Lecture 8

Reminder: HW 1 is due TONIGHT

HW 2 will be posted today or tomorrow

due 3/6

Reminder: trying to build space groups G

① $T \trianglelefteq G$ where T is a Bravais lattice

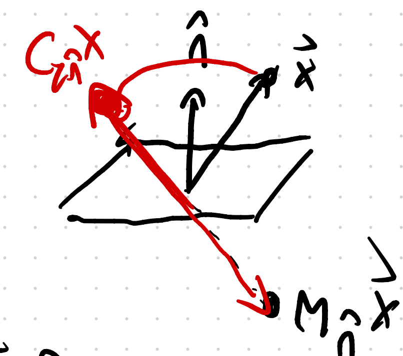
$\bar{G} = G/T$ the point group

$\bar{G} = \{ R \mid \{R|\vec{d}\} \in G \} < O(3)$

(2) if $R \in \overline{G}$:

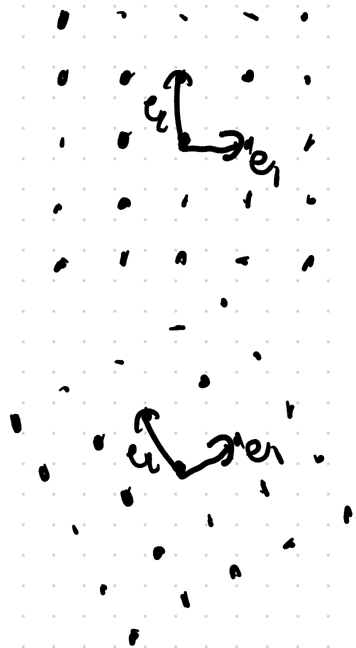
- R is a rotation by $0, \pm\frac{\pi}{3}, \pm\frac{\pi}{2}, \pm\frac{2\pi}{3}, \pi$
- R is spatial inversion I: $(x,y,z) \to (-x,-y,-z)$
- R is the product $I \times$ an allowed rotation

$$M_{\hat{n}} = I C_{2\hat{n}}$$



32 allowed crystallographic point groups

We want to combine T and $\overline{G}$ to get G



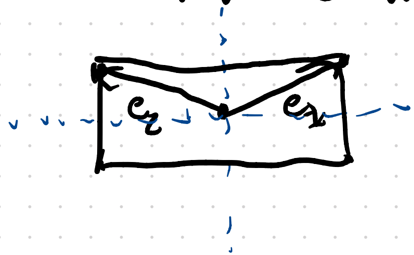
Not every T is compatible w/ every $\overline{G}$

$$T \trianglelefteq G$$

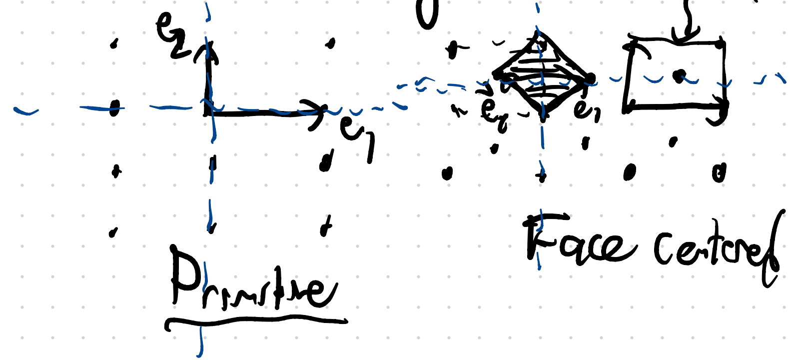
$$R \in \overline{G} \Rightarrow R\vec{t} \in T$$

6 families of Bravais lattice

→ 14 Bravais lattices



Centering:



Same point group

2mm

One way to put $\bar{G}$ and T together:

- semidirect product

$$G = T \rtimes \bar{G} = T\bar{G} = \left\{ \{E|\vec{t}\}\{R|\vec{0}\} \;\middle|\; \begin{matrix} \vec{t} \in T \\ R \in \bar{G} \end{matrix} \right\}$$

73 space groups that can be written as semidirect products - <u>Symmorphic space groups</u>

$\bar{G} \leq G$ for symmorphic space groups

$\{R|\vec{0}\} \in G$

Notation for symmorphic space groups

[letter][Hermann-Maugin symbol for the pt group]

centering
of Bravais
lattice

point
group

Example: $Pmm2$

Primitive
→ primitive
orthorhombic
Bravais lattice

point group $2mm$
ordering tells us the
twofold rotation is along z-axis

Primitive lattice vectors →
Bradley & Cracknell Table 3.1

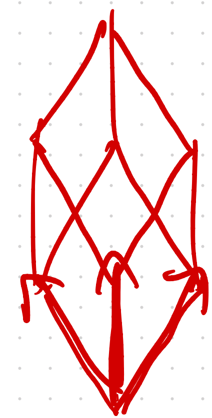
$$\vec{e}_1 = (a, 0, 0)$$
$$\vec{e}_2 = (0, b, 0)$$
$$\vec{e}_3 = (0, 0, c)$$

