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B/m Comput

So, *if* an x-ray beam reflects, it will do so at $\theta_r = \theta_i$.

But it won't always reflect.

Starts reflection 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 $d = 1$)

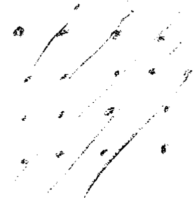
$$2d\sin\theta = n\lambda$$
$$2(1)\sin 30^\circ = (1)\lambda$$
$$\underline{\underline{\lambda = 1}}$$

Where will 2nd diffraction order be?

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

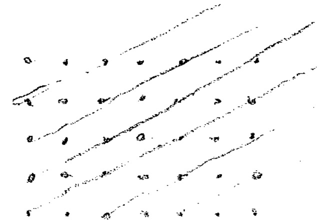
Complication: what about diagonal planes! Will x-rays diffract off of these?
Yes



(11) planes

different $\underline{d}$, angles measured from different reference angle

Even more diagonal planes



(12) planes
still different $\underline{d}$
still diff. ref. angle.

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

Notation: $(200) \Rightarrow n=2$ for (100) planes day 4 p. 2

Suppose task is to predict all angles that will reflect?

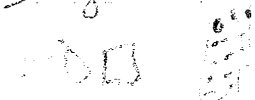
→ identify all planes, ref angles

→ identify all diff orders possible

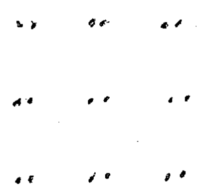
→ correct for ref angles to measure everything from x-axis

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?

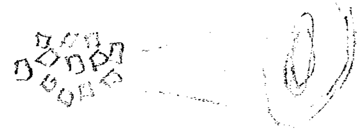


(like 2 square lattices, which each behave the same)

→ 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 }

$\boxed{\text{Scattered Wave Amplitude}}$

. . . lattice, lattice vectors $\uparrow a_1$, $\xrightarrow{a_2}$

. . .

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

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

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

general lattice vector

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

periodic function? → Fourier! $\quad$ (anyone not seen?) ↳ see theory to my 123 handout

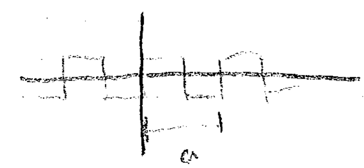
Case 1
1D lattice: $\overset{a}{\vdash\!\dashv}$ . . . .

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

p = integer
period = a

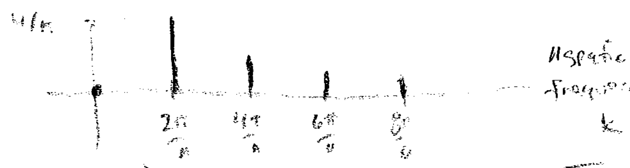
C_p, S_p are Fourier coefficients

Example:



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

Plot of coefficients



"reciprocal lattice"

terminology

"reciprocal lattice pts" are $\frac{2\pi}{a}$, $\frac{4\pi}{a}$, 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 ... (imag) + cos the ... (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)

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

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

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

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

What G's do we sum over?

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

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

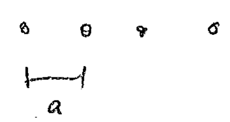
$\vec{b}_3 = \left(0, 0, \frac{2\pi}{a_3}\right)$

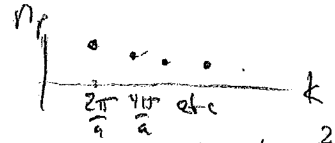
} then any combination with integer multiples

$$\boxed{\vec{G} = \underbrace{\nu_1 \vec{b}_1 + \nu_2 \vec{b}_2 + \nu_3 \vec{b}_3}_{}}$$

integers (ν not ν ... taken)

Review $\boxed{1D}$





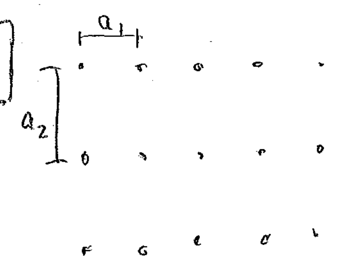
possible k's $= \frac{2\pi}{a} \times p$

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

$$n_p = \frac{1}{a} \int_0^a n(x) e^{-i 2\pi n x/a} dx$$

$n_p \rightarrow$ units of n, function of p

$\boxed{\text{simple cubic 3D}}$



$$n(x,y,z) = \sum_{v_1=-\infty}^{\infty} \sum_{v_2=-\infty}^{\infty} \sum_{v_3=-\infty}^{\infty} n_{v_1,v_2,v_3} \underbrace{e^{i\frac{2\pi v_1 x}{a_1}} e^{i\frac{2\pi v_2 y}{a_2}} e^{i\frac{2\pi v_3 z}{a_3}}}_{e^{i\left(\frac{2\pi v_1}{a_1}, \frac{2\pi v_2}{a_2}, \frac{2\pi v_3}{a_3}\right)\cdot(x,y,z)}}$$

More Compact Notation

$$\vec{r} = (x,y,z)$$

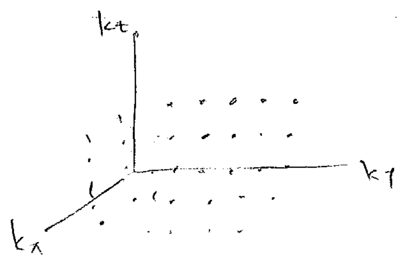
$$\vec{G} = \left(\frac{2\pi v_1}{a_1}, \frac{2\pi v_2}{a_2}, \frac{2\pi v_3}{a_3}\right) \quad \longleftrightarrow \quad v_1, v_2, v_3$$

one to one correspondence

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

$\vec{G}$ = a "reciprocal lattice vector",

aka any one of the spatial frequencies that are present



← "reciprocal lattice" the set of (k_x, k_y, k_z) values that have non-zero coefficients ($n_{\vec{G}}$ values)