

Bilbao Crystallographic Server → k-vector types and Brillouin zones

The k-vector types of space group 225 [Fm-3m]

Brillouin zone

(Diagram for arithmetic crystal class m -3 m F)

Asymmetric unit (up) Representation domain of CDML (down) Fm -3 m - Oh⁵ (225) to Fd -3 c-Oh⁸ (228)

Reciprocal-space group (Im -3 m)*, No. 229

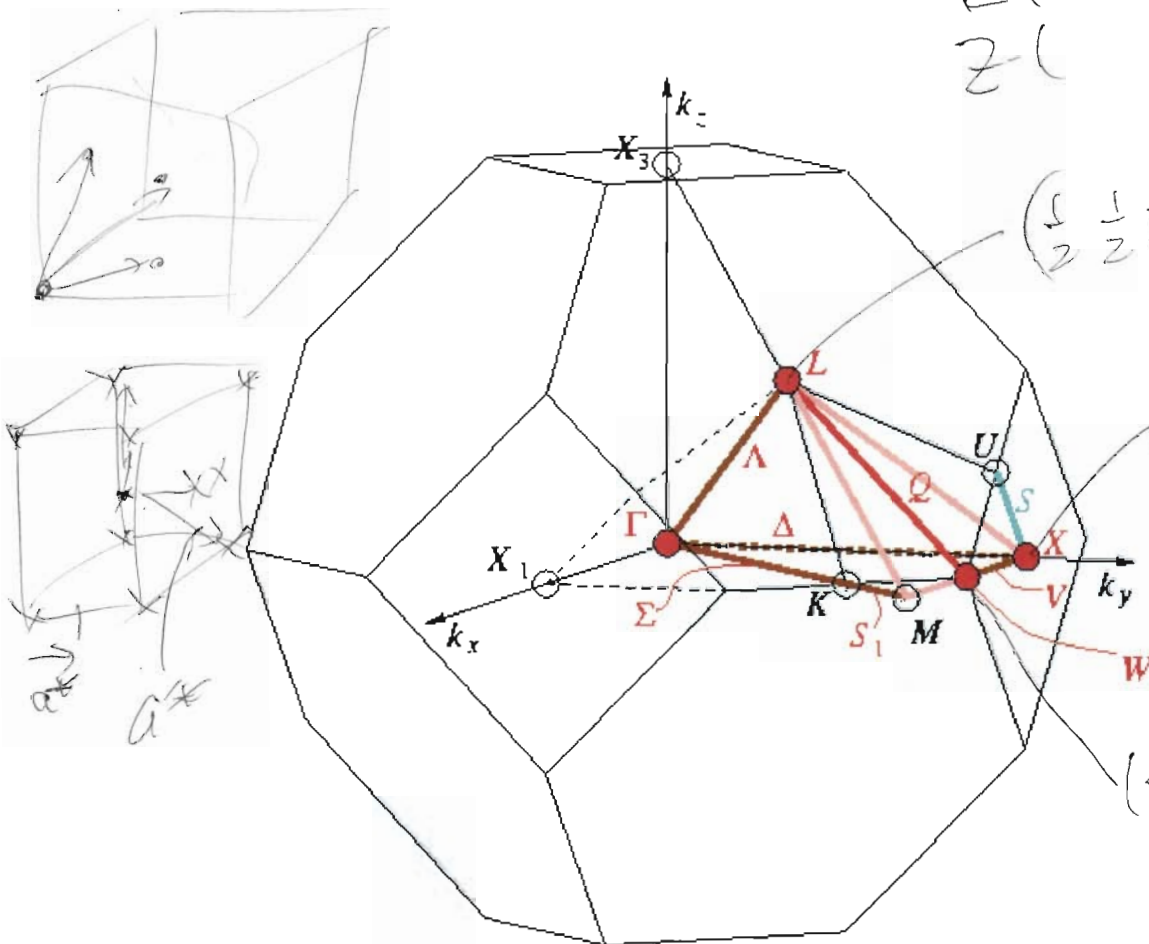
[The table with the k vectors]

$$\begin{aligned} \kappa &= \left(\frac{3}{4} \frac{3}{4} 0 \right) \\ \xi &= \left(1 \frac{1}{4} 0 \right) \end{aligned}$$

$$\left(\frac{1}{2} \frac{1}{2} \frac{1}{2} \right) = \left(\frac{1}{2} \frac{1}{2} \frac{1}{2} \right)$$

