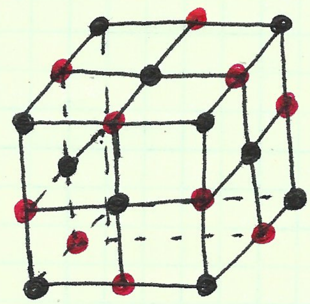
Lect 12: Examples of space group

① NaCl (O_h^5 or $Fm3m$, or $F\bar{3}42''$)



The Bravis lattice — look at black spot FCC. The fcc has three non-primitive lattice vectors

$$\begin{cases} \vec{t}_1 = (1,0\,0) \\ \vec{t}_2 = (0,1\,0) \\ \vec{t}_3 = (0,0\,1). \end{cases}$$

The primitive vectors are $\vec{a}_1 = (\tfrac{1}{2}\,\tfrac{1}{2},0)$, $\vec{a}_2 = (\tfrac{1}{2}\,0\,\tfrac{1}{2})$, $\vec{a}_3 = (0,\tfrac{1}{2},\tfrac{1}{2})$.

The translation group $\boxed{T_f = T_t \otimes \{E,\ T(0,\tfrac{1}{2}\tfrac{1}{2}),\ T(\tfrac{1}{2},0\tfrac{1}{2}),\ T(\tfrac{1}{2}\tfrac{1}{2},0)\}}$

The space group for NaCl is a symmorphic one. The crystalline point group is O_h, which has 48 symmetry operation. Hence

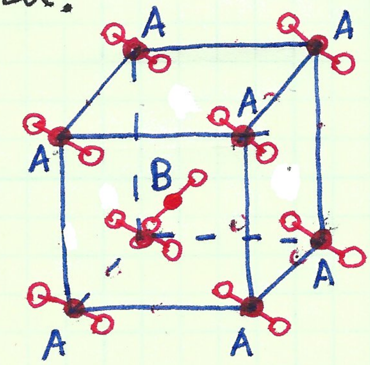
$$O_h^5 = g(E,0)\,T_f + g(R_2,0)\,T_f + \cdots + g(R_{48},0)\,T_f$$

The coset is just O_h. No fractional translation is involved.

2 TiO_2 (D_{4h}^{14} , $P\,4_2/mnm$) — non-symmorphic

The Bravais lattice is primitive tetragonal.

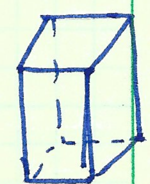
A and B sites form a pair of lattices at a relative shift along $\vec{\tau} = \frac{1}{2}(\vec{a}_1 + \vec{a}_2 + \vec{a}_3)$



The translation group T_ℓ

$\vec{t}_1 = (1,0,0)$, $\vec{t}_2 = (0,1,0)$, $\vec{t}_3 = (0,0,1)$

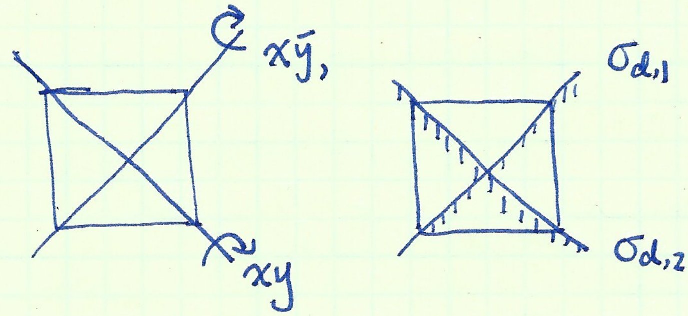
The crystalline point group D_{4h}, which has 16 elements



(points A or B sites)

$D_{4h} = D_{2h} \oplus C_{4,z} D_{2h}$.

1 We can check that the 8 operations in the $D_{2h} = \{E, C_{2,z}, C_{2,xy}, C_{2,x\bar{y}}, I, \sigma_h, \sigma_{d,1}, \sigma_{d,2}\}$,



they are all symmetries of TiO_2 cystal.

2 But for the operations in the coset of $C_{4,z} D_{2h}$, they are not the symmetry operations. $C_{4z} D_{2h} = \{C_{4z}, C_{4,z}^3, C_{2x}, C_{2,y}, S_4, S_4^3, \sigma_{v_x}, \sigma_{v_y}\}$

These operations need to be combined with the translation of $\vec{\tau}$.

