day 3 pg 4

day 4 pg 5

Alternate Fourier $n(x) = n_0 + \sum_{p=1}^{\infty} n_p e^{i2\pi px/a}$

complex; take into account sine (imag) + cosine (real)

Fourier Coefficients

compact form

$$n(x) = \sum_{p=-\infty}^{\infty} n_p e^{i2\pi px/a}$$

but constraint that $n_{-p}^* = n_p$

(forces $n(x)$ to be real function)

day 5 pg 1 { $2d\sin\theta = n\lambda$
$n=2$ vs (200) planes

To calculate coefficients

normally $a_n = \frac{2}{L}\int_0^L f(x)\cos\frac{n\pi x}{L}\,dx$ here $n_p = \frac{1}{a}\int_0^a n(x)\, e^{-i\frac{2\pi px}{a}}\,dx$

no 2 multiple because $p = -\infty$ to $+\infty$

$-i$ because we chose $+i$ above

In 3D

$$\boxed{n(\vec{r}) = \sum_{\vec{G}} n_{\vec{G}}\, e^{i\vec{G}\cdot\vec{r}}}$$

Slightly diff notation

$\vec{G}$ instead of $\frac{2\pi p}{a}$

So sum is not over all integers, but rather over all possible spatial frequencies

n_G calculated via

$$n_G = \frac{1}{\text{Volume}} \int_{\substack{\text{Volume}\\ \text{of}\\ \text{unit}\\ \text{cell}}} n(\vec{r})\, e^{-i\vec{G}\cdot\vec{r}}\, dV$$

What G's do we sum over?

rectangular lattice: $\vec{b}_1 = \left(\frac{2\pi}{a_1}, 0, 0\right)$

$\vec{b}_2 = \left(0, \frac{2\pi}{a_2}, 0\right)$

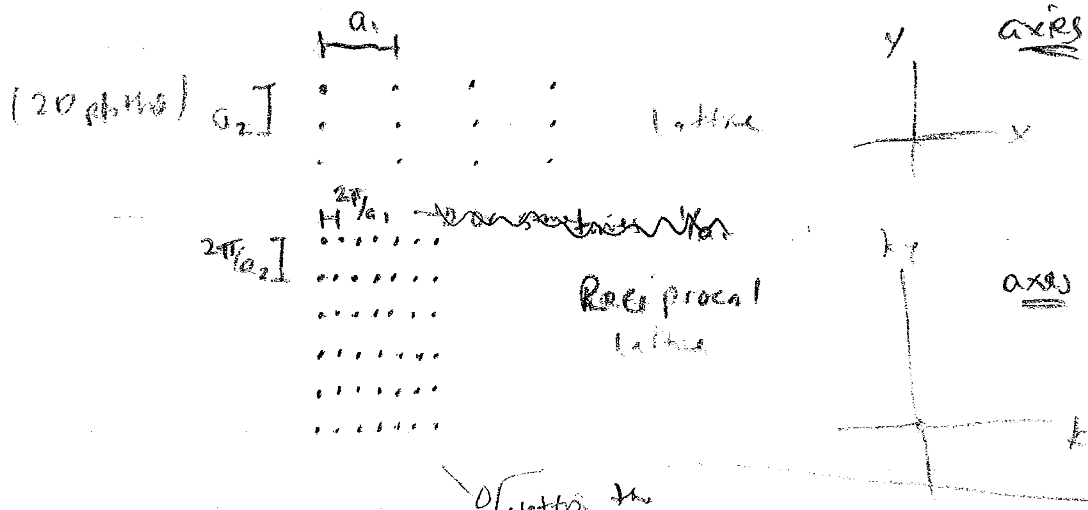
$\vec{b}_3 = \left(0, 0, \frac{2\pi}{a_3}\right)$

then any combination with integer multiples

any $\boxed{\vec{G} = v_1\vec{b}_1 + v_2\vec{b}_2 + v_3\vec{b}_3}$

integers (v was taken)

These represent points in a 3D "reciprocal lattice"



plotting the spatial frequencies we need to plot in order to represent periodic $n(x,y,z)$ in terms of Fourier components

If not rectangular, $V = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$

$$\boxed{\begin{aligned} \vec{b}_1 &= \frac{2\pi(\vec{a}_2 \times \vec{a}_3)}{V} \\ \vec{b}_2 &= \frac{2\pi(\vec{a}_3 \times \vec{a}_1)}{V} \\ b_3 &= \frac{2\pi(\vec{a}_1 \times \vec{a}_2)}{V} \end{aligned}}$$

Cool property: $\vec{a}_i \cdot \vec{b}_j = 2\pi \underbrace{\delta_{ij}}_{\text{kronecker delta}}$

test $\vec{a}_1 \cdot \vec{b}_1 = \frac{2\pi\,(\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3))}{V} = 2\pi$ ✓

$\vec{a}_1 \cdot \vec{b}_2 = \frac{2\pi}{V}\, \vec{a}_1 \cdot \underbrace{(\vec{a}_3 \times \vec{a}_1)}_{\perp \text{ to } \vec{a}_1} = 0$ ✓

Awesome theorem

The possible x-ray diffraction peaks are directly connected to the $\vec{G}$ vectors.

