Mon. Oct. 29

- last time we found that the intensity of a diffraction pattern is related to the structure factor

$$S(\vec{G}) = \int d\vec{x}\, e^{i\vec{G}\cdot\vec{x}} V(\vec{x})$$

by $I_{(hk\ell)} \propto |S_{(hk\ell)}|^2$

- we need to know the specifics of $V(\vec{x})$, which is the sum over all atoms in a unit cell

$$V(\vec{x}) = \sum_j V_j(\vec{x}-\vec{x}_j)\ , \quad j \equiv \text{atoms in unit cell}$$

- for X-rays, $V_j(\vec{x}-\vec{x}_j) = Z_j g_j(\vec{x}-\vec{x}_j)$

on order of atomic radius

$Z_j \equiv$ atomic # (# e^-#); $g_j \equiv$ short-ranged function

- plugging back into our equation for $S(\vec{G})$, we get

$$S(\vec{G}) = \sum_j f_j(\vec{G}) e^{i\vec{G}\cdot\vec{x}_j}$$

Where $f_j(\vec{G}) = \int d\vec{x}\, e^{i\vec{G}\cdot\vec{x}} V_j(\vec{x}) \rightarrow$ F.T. of V_j

f_j is called the "form factor" $V_j \sim Z_j$

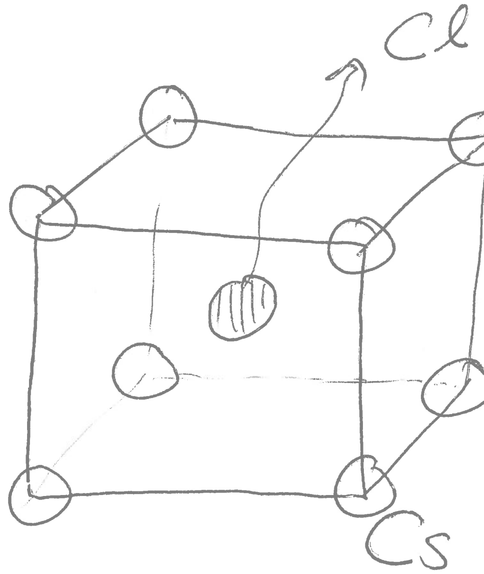
- if the lattice vectors are orthogonal (e.g. cubic)

$$S_{(hkl)} = \sum_j f_j e^{2\pi i(hx_j + ky_j + lz_j)}$$

where $[x_j, y_j, z_j] \rightarrow$ coordinates of atoms in unit cell

$\longrightarrow$

- Example: CsCl crystal type (simple cubic w/ basis)



$Cs \rightarrow [0,0,0]$

$Cl \rightarrow [\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$

$$S_{(hkl)} = \sum_j f_j e^{i2\pi(hx_j + ky_j + lz_j)}$$

$$= f_{Cs} e^{0} + f_{Cl} e^{i2\pi\left(\frac{h}{2} + \frac{k}{2} + \frac{l}{2}\right)}$$

$$= f_{Cs} + f_{Cl} e^{i\pi(h+k+l)}$$

- note $h+k+l$ = integer

$$S_{(hkl)} = f_{Cs} + f_{Cl}(-1)^{h+k+l}$$

form factors for each atomic type

- We see that for CsCl, we have partial cancellation for odd integers (sum of, h, k, l) → corresponding to lattice vectors (directions)

$$\text{odd sum} : f_{Cs} - f_{Cl} \rightarrow \text{e.g. for } [1\ 0\ 0] \text{ direction}$$

- What if we replace Cl with another Cs atom → now bcc lattice?

$$f_{Cs} - f_{Cs} = 0$$

- We see that in the [1,0,0] direction, we find another plane in between these planes from the atom in the center & we e.g. [2 0 0] have perfect destructive interference
- these "systematic absenses" are also called "selection rules"

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