Phys 425
Lecture 4

· reminders
  · problem set 1 (10/3)
  · Quiz 1 @ end of today.

Last time:

Miller indices (h, k, l) can define family of lattice planes on lattice → Planes are spaced out w/ distance

$$\boxed{d_{hkl} = \frac{2\pi}{\sqrt{h^2 + k^2 + l^2}}}$$

↳ defines the planes that give us the reciprocal lattice vector.

$$d = \frac{2\pi}{|\vec{G}_{min}|}$$

The Brillouin Zone

The 1st BZ is the equivalent of the Wigner-Seitz cell in reciprocal space. — tiles the entire space.

↳ just like any primitive, real lattice cell, the first Brillouin zone includes all physically distinct wave vectors.

Characterizing Crystal Structure

In the practical sense, you measure geometrical properties of the lattice via <u>scattering</u>.

<u>A general Scattering experiment</u>:

- Shoot EM wave into the sample (the crystal)
- represent wave as plane wave, $\mathcal{E}$

$$\mathcal{E}(\vec{r},t) = \mathcal{E}_0 e^{(i\vec{k}\cdot\vec{r}-\omega t)}$$

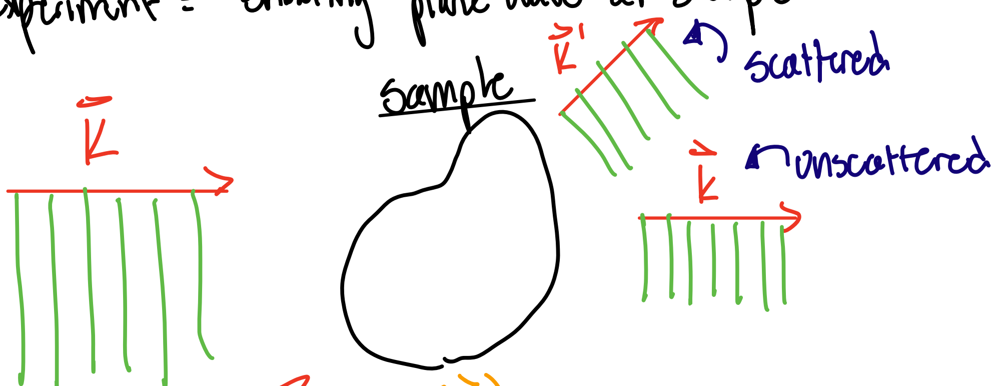
$\omega = 2\pi f$

$k = \frac{2\pi}{\lambda}$

k is a wave # (vector bc 3 different wave #s $(\vec{k}=(k_x, k_y, k_z))$)

r is position in space

- Visually
  - experiment = shooting plane wave at sample



$V(\vec{r})$ – sample can represent potential
↳ lattice potential

- wave scatters due to the potential

has same probability: go through,
elastic collision (energy exchange)

Probability of scattering is given by Fermi's golden rule.

gamma (capital)

$$\Gamma(\vec{k}', \vec{k}) =$$

→ expectation value of potential interacting in both ways.

$$\frac{2\pi}{\hbar} \underbrace{|\langle \vec{k}' | V(\vec{r}) | \vec{k} \rangle|^2}_{\to \mathcal{F}\{\text{sample}\}} \underbrace{\delta(\vec{E}_{\vec{k}'} - \vec{E}_{\vec{k}})}_{\text{we will only get a match if equal to zero}}$$

→ elastic collisions.

$$\langle \vec{k}' | V(\vec{r}) | \vec{k} \rangle$$

$$= \frac{1}{V_{\text{sample}}} \int_{-\infty}^{\infty} e^{i(\vec{k}' - \vec{k}) \cdot \vec{r}} V(\vec{r}) \, d\vec{r}$$

fourier transform of our sample.

operator

$$\langle O \rangle = \int \psi^* O \psi$$

V is a periodic function then $\langle \vec{k}' | V | \vec{k} \rangle = 0$,

unless $k' - k$ = a reciprocal lattice vector

WE ONLY SCATTER IF WE HIT AN ATOM!

$$\Rightarrow \boxed{\vec{k}' - \vec{k} = \vec{G}}$$

– In some hidden way, a law of conservation of "crystal momentum"

Laue Condition

Physically: a Laue condition tells us the condition of observing constructive interference

so, in scattering experiments,

intensity patterns will show maxima that correlates two reciprocal lattice vectors.

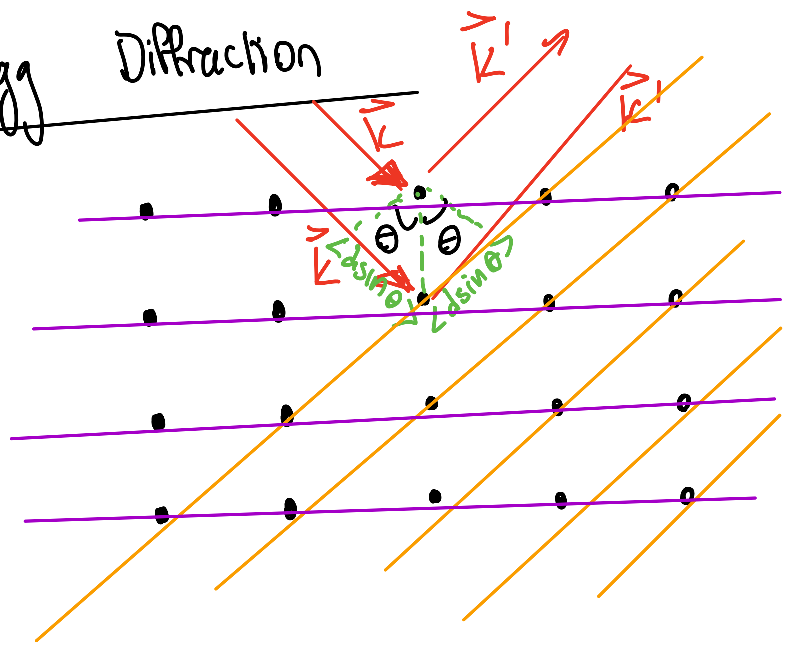
$\vec{G}$
$\downarrow$
$\vec{R}$

$$e^{i\vec{G}\cdot\vec{R}} = 1$$

Once you get intensity pattern, construct the entire lattice.

$$I \propto |\mathcal{E}(\vec{r})|^2$$

Bragg Diffraction



Once the waves scatter by 2θ, they can interfere, but they have a difference in path length.

constructive interference

$$2d\sin\theta = n\lambda$$

incoming wave

Laue condition = bragg condition

Given a set of family of lattice planes,
parameterized by the Miller indices. (h, k, l)

$$d_{hkl} = \frac{\lambda}{2\sin\theta} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$