$ ($\mathbf{c}' = 2\mathbf{c}$) (46); [2] $Ibm2$ ($\mathbf{c}' = 2\mathbf{c}$) ($Ima2$, 46); [2] $Iba2$ ($\mathbf{c}' = 2\mathbf{c}$) (45); [2] $Imm2$ ($\mathbf{c}' = 2\mathbf{c}$) (44); [2] $Ccc2$ ($\mathbf{c}' = 2\mathbf{c}$) (37); [2] $Cmc2_1$ ($\mathbf{c}' = 2\mathbf{c}$) (36); [2] $Ccm2_1$ ($\mathbf{c}' = 2\mathbf{c}$) ($Cmc2_1$, 36)

Maximal isomorphic subgroups of lowest index

IIc [2] $Cmm2$ ($\mathbf{c}' = 2\mathbf{c}$) (35); [3] $Cmm2$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (35)

Minimal non-isomorphic supergroups

I [2] $Cmmm$ (65); [2] $Cmme$ (67); [2] $P4mm$ (99); [2] $P4bm$ (100); [2] $P4_2cm$ (101); [2] $P4_2nm$ (102); [2] $P\bar{4}2m$ (111); [2] $P\bar{4}2_1m$ (113); [3] $P6mm$ (183)

II [2] $Fmm2$ (42); [2] $Pmm2$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}$) (25)

Cm C_s^3 m Monoclinic

No. 8 $A\,1\,1\,m$ Patterson symmetry $A\,1\,1\,2/m$

Origin on mirror plane m

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) $m\ \ x,y,0$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $b\ \ x,y,\frac{1}{4}$

$(\mathrm{III})H$是G的子群，但他们的平移群和晶类都不相同

$Hermann$定理(1929)

$$G \underbrace{\supset}_{\text{同平移}} M \underbrace{\supset}_{\text{同晶类}} H$$

8-8-4 空间群图表所载关于母子群的信息

H是G的最大不同构子群　　最低指数的最大同构子群

G是H的最小不同构母群　　最低指数的最小同构母群

8-6-2 patterson函数

一维： $$P(x)=a\int_0^1 \rho(X)\rho(X+x)dX$$

Patterson函数是
原子对相关函数，
其峰不代表原子位置，
代表原子对间的位矢

三维： $$\mathrm{P}(\vec{r})=\int_{V_c}\rho(\vec{R})\rho(\vec{R}+\vec{r})d\vec{R}$$

$$P(x,y,z)=V_c\int_0^1 dX\int_0^1 dY\int_0^1 dZ\rho(X,Y,Z)\rho(X+x,Y+y,Z+z)$$

把$(8-25b)$代入，得$P(x,y,z)=$

$$\frac{1}{V_c}\sum_{h'}\sum_{k'}\sum_{l'}\sum_{h}\sum_{k}\sum_{l}F(h'k'l')F(hkl)\exp[-2\pi i(hx+ky+lz)]$$

$$\int_0^1 dX \int_0^1 dY \int_0^1 dZ \exp\{-2\pi i[(h'+h)X+(k'+k)Y+(l'+l)Z]\}$$

$$= \frac{1}{V_c}\sum_h \sum_k \sum_l |F(hkl)|^2 \exp[-2\pi i(hx+ky+lz)]$$

*Patterson*函数是可实验测定的$|F|^2$的*Fourier*变换

8－6－3 Patterson函数的对称性

晶体结构的空间群符号 $\xrightarrow{(1)\text{变成点式空间群};(2)\text{加}\bar{1}}$ *Patterson* 空间群符号

第八章习题：1，4（1-2），13（1-2），14，20，23，24

https://crystalsymmetry.wordpress.com/

The Fascination of Crystals and Symmetry

Crystals are fascinating objects.

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