After these operations, the orientation of the TiO_2 trimers on A is reflected, to be in the same as B.

$$\Rightarrow D_{4h}^{14} = g(E,0)T_l \oplus g(C_{2,z},0)T_l \oplus g(C_{2,xy},0)T_l \oplus g(C_{2x\bar{y}},0)T_l$$

$$+\ g(I,0)T_l \oplus g(\sigma_h,0)T_l \oplus g(\sigma_{d,1},0)T_l \oplus g(\sigma_{d,2},0)T_l$$

$$+\ g(C_{4z},\vec{\tau})^{\star}T_l \oplus g(C_{4z}^3,\vec{\tau})^{\star}T_l \oplus g(C_{2x},\vec{\tau})^{\star}T_l \oplus g(C_{2y},\vec{\tau})^{\star}T_l$$

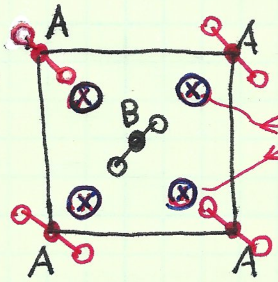
$$+\ \underbrace{g(S_4,\vec{\tau})T_l \oplus g(S_4^3,\vec{\tau})T_l}_{\text{point operations}} \oplus g(\sigma_{v_1},\vec{\tau})^{\star}T_l \oplus g(\sigma_{v_2},\vec{\tau})^{\star}T_l$$

$\boxed{\star\ \text{non-symmorphic operations.}}$

$\boxed{\text{screw rotations:}}$

$g(C_{4z},\vec{\tau})$ and $g(C_{4z}^3,\vec{\tau})$: screw axis located at $x=y=1/2$

Top view



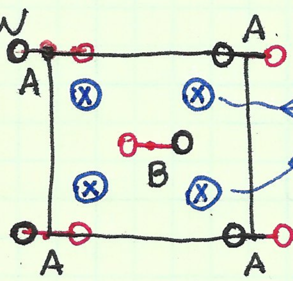
locations of screw axes

around these axes $g'(C_{4z},(00\tfrac{1}{2}))$, $g'(C_{4z}^3,(00\tfrac{1}{2}))$.

$g(C_{2x},\vec{\tau})$, $g(C_{2xy},\vec{\tau})$: screw axes located at $y=z=1/2$

$x=z=1/2$

Front view

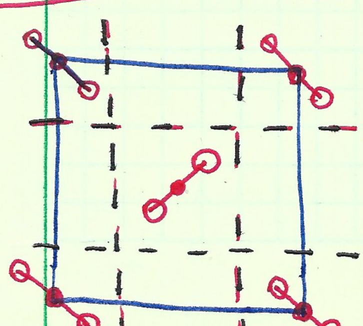


locations of screw axes.

Around these axes $g'(C_x, 0\tfrac{1}{2}0)$

$\boxed{\text{glide reflections}}$

$g(\sigma_{v_1},\vec{\tau})$: glide planes // xz plane located at $y=a/4,\ 3a/4$

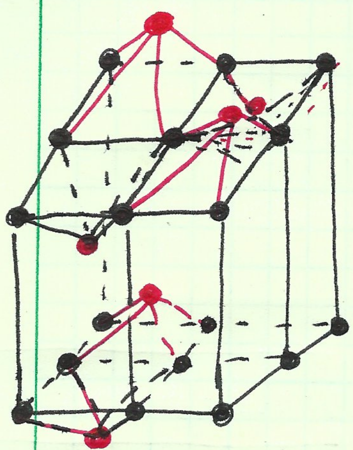


$y=3a/4$

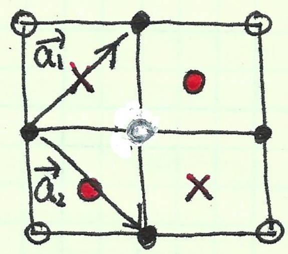
$y=a/4$,

$g(\sigma_{v_2},\vec{\tau})$ glide planes // yz located at $x=a/4,\ 3a/4$

3 Fe Se   P4/n mm



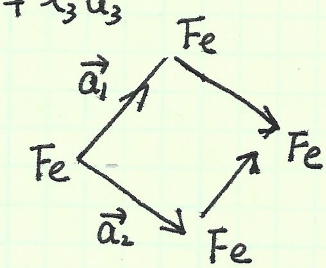
Top view:



- Fe atoms form a square lattice in the centeral layer (two sublatt
- Se atoms form two layers – above and below, which sandiwich the Fe layer.

> - On unite cell antains two Fe atoms (● and ○)
> - The primitive tetragonal Bravis lattice
> - lattice point group symmetry D_{4h}

1 The translation group $T_l = l_1 \vec{a}_1 + l_2 \vec{a}_2 + l_3 \vec{a}_3$



2 We choose the Fe site as the origin.

The point group around Fe is D_{2d}.

