To probe spatial structure, need appropriate length and energy scales

Convenient units

Photons $\lambda \sim \frac{12.4\ \text{Å}}{E/\text{keV}}$ $\quad E = h\nu = hc/\lambda$, $\lambda = hc/E$

neutrons $\lambda \sim \frac{0.28\ \text{Å}}{(E/\text{eV})^{1/2}}$ $\quad E = \frac{\hbar^2 k^2}{2m} = h^2/2md^2$, $\lambda = h/\sqrt{2mE}$

electrons $\lambda \sim \frac{12\ \text{Å}}{(E/\text{eV})^{1/2}}$ ← not as useful since do not penetrate solid

Since in CM $d \sim (1-10)$ Å need photons $E \sim$ 1-10 keV

$\Rightarrow$ x rays

need neutrons $E \sim .1$ eV

X ray photons synchrotrons SLAC
LBL
SPRING-8
:

neutrons : nuclear reactor
spallation neutron source ORNL

SS-1A

photons: $E = h\nu = hc/\lambda$

$$\lambda = \frac{hc}{E} = \frac{6.63\cdot10^{-34}\ 3\cdot10^{8}}{E} \leftarrow \text{in meters}$$

E in Joules

$$= \frac{6.63\cdot10^{-34}\ 3\cdot10^{8}\ 10^{10}}{(1.67\cdot10^{-19})\ 10^{+3}} \leftarrow \text{Å}$$

Å, eV, keV

$$= 12.4\ \text{Å}/E \text{ in keV}$$

neutrons: $E = \frac{\hbar^2 k^2}{2m} = \frac{h^2}{2m\lambda^2}$

$$\lambda = \frac{h}{\sqrt{2mE}} = \frac{6.63\cdot10^{-34}}{\sqrt{2(1.67\cdot10^{-27})}\ \sqrt{E}} \quad \leftarrow m,\ \leftarrow J$$

$$= \frac{6.63\cdot10^{-34}\ \ 10^{10}}{\sqrt{2}\ \sqrt{1.67\cdot10^{-27}\ \ 1.6\cdot10^{-19}}} \Rightarrow \frac{6.63\ \cdot10^{-1}}{\sqrt{2(1.67)(1.6)}}$$

$\leftarrow$ Å, $\uparrow$ eV

free e^- in electric field

$$\ddot{\vec{r}} = -\frac{e}{m}\vec{E}(\vec{r},t)$$

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

($\vec{k}$: direction of propagation)

Q: what do you know about $\vec{E}_0$ and $\vec{k}$?

EM waves are transverse: $\vec{E}$ and $\vec{B}$ are $\perp$ to direction of propagation: Two "polarizations"

$$\vec{\nabla}\cdot\vec{E} = \rho/\epsilon_0 \to 0$$

$$\vec{\nabla}\cdot\vec{E} = \frac{\partial E_x}{\partial x} + \frac{\partial E_y}{\partial y} + \frac{\partial E_z}{\partial z}$$

$$= (E_{0x}k_x + E_{0y}k_y + E_{0z}k_z)\, e^{i\vec{k}\cdot\vec{r}} e^{-i\omega t}$$

$$\vec{E}_0\cdot\vec{k} = 0$$

$$\vec{E}_0 \perp \vec{k}$$

Accelerated charges produce EM fields!

So the solid radiates out its own field due to the one that is incident

↳ "Scattering" of light off solid

SS-2A

How do we know $\vec{k}$ is propagation direction

A bit more E & M

Maxwell Eqns

$\oint \vec{E}\cdot\hat{n}\,dA = \frac{Q}{\epsilon_0}$	$\vec{\nabla}\cdot\vec{E} = \rho/\epsilon_0$ Coulomb's Law (ρ: charge density)
$\oint \vec{B}\cdot\hat{n}\,dA = 0$	$\vec{\nabla}\cdot\vec{B} = 0$ No magnetic monopoles
$\oint \vec{E}\cdot d\vec{\ell} = -\frac{\partial}{\partial t}\int \vec{B}\cdot\hat{n}\,dA$	$\vec{\nabla}\times\vec{E} = -\partial\vec{B}/\partial t$ Faraday's law
$\oint \vec{B}\cdot d\vec{\ell} = \mu_0 I$,	$\vec{\nabla}\times\vec{B} = \mu_0\vec{j} - \frac{1}{c}\frac{\partial\vec{E}}{\partial t}$ Ampere's law ($\vec{j}$: current density; $\frac{\partial\vec{E}}{\partial t}$: "Maxwell Displacement Current")