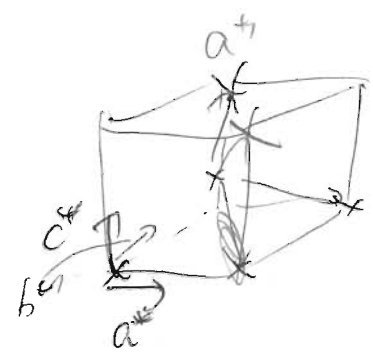
Wien.
 $\left(\frac{1}{2} \frac{1}{2} \frac{1}{2} \right) = \left(0 0 \frac{1}{2} \right)$
 C*

$$\left(\frac{1}{2} \frac{1}{4} \frac{3}{4} \right) = \left(1 \frac{1}{2} 0 \right)$$



[The PostScript file with the Brillouin zone]

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \\ 1 \\ -1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix}$$



$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \\ 1 \\ -1 \end{pmatrix} \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}$$

Wien

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \times$$

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \times$$

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

$$\begin{pmatrix} 1 \\ \frac{1}{2} \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 3 \\ 2 \end{pmatrix}$$

Bilbao Crystallographic Server → k-vector types and Brillouin zones

The k-vector types of space group 225 [*Fm-3m*]

(Table for arithmetic crystal class $m-3mF$)

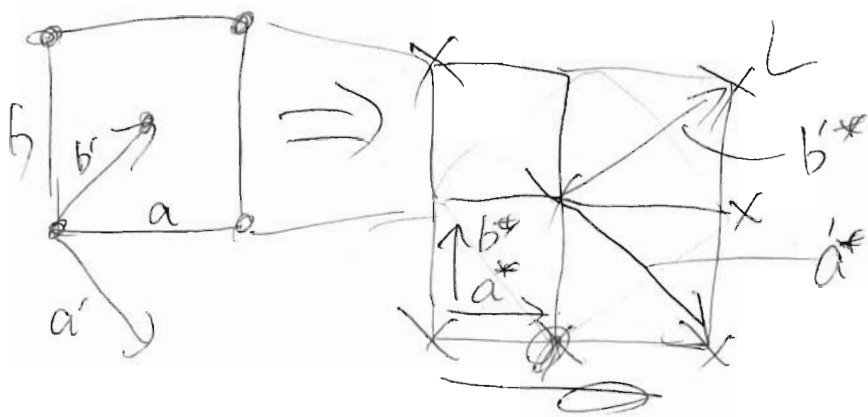
$Fm-3m-O_h^5$ (225) to $Fd-3c-O_h^8$ (228)

Reciprocal-space group ($Im-3m$)*, No. 229

[Brillouin zone]

k-vector label		Wyckoff position			Parameters
CDML		ITA			ITA
GM	0,0,0	2	a	m-3m	0,0,0
X	1/2,0,1/2	6	b	4/mm.m	0,1/2,0
L	1/2,1/2,1/2	8	c	.-3m	1/4,1/4,1/4
W	1/2,1/4,3/4	12	d	-4m.2	1/4,1/2,0
DT	u,0,u	12	e	4m.m	x,0,0: 0<x<1/2
LD	u,u,u	16	f	.3m	x,x,x: 0<x<1/4
V	1/2,u,1/2+u	24	g	mm2..	x,1/2,0: 0<x<1/4
SM	u,u,2u	24	h	m.m2	x,x,0: 0<x<3/8
S	1/2+u,2u,1/2+u	24	h	m.m2	x,1/2,x: 0<x<1/8
S ~ S ₁ [KM]					x,x,0: 3/8<x<1/2
SM + S ₁ [GM M]		24	h	m.m2	x,x,0: 0<x<1/2
Q	1/2,1/4+u,3/4-u	48	i	..2	1/4,1/2-y,y: 0<y<1/4
A	u,-u+v,v	48	j	m..	x,y,0: 0<x<y<3/8 +
					+ x,y,0: 0<x<3/4-y<y<1/2
B	1/2+u,u+v,1/2+v				48
B ~ B ₁ [KMW]		x,y,0: 3/4-y<= x<= y<1/2			
A + B ₁ [GM MX]		48	j	m..	x,y,0: 0<x<y<1/2
C	u,u,v	48	k	..m	x,x,z: 0<z<x<=1/4 +
					+ x,x,z: 0<z<3/4-2x<x
J	u,v,u [XUL]	48	k	..m	x,y,x: 0<x<y<1/2-x +
					+ x,y,x: 0 < x < 1/8 < 1/2 - x < y < 1/2 +
					+ x,y,x: 1/8<x<1/2-x<y< 3/4-2x
J ~ J ₁ [GM LX ₃] + [LKM]					x,x,z: 0<x<z<1/2-x +
C + J ₁ [GM MX ₃] \ [GM L]		48	k	..m	+ x,x,z: 0<z<3/8-1/2 z<x< 1/2-z
		48	k	..m	x,x,z: 0<z < 1/2 - x < 1/2, x z