D_{2d}: $\{E, S_4, C_{z,2}, S_4^3, \sigma_{xy}, \sigma_{x\bar{y}}, C_{x,2}, C_{y,2}\}$

$\sigma_{xy}, \sigma_{x\bar{y}}$: reflection w/r the vertical planes passing the diagonal directions

$C_{x,2}, C_{y,2}$: 2-fold axes around x and y axes

$D_{4h} = D_{2d} \oplus I\, D_{2d}$ where I is the inversion operation. w/r to the Fe atom.

or $D_{4h} = D_{2d} \oplus \sigma_h D_{2d}$, where σ_h is the reflection w/r to Fe-Fe plane

However, I and σ_h are NOT crystalline symmetries. They do not map the two sublattices of the Se atoms invariant. They can be combined with a translation along the x-direction at the distance of one bond length, which switches two Fe sublattices and also two Se lattices.

$$I \cdot D_{2d} = \sigma_h D_{2d} = \{ I,\ C_{z,4}^{3},\ \sigma_h,\ C_{z,4}^{1},\ C_{x\bar{y}}^{2},\ C_{xy}^{2},\ \sigma_x,\ \sigma_y \}.$$

Then P4/n mm group $= D_{2d}\, T_e$

$$+\ g(I, \vec{\tau}_x)\, T_e + g(C_{z,4}^{3}, \vec{\tau}_x)\, T_e + \underline{g(\sigma_h, \vec{\tau}_x)}\, T_e + g(C_{z,4}^{1}, \vec{\tau}_x)\, T_e$$

$$+\ \underline{g(C_{x\bar{y}}^{2}, \vec{\tau}_x)}\, T_e + \underline{g(C_{xy}^{2}, \vec{\tau}_x)}\, T_e + \underline{g(\sigma_x, \vec{\tau}_x)\, T_e + g(\sigma_y, \vec{\tau}_x)}\, T_e$$

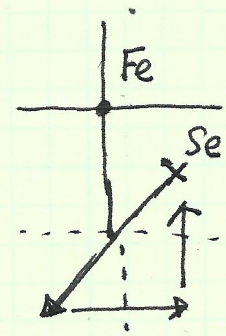
$\vec{\tau}_x = a\hat{x}$, a is the Fe-Fe bond length.

$g(I, \vec{\tau}_x)$: inversion with respect to the Fe-Fe bond center.

$g(C_4^1, \vec{\tau}_x)$ and $g(C_4^3, \vec{\tau}_x)$: since $\vec{\tau}_x$ is perpendicular to $\hat{z}$, they remain point operations. The fixed points are located at the $\hat{z}$-axes passing Se-atoms, i.e. Se's are the location of 4-fold axes.

- $g(\sigma_y, \vec{\tau}_x)$: Since $\vec{\tau}_x \perp yz$ plane, this is still a reflection.

  Check the fixed lines: The vertical planes yz passing the Se-Se atoms.



$$g(\sigma_y, \vec{\tau}_x) = g(\sigma_y, \vec{\tau}_y)\, T(-\vec{\tau}_x - \vec{\tau}_y)$$

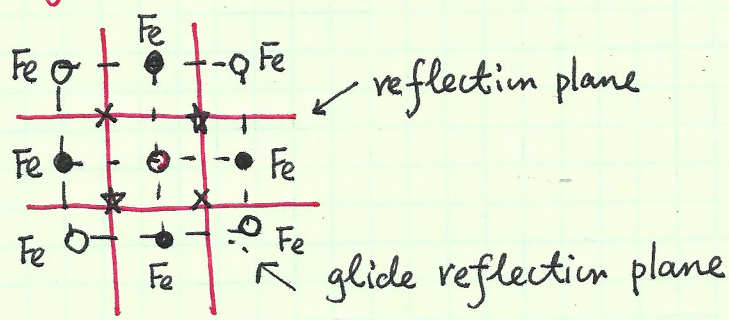
where $T(-\vec{\tau}_x - \vec{\tau}_y)$ belong to the lattice translation group, and $g(\sigma_y, \vec{\tau}_y)$ is a glide reflection.

Similarly $g(\sigma_x, \vec{\tau}_x)$ is a glide translation, but it can be represented as $g(\sigma_x, \vec{\tau}_x) = g(\sigma_x, \vec{\tau}_y)\, T(\vec{\tau}_x + \vec{\tau}_y)$.

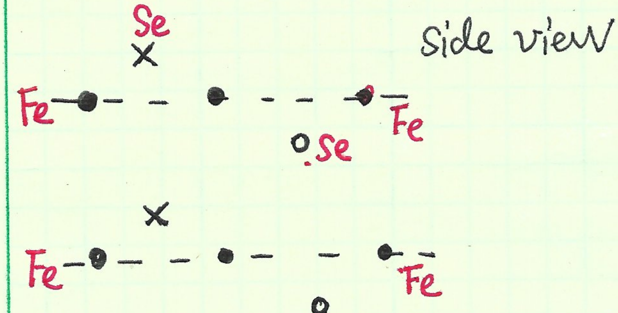
Hence, these two cosets can still be represented as point operations.

(xz and yz planes passing Se-Se atoms are reflection planes.

xz and yz planes passing Fe-Fe atoms are glide-reflection planes).

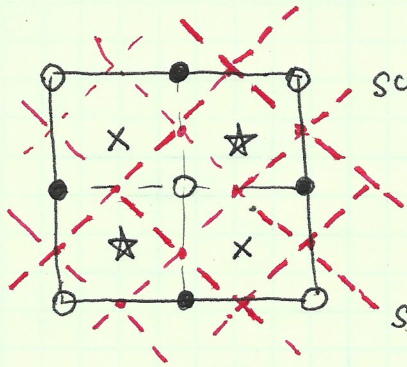


- $g(\sigma_h, \vec{\tau})$: The Fe-Fe plane is a glide reflection plane.



