Lect 11 Crystal symmetry (II) — non-symmorphic symms

* Screw rotation
* glide reflection

} we will explain these two symmety operations

§: Fractional translation $\vec{t}$

Consider a general crystalline space group operation

$$g(R,\vec{\alpha}) = T(\vec{l})\, g(R,\vec{t}\,), \quad \text{where } \vec{\alpha} = \vec{l} + \vec{t}, \ \vec{l}: \text{integer}$$

$$\vec{t} = \sum_{j=1}^{3} \vec{a}_j t_j \quad \text{with } 0 \leq t_j < 1. \leftarrow \text{if } \vec{t} \neq 0, \text{ it's fractional translation.}$$

- For each R, there exists a unique $\vec{t}$.

Proof: If there exist two $\vec{t}_1$ and $\vec{t}_2$, then we calculate

$$g(R\vec{t}_1)[g(R,\vec{t}_2)]^{-1} = g(R,t_1)\, g(R^{-1}, -R^{-1}t_2) = g(E, t_1 - t_2)$$

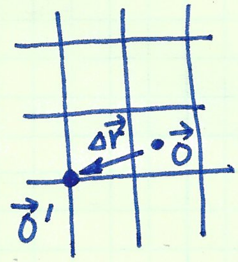
hence $\vec{t}_1 - \vec{t}_2 = \vec{l}$. Since $t_{1,j}$ and $t_{2,j}$ are smaller than 1, this is impossible.

§: Shift of point operation center — simplications of $\vec{t}$

Translations are independent of the choice of the origin, but rotations do care. If we suitably choose a point operation center, it can simplify the structure of $\vec{t}$. But can we simplify it to zero?

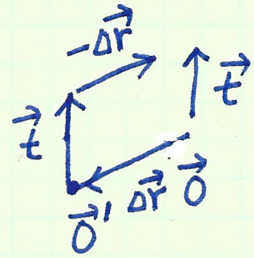
Consider two different choices of origins $\vec{O}$ and $\vec{O}'$.

And the relative vector $\overrightarrow{OO'} = \Delta\vec{r}$.



An operation with respect to the origin $\vec{O}$ is denoted as $g(R,\vec{t})$, and the same operation with respect to $\vec{O}'$ is denoted as $g'(\vec{R},\vec{t}')$. What's the relation between $\vec{t}$ and $\vec{t}'$.?

We start with the following relation



$$\boxed{\begin{array}{cc} T^{-1}(\Delta\vec{r})\ \underset{\substack{\uparrow \\ \text{w/r to } \vec{O}'}}{g'(R,\vec{t})}\ T(\Delta\vec{r}) = & \underset{\substack{\uparrow \\ \text{w/r to } \vec{O}'}}{g(R,\vec{t})} \end{array}}$$

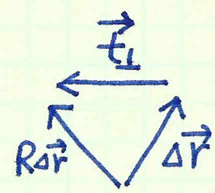
Hint: Check the operation for the point of $\vec{O}$.

On the other hand, $\text{LHS} = g'(R, (R-E)\Delta\vec{r} + \vec{t}) = g'(R,\vec{t}')$

hence, the correspondence is $\boxed{\vec{t}' = \vec{t} + (R-E)\Delta\vec{r}.}$

We check for all the point operations C_N $(N=1,2,3,4,6)$ and rotary reflections S_N $(N=1,2,3,4,6)$. S_1 is just the reflection σ, and S_2 is inversion I. $S_{3,4,6}$, are defined as usual.

- C_1: Since $R=E$, it is a trival case such that $\vec{t}'=\vec{t}$.
- C_N, then $\vec{t}'-\vec{t} = (R-E)\Delta\vec{r}$.



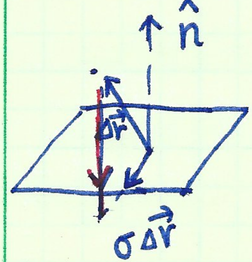
$(R-E)\Delta\vec{r} \perp \hat{n}$, where $\hat{n}$ is the rotation axis.

Hence, express $\vec{t} = \vec{t}_{\parallel} + \vec{t}_{\perp}$, where $\vec{t}_{\parallel} \parallel \hat{n}$ and $\vec{t}_{\perp} \perp \hat{n}$.

$\vec{t}_{\perp}$ can be cancelled by choosing $\boxed{(R-E)\Delta\vec{r} = -\vec{t}_{\perp}}$, then $\vec{t}' = \vec{t}_{\parallel}$.