Poynting vector

$\vec{S} = \frac{1}{\mu_0}\vec{E}\times\vec{B}$

gives direction of energy flow

Energy flux

$\vec{p}$

If $\vec{E} = \vec{E}_0 e^{i\vec{k}\cdot\vec{r}} e^{-i\omega t}$

Then $\partial\vec{B}/\partial t = -\vec{\nabla}\times\vec{E} = -\begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ E_{0x} & E_{0y} & E_{0z} \\ k_x & k_y & k_z \end{vmatrix} i e^{i\vec{k}\cdot\vec{r}} e^{-i\omega t}$

$\vec{E}_0\times\vec{k}$

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

Check units

$[k/\omega] \sim 1/c$ ⤷ $\vec{B} = -(\vec{E}_0\times\vec{k})\, e^{i\vec{k}\cdot\vec{r}} e^{-i\omega t}/\omega$

$\omega = ck$ speed of light

$$c = \frac{1}{\sqrt{\mu_0\epsilon_0}}$$

SS 28

Poynting Vector Example:
Energy loss in wire

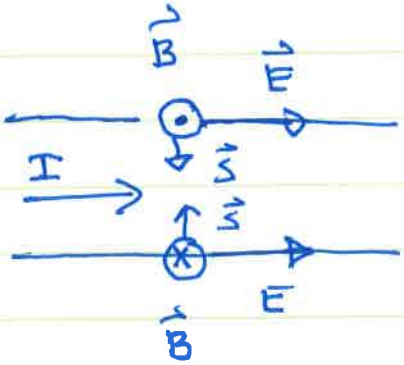
$$dW = dq\,V$$

$$P = dW/dt = dq/dt\,V = I V$$

$(2\pi r)|\vec{B}| = \mu_0 I$ $\quad$ $|\vec{B}| = \dfrac{\mu_0 I}{2\pi R}$ $\quad$ $\vec{B}$ points circularly around wire axis

$\oint \vec{B}\cdot d\vec{\ell} = \mu_0 I$

$|\vec{E}| = V/L$ $\quad$ $\vec{E}$ points along wire



$\vec{S} = \dfrac{1}{\mu_0}\vec{E}\times\vec{B}$

points inward

Energy flows into wire $\Rightarrow$ Joule heating

Energy flux $\quad |\vec{S}| = \dfrac{1}{\mu_0}\dfrac{V}{L}\dfrac{\mu_0 I}{2\pi R} = \dfrac{VI}{\underbrace{2\pi RL}_{\text{Area}}}$

$$\frac{\text{Energy}}{\text{Time}} = |S|(\text{Area}) = VI \quad \surd\surd$$

Poynting vector

$$\vec{S} = \frac{1}{\mu_0}\vec{E}\times\vec{B} \sim -\vec{E}_0\times(\vec{E}_0\times\vec{k})\frac{1}{\mu_0}$$

$$\vec{A}\times(\vec{B}\times\vec{C}) = \vec{B}(\vec{A}\cdot\vec{C}) - \vec{C}(\vec{A}\cdot\vec{B})$$

$$\vec{E}_0\times(\vec{E}_0\times\vec{k}) = -\left[\vec{E}_0(\underbrace{\vec{E}_0\cdot\vec{k}}_{\vec{\omega}}) - \vec{k}(\vec{E}_0\cdot\vec{E}_0)\right]$$