Screw rotation

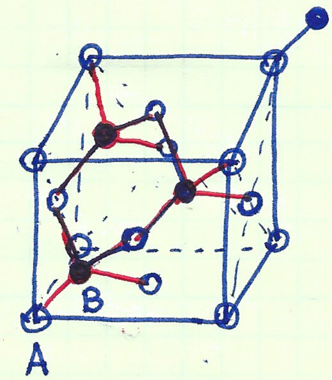
$g(C^2_{xy}, \vec{\tau}_x)$ and $g(C^2_{x\bar{y}}, \vec{\tau}_x)$ — screw axes along 11, $1\bar{1}$



④ Diamond (O_h^7 or $Fd3m$)

Two sublattices and each of them forms a Fcc lattice. The two sets of fcc lattices are off-set along the 111 direction at $\vec{\tau}_1 = \frac{a}{4}(111)$. The cosets after modula the fcc translation group is O_h, which contains 48 elements. Among them, $O_h = T_d \oplus T_d I$ 24 elements are T_d group elements, which do not involve the transformation among two sublattices. The rest 24 group elements of O_h, which contains the inversion I, combined with $\vec{\tau}$, transform one sublattice to another sublattice.

transform one sublattice to another sublattice



$$O_h^7 = g(E,0)\,T_f + \cdots\ g\{R_{24},0\}\,T_f$$

$$+\, g(I,\tau_1)\,T_f + \cdots\ g\{R_{48},\tau_1\}\,T_f$$

$\{E, R_1, \cdots R_{24}\}$ are T_d group operations which do not contain the inversion

$S_4 \sim T_d \sim O$ which contains 24 elements, and 5 classeal.

T_d: E

24
- $3C_4^2$ 2-rotation around the (001), (100), and (010)
- $8C_3'$ 3-fold rotations around the body-diagonal lines
- $6\sigma_v$ reflections with respect to the (110) $(1\bar{1}0)$ (011) $(01\bar{1})$ (101) $(10\bar{1})$ planes
- $6S_4'$ rotary-reflection around (001) (100) and (010)

The other 24 elements including $\{I, \cdots R_{48}\}$ are

- I : inversion
- $\sigma_{x,y,z}$: reflection with respect to yz; zx, xy-plane
- $8IC_3$ $(\bar{3})$: rotary-reflection
- $6C_2''$: 2-fold rotation around the lines connecting middle points of opposite edges
- $6C_4'$: 4-fold rotation around (001), (100) and (010)

The latter 24 operations need to combine with the fractional translation $\vec{\tau}_1 = \frac{1}{4}(111)$. $\{g(I,\tau_1), \cdots g\{R_{48},\tau_1\}\}$: transform $A \longleftrightarrow B$ sublattice

③

The transformation of the xyz for each coset

Case I: we set the origin at a diamond

Case II: we set the origin at $(\frac{1}{8}\ \frac{1}{8}\ \frac{1}{8})$, i.e. the A-B middle point

Class of O_h	space group	$g\vec{r}$	space group	$g\vec{r}$
E	$g(E,0)$	$x\ y\ z$	$g(E,0)$	$x\ y\ z$
$3C_4^2$	$g(C_{2z},0)$	$\bar{x}\ \bar{y}\ z$	$g(C_{2z};\frac14\frac14 0)$	$\bar{x}+\frac14,\ \bar{y}+\frac14,\ z$
	$g(C_{2x},0)$	$x\ \bar{y}\ \bar{z}$	$g(C_{2x};0\frac14\frac14)$	$x,\ y+\frac14,\ z+\frac14$
	$g(C_{2y},0)$	$\bar{x}\ y\ z$	$g(C_{2y};\frac14 0\frac14)$	$\bar{x}+\frac14,\ y,\ \bar{z}+\frac14$
$6S_4^1$	$g(S_{4z}^3,0)$	$y\ \bar{x}\ \bar{z}$	$g(S_{4z}^3;0\frac14\frac14)$	$y,\ \bar{x}+\frac14,\ \bar{z}+\frac14$
	$g(S_{4z},0)$	$\bar{y}\ x\ \bar{z}$	$g(S_{4z};\frac14 0\frac14)$	$\bar{y}+\frac14,\ x,\ \bar{z}+\frac14$
	$g(S_{4x}^3,0)$	$\bar{x}\ z\ \bar{y}$	$g(S_{4x}^3,\frac14 0\frac14)$	$\bar{x}+\frac14,\ z,\ \bar{y}+\frac14$
	$g(S_{4x},0)$	$\bar{x}\ \bar{z}\ y$	$g(S_{4x},\frac14\frac14 0)$	$\bar{x}+\frac14\ \ \bar{z}+\frac14,\ y$
	$g(S_{4y}^3,0)$	$\bar{z}\ \bar{y}\ x$	$g(S_{4y}^3,\frac14\frac14 0)$	$\bar{z}+\frac14\ \ \bar{y}+\frac14,\ x$
	$g(S_{4y},0)$	$z\ \bar{y}\ \bar{x}$	$g(S_{4y}\ 0\frac14\frac14)$	$z\ \ \bar{y}+\frac14,\ x+\frac14$
σ_v	$g(\sigma_{xy},0)$	$y\ x\ z$	$g(\sigma_{xy},0)$	$y\ x\ z$
	$g(\sigma_{x\bar{y}},0)$	$\bar{y}\ \bar{x}\ z$	$g(\sigma_{x\bar{y}}.\frac14\frac14 0)$	$\bar{y}+\frac14\ \ \bar{x}+\frac14,\ z)$
	$g[\sigma_{yz}\ 0]$	$x\ z\ y$	$g[\sigma_{yz},0]$	$x\ z\ y$
	$g[\sigma_{\bar{y}z},0]$	$x\ \bar{z}\ \bar{y}$	$g[\sigma_{\bar{y}z},0\frac14\frac14]$	$x\ \ \bar{z}+\frac14\ \ \bar{y}+\frac14$
	$g[\sigma_{xz},0]$	$z\ y\ x$	$g(\sigma_{xz}.0)$	$z\ y\ x$
	$g[\sigma_{\bar{x}z},0)$	$\bar{z}\ y\ \bar{x}$	$g[\sigma_{\bar{x}z},\frac14 0\frac14)$	$\bar{z}+\frac14,\ y,\ \bar{x}+\frac14$