Hence, the component of translation along the rotation axis $\hat{n}$ is independent on the choice of the origin. But the perpendicular part $\vec{t}_{\perp}$ can be set to zero by choosing $\Delta\vec{r}$ satisfying $(E-R)\Delta\vec{r} = \vec{t}_{\perp}$.

- S_1 or σ. Then $\vec{t}' - \vec{t} = (\sigma - E)\Delta\vec{r} \parallel \hat{n} \leftarrow$ axis perpendicular to $\hat{n}$.



hence $\vec{t} = \vec{t}_{\parallel} + \vec{t}_{\perp}$, then the transverse part $\vec{t}_{\perp}$ is invariant. But the longitudinal part $\vec{t}_{\parallel}$ can be cancelled to zero by choosing $\Delta\vec{r}$

$$\boxed{-\vec{t}_{\parallel} = (\sigma - E)\Delta\vec{r}} \leftarrow \text{For example, we take } \Delta\vec{r} = \vec{t}_{\parallel}/2.$$

$$\boxed{T(t_{\parallel}\hat{n})\,\sigma(\underset{\substack{\uparrow \\ \text{xy plane at } z=z_0}}{z_0}) = \sigma\left(z_0 + \frac{t_{\parallel}}{2}\right)} \leftarrow \text{shift of the location of the reflection plane.}$$

- S_2, S_3, S_4, S_6. Their matrices' eigenvalues do not contain 1, i.e., $S_{2,3,4,6}$ do not keep any direction invariant! Hence

$$(R-E)\Delta\vec{r} = -\vec{t} \text{ can always be solved as}$$

$$\Delta\vec{r} = -(R-E)^{-1}\vec{t}.$$

Hence, only 2 cases that $\vec{t}$ can not be set to zero by a shift of the center of R-operation.

They are •) $g(C_N, \vec{t}_{\parallel})$ with $N = 2, 3, 4, 6$ — screw rotation (screw axis)

•) $g(\sigma, \vec{t}_{\perp})$ — glide reflection (glide plane).

non-symmorphic symmetries

•§ Constraints on $\vec{t}_{\parallel}$ and $\vec{t}_{\perp}$

Consider $g(R, \vec{t})$, and the cyclic group generated by R's powers. Here we denote such a group as C_N if R is a proper point operation, and S_N if R is improper. (S_1 is just reflection, S_2 is inversion, S_3 is C_{3h}, S_6 is C_{3i}).

Let's assume $R^M = E$, then we ask $[g(R, \vec{t})]^M = ?$

$$[g(R, t)]^M = g[R^M, (R^{M-1} + \cdots R + 1)\vec{t}\,] = g(E, MP\vec{t}\,)$$

where $P = \frac{1}{M}(1 + R + \cdots R^{M-1})$. Hence $\boxed{MP\vec{t} \text{ has to be a lattice vector.}}$

P is actually a projection operater to the identity Rep of the cyclic group spanned by R's power. Hence, $P\vec{t}$ is invarint under R's operation, i.e. $\boxed{R(P\vec{r}) = P\vec{r}}$.

In the case of C_N, let's denote the rotation axis $\hat{n}$. Then

$P\vec{r} = \vec{r}$ for C_1, and $\boxed{P\vec{r} = \hat{n}\,(\hat{n} \cdot \vec{r})}$

In the case of σ, we have $\boxed{P\vec{r} = \vec{r} - \hat{n}(\hat{n} \cdot \vec{r})}$

Otherwise I, $S_{3,4,6}$ do not have invariant vector, except $\vec{r} = 0$, $P\vec{r} = 0$

We have the following results

1° C_1 : $R = E \Rightarrow \vec{t} = 0$ (it's not allowed to have a pure fractional translation).

2° C_N but $N \geq 2$. $M\hat{n}(\hat{n}\cdot\vec{t}) = M\vec{t}_{\parallel} = r\vec{a}_{\parallel}$

where $\vec{a}_{\parallel}$ is the shortest lattice vector along the rotation axis

$$\boxed{\vec{t}_{\parallel} = \frac{r}{M}\vec{a}_{\parallel}}$$

3° $\sigma \Rightarrow M = 2 \Rightarrow 2[\vec{t} - \hat{n}(\hat{n}\cdot\vec{t})] = 2\vec{t}_{\perp} = r\vec{a}_{\perp}$

$$\boxed{\vec{t}_{\perp} = \frac{1}{2}\vec{a}_{\perp}}$$

glide distance in the reflection plane, and $\vec{a}_{\perp}$ is the shortest lattice vector $\parallel \vec{t}_{\perp}$.

4° S_N but $N > 1$. Since $P\vec{r} = 0$, there's no constraint on $\vec{t}$.