$\vec{E}_0\cdot\vec{k} = 0$ from $\vec{\nabla}\cdot\vec{E} = 0$

$$\vec{S} \sim \frac{\vec{k}}{\vec{\omega}}(E_0^2)\frac{1}{\mu_0}$$

↗ direction of energy flow

Actually $\vec{S}$ is energy flux: Energy flow per time per area. See this because

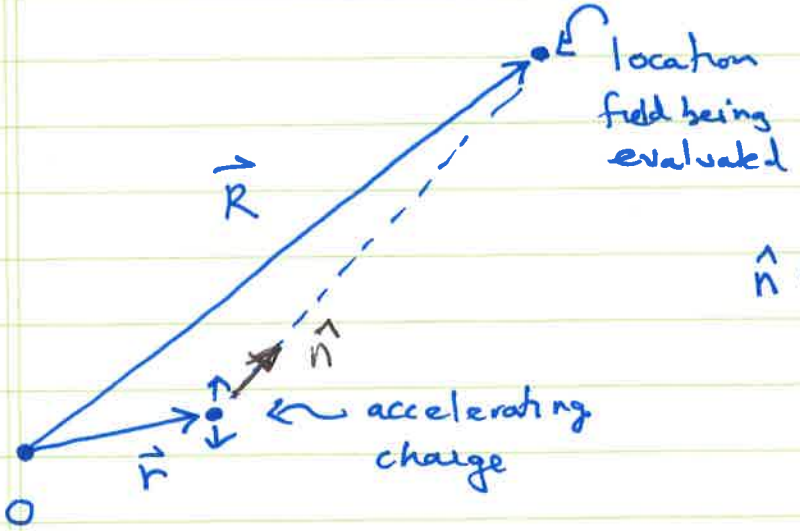
$$|\vec{S}| = \frac{k}{\omega}E_0^2\frac{1}{\mu_0} = \frac{1}{c}\epsilon_0 E_0^2 \underbrace{\frac{1}{\mu_0\epsilon_0}}_{c^2}$$

$$= c(\epsilon_0 E_0^2)$$

↑ speed ↑ Energy density

An advanced EM course gives formula for scattered E-field

$$\vec{E}_s = \frac{e^2}{mc^2}\,\hat{n}\times(\hat{n}\times\vec{E}_0)\,e^{i\vec{k}\cdot\vec{r}}\,e^{-i\omega t}\,\frac{e^{ik|\vec{R}-\vec{r}|}}{|\vec{R}-\vec{r}|}$$



$$\hat{n} = \frac{\vec{R}-\vec{r}}{|\vec{R}-\vec{r}|}$$

It is a good approximation to write

$$\hat{n} = \frac{\vec{R}-\vec{r}}{|\vec{R}-\vec{r}|} \approx \frac{\vec{R}}{|\vec{R}|} \qquad \text{ie} \qquad \vec{R}_D = R_D\hat{n} \sim \vec{R}$$

except up in the exponential where the rapidly oscillating phase is sensitive to small differences in location $\vec{r}$

$$k|\vec{R}-\vec{r}| = k\sqrt{R_D^2 - 2\vec{r}\cdot\vec{R}_D + r^2}$$

$$= kR_D\left[1 - \frac{2\vec{r}\cdot\vec{R}_D}{R_D^2} + \frac{r^2}{R_D^2}\right]^{1/2}$$

$$\approx kR_D\left[1 - \frac{\vec{r}\cdot\vec{R}_D}{R_D^2}\right]$$

$$\vec{k}' = k\frac{\vec{R}_D}{R_D} = k\hat{n} \equiv \vec{k} + \vec{q}$$ ← momentum change

$$\frac{e^{ik|\vec{R}-\vec{r}|}}{|\vec{R}-\vec{r}|} = \frac{e^{i\left[kR_D - k\vec{r}\cdot\vec{R}_D/R_D\right]}}{R_D}$$

$$= \frac{e^{ikR_D}}{R_D} e^{-i\vec{k}'\cdot\vec{r}} = \frac{e^{ikR_D}}{R_D} e^{-i(\vec{k}+\vec{q})\cdot\vec{r}}$$