Class O_h	Case I: space group	Case I: $g\vec{r}$	Case II: space group	Case II: $g\vec{r}$
$8C_3^1$	$g(C^1_{xyz},0)$	$y\,z\,x$	$g(C^1_{xyz},0)$	$y\,z\,x$
	$g(C^2_{xyz},0)$	$z\,x\,y$	$g(C^2_{xyz}\ 0)$	$z\,x\,y$
	$g(C^1_{\bar{x}\bar{y}z},0)$	$y\,\bar{z}\,\bar{x}$	$g(C^1_{\bar{x}\bar{y}z},\ 0\tfrac14\tfrac14)$	$y\ \ \bar{z}+1/4\ \ x+1/4$
	$g(C^2_{\bar{x}\bar{y}z},0)$	$\bar{z}\,x\,\bar{y}$	$g(C^2_{\bar{x}\bar{y}z},\ \tfrac14 0\tfrac14)$	$\bar{z}+1/4\ \ x,\ \bar{y}+1/4$
	$g(C^1_{\bar{x}y\bar{z}},0)$	$\bar{y}\,\bar{z}\,x$	$g[C^1_{\bar{x}y\bar{z}}\ \ \tfrac14\tfrac14 0)$	$\bar{y}+1/4\ \ \bar{z}+1/4\ \ x$
	$g(C^2_{\bar{x}y\bar{z}},0)$	$z\,\bar{x}\,\bar{y}$	$g[C^2_{\bar{x}y\bar{z}}\ \ 0\tfrac14\tfrac14)$	$z\ \ \bar{x}+1/4\ \ \bar{y}+1/4$
	$g(C^1_{x\bar{y}\bar{z}},0)$	$\bar{y}\,z\,\bar{x}$	$g[C^1_{x\bar{y}\bar{z}},\ \tfrac14 0\tfrac14)$	$\bar{y}+1/4,\ z,\ x+1/4$
	$g(C^2_{x\bar{y}\bar{z}},0)$	$\bar{z}\,\bar{x}\,y$	$g[C^2_{x\bar{y}\bar{z}},\ \tfrac14\tfrac14 0)$	$\bar{z}+1/4,\ \bar{x}+1/4,\ y$