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$$\begin{array}{l}
 a^*, b^* \quad a^* b^* \\
 X = \begin{pmatrix} L & 0 \\ 2 & 2 \end{pmatrix} \quad \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ 2 & 2 \end{pmatrix} \\
 L \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ 2 & 2 \end{pmatrix} \quad \begin{pmatrix} 0 & \frac{1}{2} \\ 1 & 1 \end{pmatrix}
 \end{array}$$

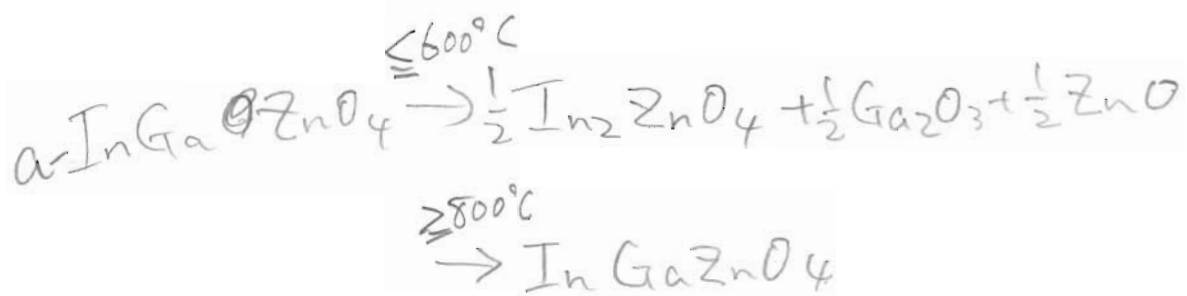
$$|a'| < |a| \quad |a^*| > |a^*|$$

$$\begin{pmatrix} a' \\ b' \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}$$

$$\begin{pmatrix} a'^* \\ b'^* \end{pmatrix} = \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}^T \begin{pmatrix} a^* \\ b^* \end{pmatrix}$$

$$x = a^* \frac{1}{2} = a'^* + b'^*$$

$$\begin{aligned}
 \begin{pmatrix} x & y \end{pmatrix} \begin{pmatrix} a^* \\ b^* \end{pmatrix} &= \begin{pmatrix} x & y' \end{pmatrix} \begin{pmatrix} a'^* \\ b'^* \end{pmatrix} \\
 &= \begin{pmatrix} x' & y' \end{pmatrix}^T \begin{pmatrix} a'^* \\ b'^* \end{pmatrix} \\
 \begin{pmatrix} x \\ y \end{pmatrix} &= T^t \begin{pmatrix} x' \\ y' \end{pmatrix}
 \end{aligned}$$



Bilbao Crystallographic Server → k-vector types and Brillouin zones

The k-vector types of space group 230 [*Ia-3d*]