Thus

$$\vec{E}_S = \frac{e^2}{mc^2}\frac{e^{ikR_D}}{R_D}\left[\hat{n}\times(\hat{n}\times\vec{E}_0)\right] e^{-i\omega t} e^{-i\vec{q}\cdot\vec{r}}$$

Key physical point: the phase of the scattered $\vec{E}$ field is sensitive to position of e^- and hence spatial structure of atoms to which e^- are bound.

project: FTID

FOURIER TRANSFORM AND RECIPROCAL LATTICE —

One dimensional example

$X_n = na \qquad n = 0, 1, 2, 3, 4, \ldots$

$f_k = \sum_n e^{ikx_n}$ Wave number k has units $1/\text{Length}$

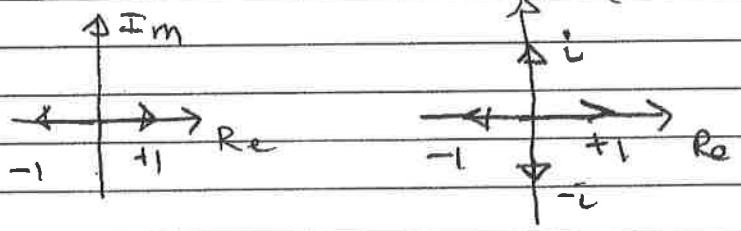
$k = \pi/a \qquad e^{ikx_n} = e^{i(\pi/a)na} = e^{i\pi n} = (-1)^n$

$f_{\frac{\pi}{a}} = \sum_n (-1)^n = 1 - 1 + 1 - 1 + 1 - 1 \ldots \rightarrow \not\exists$

$k = \pi/2a \qquad e^{ikx_n} = i^n = 1, i, -1, -i, 1, i, \ldots$

again $f_{\pi/2a} \rightarrow \not\exists$

Pictorially



Cancellation will occur $\forall k$ except $k = 2\pi/a\, l$

(really
Do not need to consider k outside $[0, 2\pi/a]$ because

$e^{i(k + 2\pi/a)x_n} = e^{ikx_n}$

"Brillouin Zone")

$k = 2\pi/a\, l$ ← "Reciprocal lattice vector"

more appropriate when we consider $d > 1$

$e^{ikx_n} = 1 \qquad \forall x_n$ in lattice

project:

X ray Scattering at UCD

Fadley group (Advanced Light Source) LBL : synchrotron

esp layered materials

also x ray in, e^- out "photoemission"

Savrasov group – theoretical calculation of phonons (lattice vibrations)
probed by inelastic x ray scattering

$|\vec{k}| \neq |\vec{k}'|$ $E_k \neq E_{k'}$

$E_{k'} - E_k \rightarrow$ phonons

Pickett group / LLNL DAC group $CaLi_2$ under pressure

superconductor under pressure

x ray diffraction at APS at ANL

another synchrotron

Where do x rays come from?

Accelerated e^- hitting anode (Röntgen @ 1895)
Nobel prize 1901

project:

SF-1

The Structure Factor

The scattering amplitude for X-rays off a crystal $\sim |F|^2$ where

$$F_{\Delta\vec{k}} = \int dV\, n(\vec{r})\, e^{-i\Delta\vec{k}\cdot\vec{r}}$$

$n(\vec{r})$: charge density

We have argued $\Delta\vec{k}$ is big only if it matches a reciprocal lattice vector $\Delta\vec{k} = \vec{G}$, the von Laue condition

$$f_{\vec{G}} = \int dV\, n(r)\, e^{-i\vec{G}\cdot\vec{r}}$$

$$= N \int_{\text{cell}} dV\, n(r)\, e^{-i\vec{G}\cdot\vec{r}} \qquad \text{N identical cells}$$

$$\equiv N S_G$$

If there are S atoms in the cell, at positions r_j

$$n(r) = \sum_{j=1}^{S} n_j(r - r_j)$$

$$S_G = \sum_j \int dV\, n_j(r - r_j) e^{-iG\cdot r} \qquad r = \rho + r_j \quad \rho = r - r_j$$

$$= \sum_j \left[\int dV\, n_j(\rho) e^{-iG\cdot\rho}\right] e^{-i\vec{G}\cdot\vec{r}_j}$$