The other 24

I	$g(I,\tau_1)$	$\bar{x}+1/4,\ \bar{y}+1/4,\ \bar{z}+1/4$	$g(I,0)$	$\bar{x}\ \ \bar{y}\ \ \bar{z}$
$3\sigma_{xyz}$ glide reflection	$g(\sigma_z,\tau_1)$	$x+1/4\ \ y+1/4\ \ \bar{z}+1/4$	$g(\sigma_z,\ \tfrac14\tfrac14 0)$	$x+1/4\ \ y+1/4\ \ \bar{z}$
	$g(\sigma_x,\tau_1)$	$\bar{x}+1/4\ \ y+1/4\ \ z+1/4$	$g(\sigma_x\ \ 0\tfrac14\tfrac14)$	$\bar{x}\ \ y+1/4\ \ z+1/4$
	$g(\sigma_y,\tau_1)$	$x+1/4\ \ \bar{y}+1/4\ \ z+1/4$	$g(\sigma_y,\ \tfrac14 0\tfrac14)$	$x+1/4\ \ \bar{y}\ \ z+1/4$
$6C_4^1$ screw rotation	$g(C^1_{4(z)},\tau_1)$	$\bar{y}+1/4\ \ x+1/4\ \ z+1/4$	$g(C^1_{4(z)},\ 0\tfrac14\tfrac14)$	$\bar{y},\ x+1/4,\ z+1/4$
	$g(C^3_{4(z)},\tau_1)$	$y+1/4\ \ \bar{x}+1/4,\ z+1/4$	$g(C^3_{4(z)},\ \tfrac14 0\tfrac14)$	$y+1/4,\ \bar{x},\ z+1/4$
	$g(C^1_{4(x)},\tau_1)$	$x+1/4\ \ \bar{z}+1/4\ \ y+1/4$	$g(C^1_{4x},\ \tfrac14 0\tfrac14)$	$x+1/4,\ \bar{z},\ y+1/4$
	$g(C^3_{4(x)},\tau_1)$	$x+1/4\ \ z+1/4\ \ \bar{y}+1/4$	$g(C^3_{4x},\ \tfrac14\tfrac14 0)$	$x+1/4\ z+1/4,\ \bar{y}$
	$g(C^1_{4(y)},\tau_1)$	$z+1/4\ \ y+1/4\ \bar{x}+1/4$	$g(C^1_{4(y)},\ \tfrac14\tfrac14 0)$	$z+1/4,\ y+1/4,\ \bar{x}$
	$g(C^3_{4(y)},\tau_1)$	$\bar{z}+1/4\ \ y+1/4\ x+1/4$	$g(C^3_{4(y)},\ 0\tfrac14\tfrac14)$	$\bar{z},\ y+1/4,\ x+1/4$

$6C_2'$	$g(C_{xy}, \tau_1)$	$(y+1/4, x+1/4, \bar{z}+1/4)$	$g(C_{xy}, 1/4\, 1/4\, 0)$	$(y+1/4, x+1/4, \bar{z})$
	$g(C_{x\bar{y}}, \tau_1)$	$(\bar{y}+1/4, \bar{x}+1/4, \bar{z}+1/4)$	$g(C_{x\bar{y}}$, [illegible] $0)$	$(\bar{y}, \bar{x}, \bar{z})$
	$g(C_{yz}, \tau_1)$	$(\bar{x}+1/4, z+1/4, y+1/4)$	$g(C_{yz}, 0\, 1/4\, 1/4)$	$(\bar{x}, z+1/4, y+1/4)$
	$g(C_{y\bar{z}}, \tau_1)$	$(\bar{x}+1/4, \bar{z}+1/4, \bar{y}+1/4)$	$g(C_{y\bar{z}}, 0)$	$(\bar{x}, \bar{z}, \bar{y})$
	$g(C_{xz}, \tau_1)$	$(z+1/4, \bar{y}+1/4, x+1/4)$	$g(C_{xz}, 1/4\, 0\, 1/4)$	$(z+1/4, \bar{y}, x+1/4)$
	$g(C_{x\bar{z}}, \tau_1)$	$(\bar{z}+1/4, \bar{y}+1/4, \bar{x}+1/4)$	$g(C_{x\bar{z}}, 0)$	$(\bar{z}, \bar{y}, \bar{x})$
$8IC_3'$	$g(IC^1_{xyz}, \tau_1)$	$\bar{y}+1/4, \bar{z}+1/4\ \bar{x}+1/4$	$g(IC^1_{xyz})$	$(\bar{y}\ \bar{z}\ \bar{x})$
	$g(IC^2_{xyz}, \tau_1)$	$\bar{z}+1/4\ \bar{x}+1/4\ \bar{y}+1/4$	$g(IC^2_{xyz})$	$(\bar{z}\ \bar{x}\ \bar{y})$
	$g(IC^1_{\bar{x}\bar{y}z}, \tau_1)$	$\bar{y}+1/4\ z+1/4, x+1/4$	$g(IC^1_{\bar{x}\bar{y}z}, 0\, 1/4\, 1/4)$	$\bar{y}\ z+1/4\ x+1/4$
	$g(IC^2_{\bar{x}\bar{y}z}, \tau_1)$	$z+1/4\ \bar{x}+1/4\ y+1/4$	$g(IC^2_{\bar{x}\bar{y}z}, 1/4\, 0\, 1/4)$	$z+1/4\ \bar{x}\ y+1/4$
	$g(IC^1_{\bar{x}y\bar{z}}, \tau_1)$	$y+1/4\ z+1/4\ \bar{x}+1/4$	$g(IC^1_{\bar{x}y\bar{z}}, 1/4\, 1/4\, 0)$	$y+1/4\ z+1/4\ \bar{x}$
	$g(IC^2_{\bar{x}y\bar{z}}, \tau_1)$	$\bar{z}+1/4\ x+1/4\ y+1/4$	$g(IC^2_{\bar{x}y\bar{z}}, 0\, 1/4\, 1/4)$	$\bar{z}\ x+1/4\ y+1/4$
	$g(IC^1_{x\bar{y}\bar{z}}, \tau_1)$	$y+1/4\ \bar{z}+1/4, x+1/4$	$g(IC^1_{x\bar{y}\bar{z}}, 1/4\, 0\, 1/4)$	$y+1/4\ \bar{z}\ x+1/4$
	$g(IC^2_{x\bar{y}\bar{z}}, \tau_1)$	$z+1/4\ x+1/4\ \bar{y}+1/4$	$g(IC^2_{x\bar{y}\bar{z}}, 1/4\, 1/4\, 0)$	$z+1/4\ x+1/4\ \bar{y}$