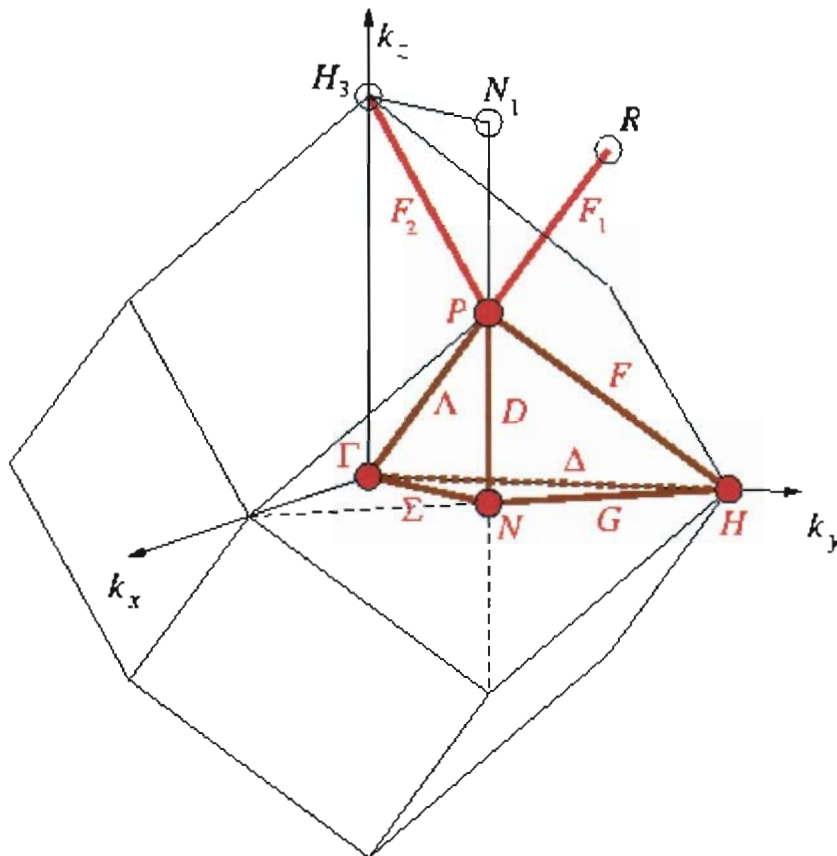
Brillouin zone

(Diagram for arithmetic crystal class $m\bar{3}m$)

$Im\bar{3}m-O_h^9$ (229), $Ia\bar{3}d-O_h^{10}$ (230)

Reciprocal-space group ($Fm\bar{3}m$)*, No. 225

[The table with the k vectors]



[The PostScript file with the Brillouin zone]

Bilbao Crystallographic Server → k-vector types and Brillouin zones

The k-vector types of space group 230 [*Ia-3d*]

(Table for arithmetic crystal class $m-3m$)

$Im-3m-O_h^9$ (229), $Ia-3d-O_h^{10}$ (230)

Reciprocal-space group ($Fm-3m$)*, No. 225

[Brillouin zone]

k-vector label		Wyckoff position			Parameters
CDML		ITA			ITA
GM	0,0,0	4	a	$m-3m$	0,0,0
H	1/2,-1/2,1/2	4	b	$m-3m$	0,1/2,0
P	1/4,1/4,1/4	8	c	-4 3m	1/4,1/4,1/4
N	0,0,1/2	24	d	m.mm	1/4,1/4,0
DT	u,-u,u	24	e	4m.m	0,y,0: 0<y<1/2
LD	u,u,u	32	f	.3m	x,x,x: 0<x<1/4
F	1/2-u,-1/2+3u,1/2-u ex hspace-0.5em	32	f	.3m	x,1/2-x,x: 0<x<1/4
	F ~ F ₁ [PR]				x,x,x: 1/4<x<1/2
	F ~ F ₂ [PH ₃]				x,x,1/2-x:0<x<1/4
	LD + F ₁ [GM R] \ [P]				x,x,x: 0<x<1/2, x !=1/4
D	u,u,1/2-u	48	g	2.mm	1/4,1/4,z: 0<z<1/4
SM	0,0,u	48	h	m.m2	x,x,0: 0<x<1/4
G	1/2-u,-1/2+u,1/2	48	i	m.m2	x,1/2-x,0: 0<x<1/4
A	u, -u, v	96	j	m..	x,y,0: 0<x<y<1/2-x
B	u+v,-u+v,1/2-v	96	k	..m	x,1/2-x,z: 0<z<x<1/4
	B ~ B ₁ [PN ₁ H ₃]				x,x,z: 0<x<1/2-x<z<1/2
C	u,u,v	96	k	..m	x,x,z: 0<z<x<1/4
J	u, v, u	96	k	..m	x,y,x: 0<x<y<1/2-x
	J ~ J ₁ [GM PH ₃]				x,x,z: 0<x<z<1/2-x
	C + B ₁ + J ₁ [GM NN ₁ H ₃] \				96
	\ [P, PH ₃]	with z x, z !=1/2-x			
GP	u,v,w	192	l	1	x,y,z: 0<z<x<y<1/2-x

⑧ → ~~⑨~~ (木村部) カサカサ, 尻中, 平山, カサカサ, 三木, 赤津, 田, 若甲

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