Space Groups & Point Groups

- Space group = Full symmetry group of crystal structure (all rigid motions)
  - Translation symmetries (Bravais lattice) form a subgroup
- Point group ≈ Symmetries leaving some point fixed (maybe not an atomic position)

  Rotations, reflections, inversions, ...

- ~~Alter~~
- To precisely define point group, need to be more careful.

- General space group operation specified by "Seitz symbol"

$$\{R|\vec{t}\}: \vec{a} \to R\vec{a} + \vec{t}$$

Some orthogonal matrix

translation vector, not necessarily Bravais lattice vector.

ex: $\{R|0\}$ is rotation about the origin ~~$\vec{x}$~~

(if R is rotation matrix)

$\{\mathbb{1}|\vec{\tau}\}$ is pure translation.

Precise definition of point group:

- Given a space group, take all operations $\{R|\vec{\tau}\}$.
- In each operation, set $\vec{\tau} \to 0$, left with set of $\{R|0\}$'s. $\longrightarrow$ This is the point group.

Why define point group like this?

(Many)

- Macroscopic (averaged) properties only know about R-part of $\{R|\vec{\tau}\}$, don't care about $\vec{\tau}$-part. $\Big\}$ "Neumann's principle"

e.g. elasticity

- Can show: For Bravais lattice, every lattice point has the full point group symmetry.

  - Turns out that only 7 point groups possible for a Bravais lattice → 7 "crystal systems"
  - If we consider the full space group, there are 14 distinct Bravais lattices.

    ↳ "Same" Bravais lattice = "same" space group

    Essentially, two groups are the same if they have the same multiplication table. Don't care about things like lattice constant.

Lattice w/ Basis: 230 space groups & 32 point groups

Q: For a crystal structure with a given space group, is there always some point in the unit cell with full point group symmetry?

A: Not in general!

- For "symmorphic" space groups, some such point always exists somewhere in unit cell.

- For "non-symmorphic" space groups, it's impossible to find such a point.

Examples:

- All Bravais lattices have a symmorphic space group.

- Diamond structure has a non-symmorphic space group.
    - The point group has full symmetry of the cube.
    - But the space group has no 4-fold rotation. Instead, there is a 4-fold screw axis, which leaves no point fixed.