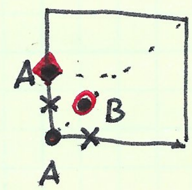
The nature of 2nd class transformations

① $g(I, \vec{\tau}_1)$ ⇒ inversion center located at A–B bond middle points

② $g(\sigma_z, \vec{\tau}_1)$ ⇒ glide reflection: glide plane // xy, located at $z = \frac{1}{8}a$, and glide $\frac{a}{4}\hat{x} + \frac{a}{4}\hat{y}$ in the plane.

$g(\sigma_x, \vec{\tau}_1)$, $g(\sigma_y, \vec{\tau}_1)$: glide planes // yz, xz, respectively they pass the middle points of a A–B bond and translate along $\frac{a}{4}(\hat{y}+\hat{z})$ and $\frac{a}{4}(\hat{x}+\hat{z})$, respectively.

③ $g(C^1_{4,z}, \tau_1)$: ⇒ screw rotation — screw axis // $\hat{z}$, with $x=0$, $y=1/4$ followed by translation along z-axis at $1/4\, a$



$g(C^3_{4,z}, \tau_1) \neq g^3[C^1_{4z}, \tau_1]$

it's screw axis // $\hat{z}$ ⇒ $\begin{cases} x = 1/4 \\ y = 0 \end{cases}$

• A $z=0$
○ B $z=1/4$
◇ A $z=1/2$

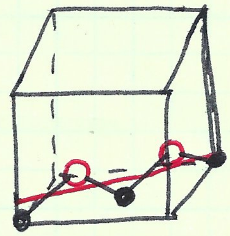
$g(C^1_{4x}, \tau_1)$: screw axis // $\hat{x}$ with $\begin{cases} y=0 \\ z=1/4 \end{cases}$

$g(C^3_{4x}, \tau_1)$: screw axis // $\hat{x}$ with $\begin{cases} y=1/4 \\ z=0 \end{cases}$

$g(C^{1,3}_{4y}, \tau_1)$: screw axis // $\hat{y}$ with $\begin{cases} x=1/4 \\ z=0, \end{cases}$ and $\begin{cases} x=0 \\ z=1/4 \end{cases}$

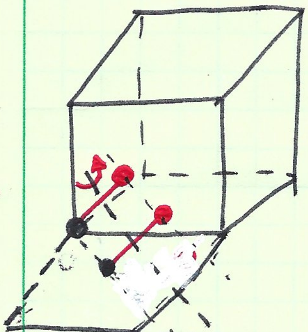
④ $6C_2'$: $g(C_{xy}, \tau_1)$ screw axis $// xy$, but with $z = 1/8$, or $z = 5/8$

followed by translation $\frac{a}{4}(\hat{x} + \hat{y})$

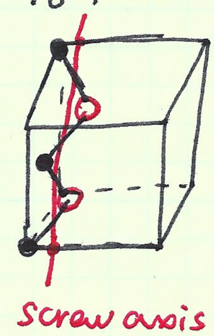


$g(C_{x\bar{y}}, \tau_1)$: pure rotation, axis $// x\bar{y}$

at $z = 1/8$

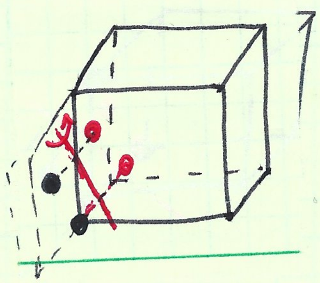


$g(C_{yz}, \tau_1)$ screw axis $// yz$, but $x = 1/8$, or $x = 5/8$

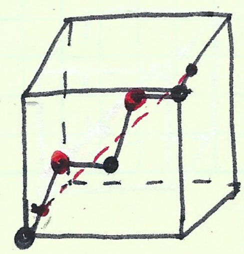


$g[C_{y\bar{z}}, \tau_1]$: pure rotation, axis $// y\bar{z}$

with $x = 1/8$

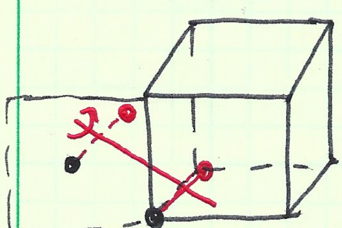


$g[C_{xz}, \tau_1]$ screw axis $// xz$ with $y = 1/8$, $5/8$



$g[C_{x\bar{z}}, \tau_1]$, pure rotation axis $// x\bar{z}$

passing A.B bond middle point



$8IC_3'$ are all point operation

① $g(IC^1_{xyz}, \tau/4)$ and $g(IC^2_{xyz}, \tau/4)$ are point operations with respect to $(1/8\ 1/8\ 1/8) \rightarrow$ A B bond middle point

② $g(IC^1_{\bar{x}\bar{y}z}, \tau_1)$ — fixed point $x=-1/8$. $y=3/8$, $z=1/8$ . .