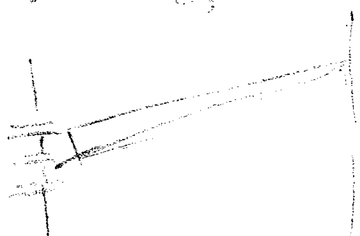
Specifically, $\boxed{\Delta \vec{k} = \vec{G}}$

$\vec{k}_{peak} - \vec{k}_{incident} = \vec{G}$

will give you all diffraction peaks if you try all $\vec{G}$ vectors!

Proof.

first back to 12.3



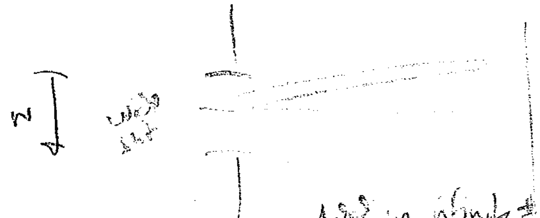
recall plane wave $\vec{E} = \vec{E}_0 e^{i(\vec{k}\cdot\vec{r} - \omega t + \phi)}$

diffraction from 3 slits $E = E_0 e^{i(kr - \omega t + \phi)}$

$$E = \sum_i E_i$$
$$= E_0 \left(e^{-i\phi} + 1 + e^{+i\phi}\right)$$

phase shift via $e^{i\phi}$

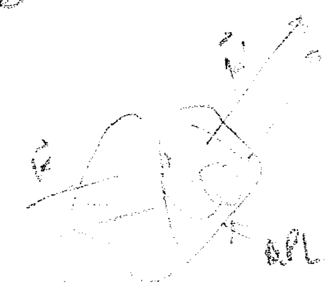
$$\phi = 2\pi\left(\frac{\Delta PL}{\lambda}\right) \quad \Delta d\sin\theta$$



Add up infinite # of phase shifts

$$E \propto \int_{-\frac{w}{2}}^{\frac{w}{2}} e^{i\Delta\phi}\, dy$$

back to our case



$$E \propto \int_{\text{volume}} e^{i\Delta\phi}\, dV$$

before $\Delta\phi = 2\pi \frac{\Delta PL}{\lambda}$

Now $\Delta\phi = \vec{k}\cdot\vec{r} - \vec{k}'\cdot\vec{r}$

$= -\Delta\vec{k}\cdot\vec{r}$

$\Delta\vec{k} = \vec{k}' - \vec{k}$

But... x-rays sensitive to electron density, so need to weight by $n(\vec{r})$:

$$F = \int_{\substack{\text{volume}\\ \text{of}\\ \text{crystal}}} n(\vec{r})\, e^{-i\Delta\vec{k}\cdot\vec{r}}\, dV$$

scattering amplitude $E \propto F$

Plug in Fourier representation of $n(\vec{r})$.

$$F = \int_{\substack{\text{vol of}\\ \text{xtal}}} \left(\sum_{\vec{G}} n_{\vec{G}}\, e^{i\vec{G}\cdot\vec{r}}\right) e^{-i\Delta\vec{k}\cdot\vec{r}}\, dV$$

$$= \sum_{\vec{G}} \int_{\substack{\text{vol of}\\ \text{xtal}}} n_{\vec{G}}\, e^{i(\vec{G}-\Delta\vec{k})\cdot\vec{r}}\, dV$$

this $= 0$ unless $\boxed{\Delta\vec{k} = \vec{G}}$! (HW problem)

(due to oscillations)

day 6 pg 1

That's a huge part of the reason why those RLVs are useful

One step further: magnitude of k is not changing, only direction, so $k = k'$

$$\vec{k}' - \vec{k} = \vec{G} \rightarrow \vec{k}' = \vec{G} + \vec{k}$$

$$\vec{k}'\cdot\vec{k}' = (\vec{G}+\vec{k})\cdot(\vec{G}+\vec{k})$$

$$\cancel{k^2} = G^2 + 2\vec{k}\cdot\vec{G} + \cancel{k^2}$$

$$G^2 + 2\vec{k}\cdot\vec{G} = 0$$