$a \neq b \neq c$

Ex: $R\bar{3}m \to$ point group $\bar{3}m = \langle C_{3\hat{z}}, m_x, I \rangle$

rhombohedral

$$\vec{e}_1 = (0, -a, c)$$
$$\vec{e}_2 = \frac{1}{2}(a\sqrt{3}, a, 2c)$$
$$\vec{e}_3 = \frac{1}{2}(-a\sqrt{3}, a, 2c)$$



Symmorphic Space groups $G = T \rtimes \bar{G}$

[centering][symbol for $\bar{G}$]

73

Most space groups are not symmorphic

Nonsymmorphic space groups $G \neq T \rtimes \bar{G}$

what does this mean

$G = T \cup T\{R_1 | \vec{d}_1\} \cup T\{R_2 | \vec{d}_2\} \cdots \cup T\{R_{n-1} | \vec{d}_{n-1}\}$

$$\bar{G} = \{E, R_1, R_2, \dots, R_{n-1}\}$$

if $G \neq T \rtimes \bar{G}$ then at least one $\vec{d}_i$ must be a fractional translation $\vec{d}_i \notin T$

In most cases G is nonsymmorphic b/c it contains either screw rotation or a glide reflection

Screw rotation: $\{C_{n\hat{r}} | \vec{d}\}$ where $\vec{d}$ has a component along $\hat{r}$ thats a fraction of a Bravais lattice vector denoted Λ_ℓ $\quad (\Lambda_\ell)^n$ is a translation by ℓ primitive lattice vectors along $\hat{r}$

$$\vec{d}\cdot\hat{r} = \frac{\ell}{n}\vec{e}$$

Ex: $\vec{e}_1 = (a,0,0)$
$\vec{e}_2 = (0,b,0)$
$\vec{e}_3 = (0,0,c)$

2_1: $\{C_{2\hat{z}} \mid \frac{1}{2}\vec{e}_3\}$

$$(x,y,z) \to (-x,-y,z+\tfrac{c}{2})$$

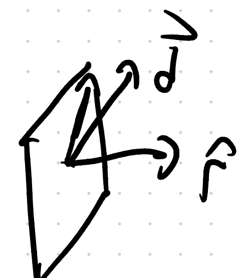
$$(\{C_{2\hat{z}} \mid \tfrac{1}{2}\vec{e}_3\})^2 = \{E \mid \vec{e}_3\}$$

3_1: $\{C_{3z} \mid \frac{1}{3}\vec{e}_3\}$ $\quad (3_1)^3 = \{E \mid \vec{e}_3\}$

3_2: $\{C_{3z} | \frac{2}{3}\vec{e}_3\}$ $(3_2)^3 = \{E | 2\vec{e}_3\}$

also $4_1, 4_2, 4_3$ $6_1, 6_2, 6_3, 6_4, 6_5$

<u>Glide reflection</u>: Mirror reflection + a translation w/ component along the mirror plane

$\{M_{\hat{r}} | \vec{d}\}$ $\vec{d} \times \hat{r} \neq 0$ 

$\{M_{\hat{r}} | \vec{d}\}^2 = \{E | \vec{d} + M_{\hat{r}}\vec{d}\} = \{E | 2(\text{component of } \vec{d} \text{ in}$

mirror plane }

Component of $\vec{d}$ in the mirror plane must be half a Bravais lattice vector

$$\vec{e}_1 = (a, 0, 0)$$

$$\{ M_{\hat{z}} \mid \tfrac{1}{2}\vec{e}_1 \} \to a$$

$$(x, y, z) \to \left(x + \tfrac{a}{2}, y, -z\right)$$

Herman Maugin symbol: m - mirror (not a glide)

a, b, c - glide w/ translation along Cartesian direction

n - glide w/ translation along a face

157 nonsymmorphic space groups

+

73 symmorphic groups

=

230 space groups

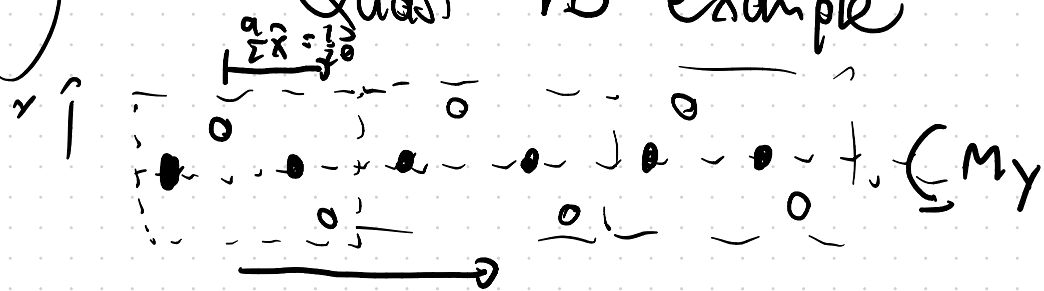
$\left(\begin{array}{l} I2_12_12_1 \ (\#24) \\ I2_13 \ (\#199) \end{array} \right)$

Body centered

d – glide w/ translation along the body diagonal

e ← distinguishes between multiple glides

Quasi - 1D example



$\vec{e} = a\hat{x}$

$\{M_y | \tfrac{1}{2}\vec{e}\}$ = glide

Space group Pa

$$\left\langle \{M_y | \tfrac{1}{2}a\hat{x}\},\ \{E | b\hat{y}\},\ \{E | a\hat{x}\} \right\rangle$$