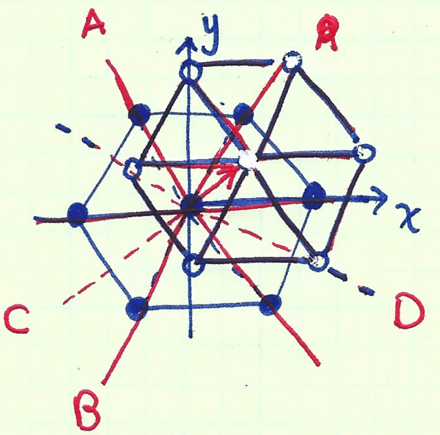
Bascically. around each bond perform 3-fold rotation and do inversion.

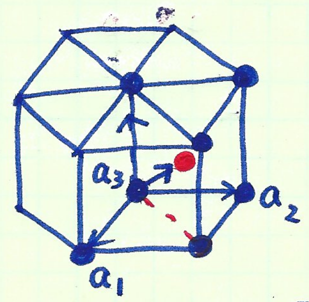
$g(S_4, \vec{\tau})$ and $g(S_4^3, \vec{\tau})$ are point operations, and the origins are at $(0, \frac{1}{2}a, \frac{3}{4}c)$. ⑦

$g(\sigma_{v1}, \vec{\tau})$ and $g(\sigma_{v2}, \vec{\tau})$ are glide reflections. The glide planes are parallel to xz-planes and located at $y = a/4,\ 3a/4$.

parallel to yz-planes and located at $x = a/4,\ 3a/4$.

③ hexagonal close-pack (D_{6h}^4) — the crystalline point group D_{6h}





$\vec{\tau} = (\frac{a}{2}\ \ \frac{\sqrt{3}}{6}a\ \ \frac{c}{2})$

D_{3h}

$g(E, 0)$ $g(C_{3z}, 0)$ $g(C_{3z}^2, 0)$, $g(C_{2y}, 0)$ $g(C_{2C}, 0)$ $g(C_{2D}, 0)$

$g(S_3^1, 0)$ $g(S_3^2, 0)$ $g(\sigma_z, 0)$

$g(\sigma_y, 0)$ $g(\sigma_C, 0)$ $g(\sigma_D, 0)$

which do not change sublattice $A \to A$, $B \to B$.

2nd class

$g(C_{z,6}, \vec{\tau})$, $g(C_{z,6}^5, \vec{\tau})$, $g(C_z^2, \vec{\tau})$

$g(C_{2x}, \vec{\tau})$ $g(C_{2A}, \vec{\tau})$, $g(C_{2B}, \vec{\tau})$

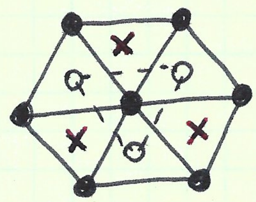
$g(I, \vec{\tau})$ $g(S_6^1, \vec{\tau})$ $g(S_6^5, \vec{\tau})$

$g(\sigma_x, \vec{\tau})$ $g(\sigma_A, \vec{\tau})$ $g(\sigma_B, \vec{\tau})$

The nature of operations of the 2nd class

① $g(C_{z,6}, \vec{\tau})$, $g(C^5_{z,6}, \vec{\tau})$ $g(C^2_z, \vec{\tau})$ — screw rotations

Screw axes are located at "X" - positions



② $g(C_{2x}, \vec{\tau})$ — screw rotation

Screw axe put on the middle point of A–B bond, i.e the A-layer is rotated to the B-layer, and after a shift along the x-axis $a/2$, it reaches the lattice in the B-layer.

$g(C_{2A}, \vec{\tau})$ — rotation, The rotation axis // the A-line direction, and it passes the A–B bond center

$g(C_{2B}, \vec{\tau})$ – rotation axis // B-line, but passes the AB bond center. After rotation, then translate the distance $\frac{a}{2}$.

③ $g(I, \vec{\tau})$ – point operation. Inversion centers are at AB middle points

$g(S_6^{1,5}, \vec{\tau})$ – point operations. The rotation axes are at the "X" position followed by a reflection with respect to the middle plane between the A B layer.

④ $g(\sigma_x, \vec{\tau})$ – glide plane parallel to the xz plane, but lie in the middle
$g(\sigma_{A,B}, \vec{\tau})$ betwo parallel lines between 2 layers, then followed by a translation of $a/2$.