$\equiv f_j$

writing $\vec{r}_j = x_j\vec{a}_1 + y_j\vec{a}_2 + z_j\vec{a}_3$

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

$$\vec{r}_j\cdot\vec{G} = 2\pi(v_1x_j + v_2y_j + v_3z_j)$$

project:
SF-2

redundant labeling since $\nu_1\nu_2\nu_3$ specify $\vec{q}$?

$$S_{\vec{q}}(\nu_1\nu_2\nu_3) = \sum_j f_j e^{-i2\pi(\nu_1 x_j + \nu_2 y_j + \nu_3 z_j)}$$

$$\Rightarrow I \sim |S_{\vec{q}}|^2$$

Intensity of x ray scattering

Example 1 bcc : 2 atoms/cell $\quad x_1 = 0 \quad x_2 = 1/2$ $\quad y_1 = 0 \quad y_2 = 1/2$ $\quad z_1 = 0 \quad z_2 = 1/2$

$$S(\nu_1\nu_2\nu_3) = f\left(1 + e^{-i\pi(\nu_1+\nu_2+\nu_3)}\right) = \begin{cases} 0 & \nu_1+\nu_2+\nu_3 = \text{odd} \\ 2f & \nu_1+\nu_2+\nu_3 = \text{even} \end{cases}$$

(f: identical atoms)

So, e.g., x ray scattering of Na, which is bcc

does not have peaks at (100), (300), (111), ... ← $\nu_1+\nu_2+\nu_3$ odd

but has peaks at (200) (110) (222) ← $\nu_1+\nu_2+\nu_3$ even

Example 2 fcc

x	0	1/2	0	1/2
y	0	1/2	1/2	0
z	0	0	1/2	1/2

$$S(\nu_1\nu_2\nu_3) = f\left[1 + e^{-i\pi(\nu_1+\nu_2)} + e^{-i\pi(\nu_1+\nu_3)} + e^{-i\pi(\nu_2+\nu_3)}\right]$$

S vanishes if one or two of $\nu_1\nu_2\nu_3$ odd

$S = 4f$ if all three $\nu_1\nu_2\nu_3$ odd or all three even

~~bcc, fcc are fcc~~

project:

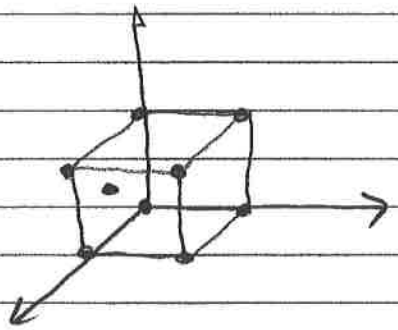
SF-3 ↙ fcc

KCl K^+ Cl^- ← same # electrons

$\Rightarrow f(K^+) \simeq f(Cl^-)$

so fcc looks like sc of a/2

sc has all $v_1 v_2 v_3$ with peaks, but here a/2 so $v_1 v_2 v_3$ need to be even to compensate for 1/2 in a/2.



KCl has peaks at (200) (220) (222) (400) (420)

KBr is also fcc but $f(K^+) \neq f(Br)$ so really ~~looks like fcc~~ follows fcc calculation of page SF-2

condition is $v_1 v_2 v_3$ all even or $v_1 v_2 v_3$ all odd

(111) (200) (220) (311) (222) (400) (331) (420)

