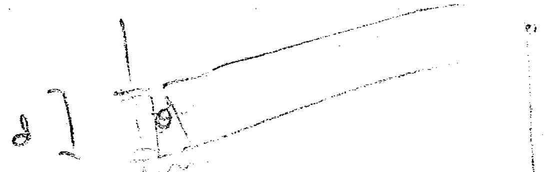
Chapter 2 — Diffraction of waves by crystals

How do we know the structures? Typically XRD / neutron

but simply: x-rays | neutron diffraction

$\lambda \approx$ a few Å — energies such that λ also $\approx$ a few Å

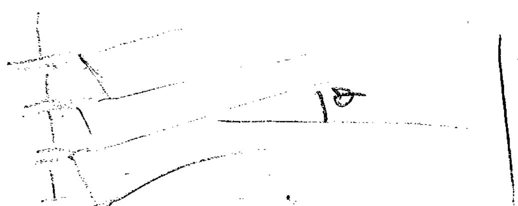
Diffraction by double slit (Phys 123)



$\Delta PL = n\lambda$ for constr. interference

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

Diffraction by grating (Phys 123)

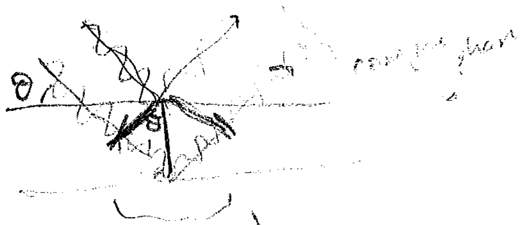


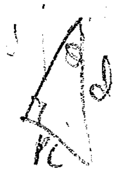
same thing:

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

Diffraction by planes (maybe / maybe not in 123)

no change wavelength





$$d\sin\theta = PL$$

$\Delta PL = n\lambda$

$$\boxed{2d\sin\theta = n\lambda}$$ Bragg's Law

Note: this assumes reflection is specular. Why is that?

★ $\boxed{\text{Sliding reflection from planes}}$

So, if an x-ray beam reflects, it will do so at $\theta_r = \theta_i$.
But it won't always reflect.

Strikes reflections from lattice

Start w/ θ close to 0 ... where is first reflection?
("diffraction order")

$\rightarrow 30^\circ$

What does that tell us about λ? (Take $d = 1$)

$$2d\sin\theta = n\lambda$$
$$2(1)\sin 30^\circ = (1)\lambda$$
$$\underline{\lambda = 1}$$

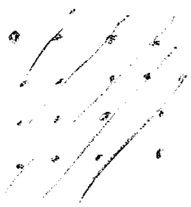
Where will 2nd diffraction order be?

$$2d\sin\theta = n\lambda$$
$$2(1)\sin\theta = (2)(1)$$
$$\sin\theta = 1$$
$$\underline{\theta = 90^\circ}$$

test it out!

From Kittel: each plane only reflects $10^{-3} - 10^{-5}$ of incident radiation
$\therefore 10^3 - 10^5$ planes contribute.
(Peter Yu: much more for neutron diff.)

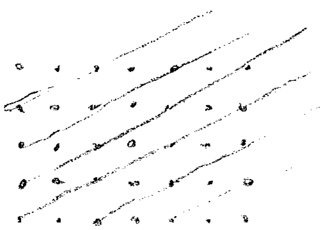
Complication: what about diagonal planes! Will x rays diffract off of these?
Yes



(11) planes

different d, angles measured from different reference angle

Even more diagonal planes



(12) planes
still different d
still diff. ref. angle.

HW: spacing for cubic: $d = \frac{a_0}{\sqrt{h^2+k^2+l^2}}$

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Suppose task is to predict all angles that will reflect?

→ identify all planes, ref angles

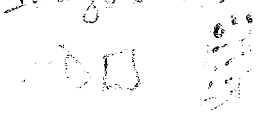
→ identify all diff orders possible

→ correct for ref angles to measure everything from x-rays

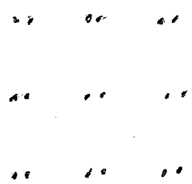
Even for simplest possible case here (2D, square lattice),

it's not trivial!

Imagine 3D structures, complicated lattices. (Now use computers)

 "Laue pattern"

Speaking of lattices, how will this behave?



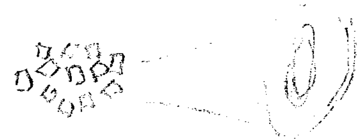
(like 2 square lattices, which each behave the same)

→ diffraction points giving info about lattice not about crystal

however, intensity of diffracted spots gives info about the unit cell.

Final notes on this section

1) "powder diffraction"



guarantees correct angle for some crystals

2) x-rays vs neutrons

→ interact w/ electrons

→ interact w/ nuclei

will they be different? Yes, sometimes, due to "bond charge"

Also: neutrons interact w/ ~1-10mm depth

(Need to start on next lecture material because it's long) day 4 pg 4

Scattered Wave Amplitude

. . . basic, lattice vectors $\uparrow a_1$ $\overrightarrow{a_2}$

. . . . . . make are periodic, with periods $\vec{a}_1$ and $\vec{a}_2$

What about electron density n? Also periodic w/ $\vec{a}_1, \vec{a}_2$

3D: $\vec{T} = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3$ u_i = integers (n was taken)

general lattice vector

Then $n(\vec{r} + \vec{T}) = n(\vec{r})$

periodic function? → Fourier! (anyone not seen?) ↳ see thing to my 123 handout

Case 1 1D lattice: $\overset{a}{\vdash\!\dashv}$ . . . .

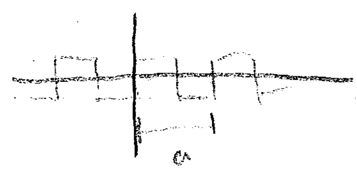
$$n(x) = n_0 + \sum C_p \cos\frac{2\pi p x}{a} + \sum S_p \sin\frac{2\pi p x}{a}$$

p = integer

period = a

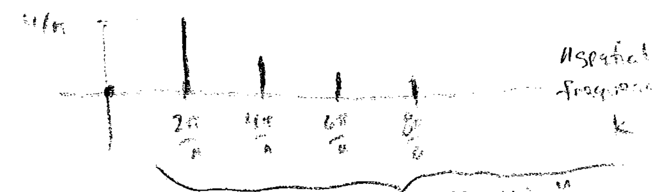
C_p, S_p are Fourier coefficients

Example:



Answer: $n(x) = 0 + \left(\begin{matrix}\text{no cosine terms,} \\ \text{since it's odd}\end{matrix}\right) + \sum_{p=1}^{\infty} \frac{4}{p\pi}\sin\frac{2\pi p x}{a}$

Plot of coefficients



terminology: $\underbrace{\qquad\qquad}_{\text{"reciprocal lattice"}}$

"reciprocal lattice pts" are $\frac{2\pi}{a_1}, \frac{4\pi}{a_1}$, etc.

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Alternate Fourier $n(x) = n_0 + \sum_{p=1}^{\infty} n_p e^{i 2\pi p x/a}$

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

Compact form

$$n(x) = \sum_{p=-\infty}^{\infty} n_p e^{i 2\pi p x/a}$$

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

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

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

no 2 needed because $p = -\infty$ to ∞

$-i$ 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?

Reciprocal 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 w/ 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)