Phys 425 - Lecture 3

Last Time:

Reciprocal lattice $\vec{R}$, the corresponding reciprocal lattice is $\vec{G}$ such that

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

$$\vec{R} = n_1\vec{a_1} + n_2\vec{a_2} + n_3\vec{a_3} \qquad \vec{G} = m_1\vec{b_1} + m_2\vec{b_2} + m_3\vec{b_3}$$

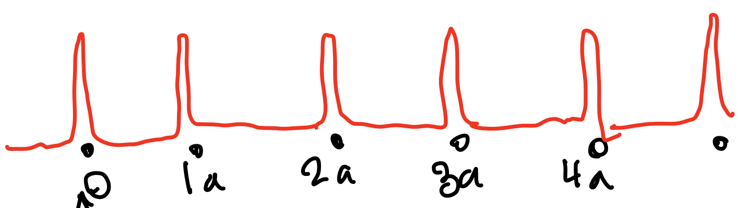
$$\Longleftrightarrow \quad \vec{a_i}\cdot\vec{b_j} = 2\pi\delta_{ij}$$

$$\delta_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if} \end{cases}$$

Vectors not reciprocal but lattice are.

Generally, we can think of the reciprocal lattice as the Fourier or wave vector (momentum representation) of the real lattice.

↳ in 1D



points are equally spaced.

Write lattice as $R_n = na$

which we represent using functional density: $\rho(r) = \sum_{n=1}^{\infty} \delta(r - R_n)$ location

Let's Fourier Transform this density

Fourier transformed $\hat{\rho}(k) = \int_{-\infty}^{\infty} e^{ikr}\rho(r)\,dr$ "Fourier transform of ρ"

wave vector

Functional density: (transform of ρ)

$$= \int_{-\infty}^{\infty} e^{ikr} \sum_n \delta(r-na)\, dr$$

$$= \sum_n \int_{-\infty}^{\infty} e^{ikr} \underbrace{\delta(r-na)}_{\text{only non-zero when } r=na}\, dr$$

$$= \sum_n e^{inak} \quad (\star) \quad \text{Poisson resummation}$$

$$= \frac{2\pi}{|a|} \sum \delta\left(k - \frac{2\pi m}{a}\right)$$

Check that e^{inak} is 1 if $k = \frac{2\pi m}{a}$ &

otherwise, you have an infinite sum of oscillating functions

$= 0$

Now compare $(\star)$ to our original definition

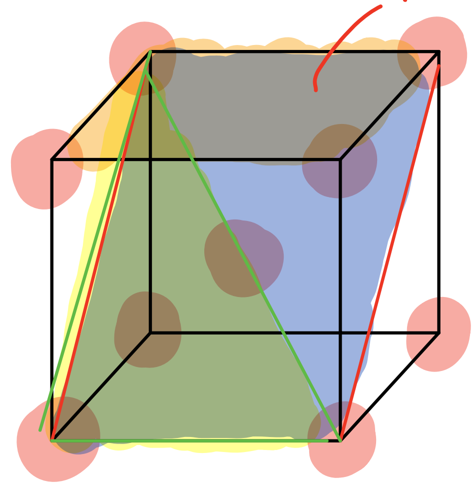
$$e^{i\vec{G}\cdot\vec{R}} = 1$$ for the reciprocal lattice.

This tells us that this is only non-zero when $k = 2\pi/a$ which is the location of every lattice point in the reciprocal lattice points.

$$G_n = \frac{2\pi}{a} m$$

Let's define a lattice plane.

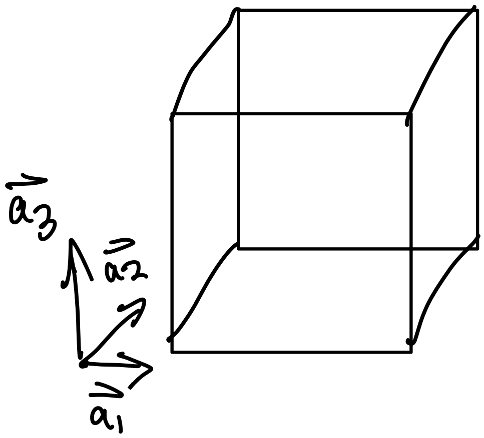
→ plane on the lattice that contains at least 3 coplanar lattice points.



Miller indices:

a set of 3 numbers (h, k, ℓ) where we identify w/

$(\vec{a}_1, \vec{a}_2, \vec{a}_3)$ so that h, k, l are the inverse intercept of the plane w/ each crystallographic axis.



eg. plane that intersects the top face.

It intersects axes when $a_3 = 1$.

$$\underbrace{\& \quad a_2 = a_1 = \infty}_{\text{never intersect}}$$

So $$(h, k, l) = \left(\frac{1}{\infty}, \frac{1}{\infty}, \frac{1}{1}\right)$$

$$= (0, 0, 1)$$

We can represent a lattice as a collection / family of lattice planes.

The directions perpendicular (or normal) to each family of planes defines the reciprocal lattice:

From math, we can write a plane as

$$\vec{a} \cdot \vec{x} = \text{const}$$

$\vec{a}$ is $\perp$ to the plane.

why? $\rightarrow$ $\vec{G} \cdot \vec{R} = 2\pi m \Rightarrow e^{i\vec{G}\cdot\vec{R}} = 1$

Not every G gives you a lattice plane.

↳ only the ones that correspond to a minimum G define a family of lattice points, in which case, the planes are spaced out with distance $d = \frac{2\pi}{|\vec{G}_{min}|}$ apart.

Miller indices are also the coefficients of G

$$\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

& the spacing of the plane is $d = \frac{2\pi}{\sqrt{h^2 + k^2 + l^2}}$