↑ ↑ ↑

"extra peaks" not in KCl

See Figure 17 of Kittel

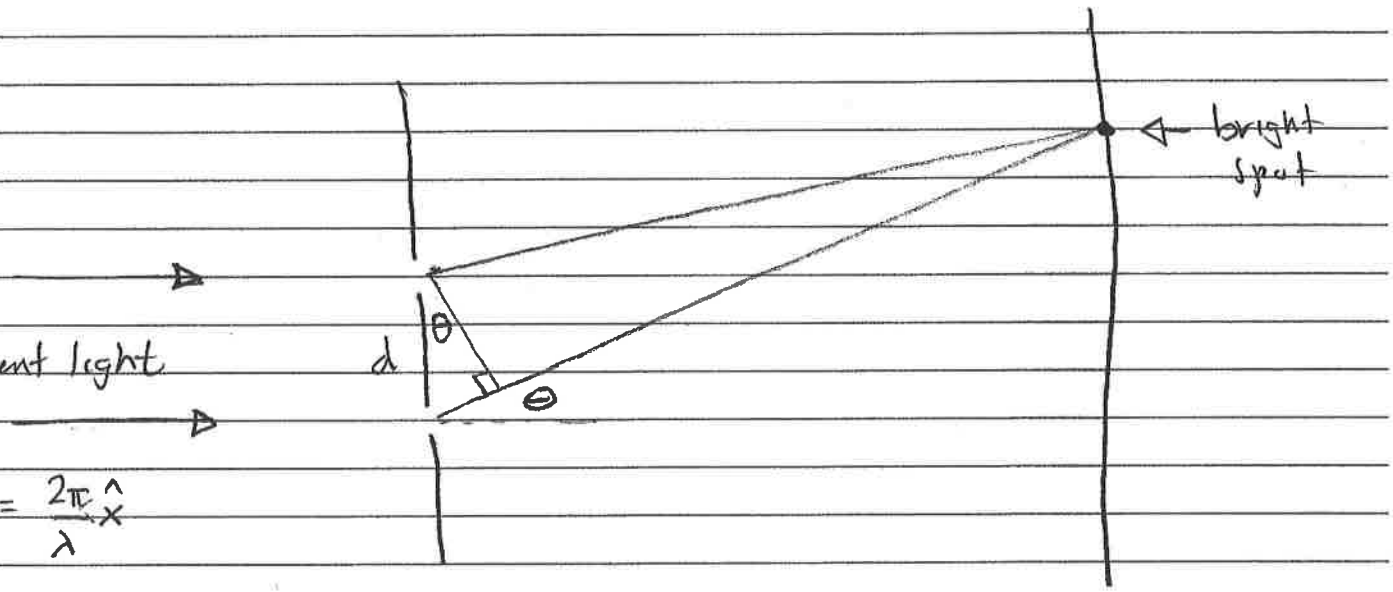
project:

D1

Diffraction

{ X rays on crystals yield intense peaks of scattered radiation for certain special λ and angles. (liquid no!)

Analogy with problem of 2 slit interference



bright spot if $d\sin\theta = \ell\lambda$

$$\vec{k}' = \frac{2\pi}{\lambda}(\cos\theta\,\hat{x} + \sin\theta\,\hat{y})$$

Only certain scattering vectors $\vec{q} = \vec{k}' - \vec{k}$ give bright spots

$$\cos\theta - 1 = -2\sin^2\frac{\theta}{2}$$

$$\vec{q} \approx \frac{2\pi}{\lambda}\frac{\ell\lambda}{d}\hat{y} = \frac{2\pi\ell}{d}\hat{y}$$

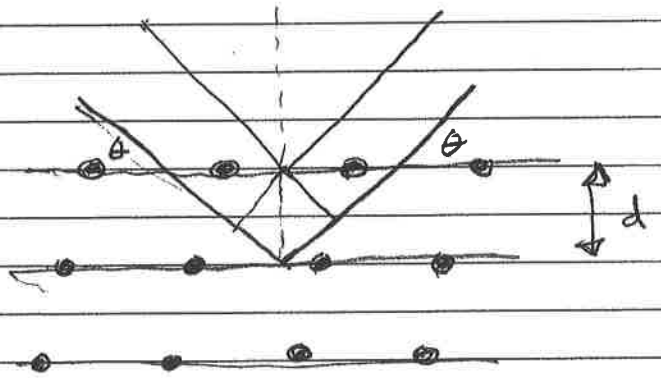
From positions of bright spots, can infer slit separation d.

This is basically the idea of x-ray diffraction except 3d lattice of atoms ⟷ 2 slits so more complicated.

project:

D2

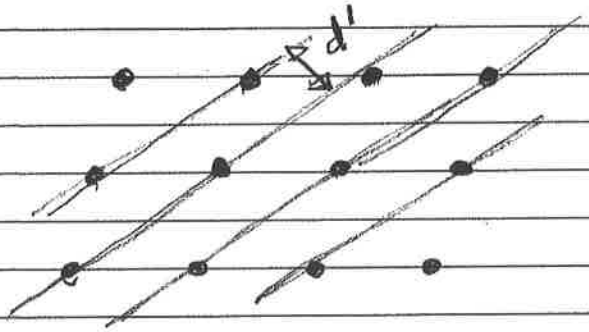
Bragg Formulation: Scattering off planes of atoms must result in constructive interference



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

for constructive interference.

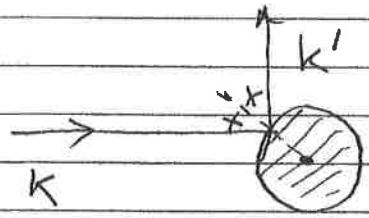
Note there are many ways to define the planes of atoms! ⇒ many Bragg peaks.



project:
SC-1

Some General Remarks on Scattering

Arises in classical physics

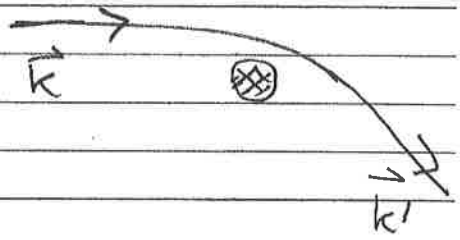


Hard sphere

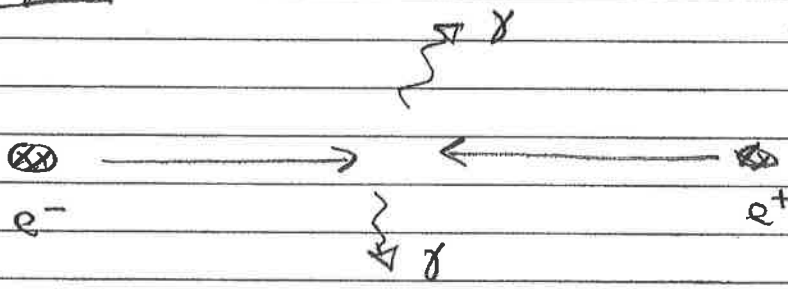
Maybe you are doing this problem in classical mechanics

Kepler problem $V(r) = 1/r$ Comet around sun

Need to solve orbit eqn (hyperbolas



Particle physics



$e^+ + e^- \to e^+ + e^-$

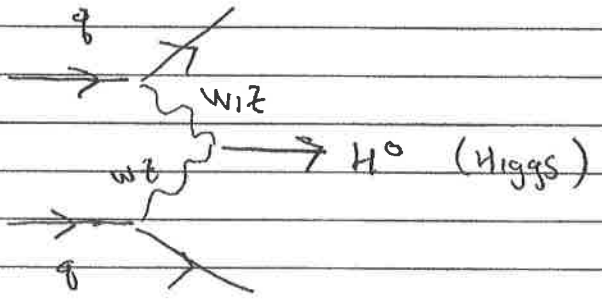
LEP 45 GeV 10^9 e^-

large e^-

LHC p+p

7 TeV

10^{12}



$e^- + e^- \to \mu^+ + \mu^-$

$e^+ + e^- \to q\bar{q}$

→ hadrons

J/ψ $c\bar{c}$

In our case $e^- + \text{nucleus} \to e^- + \text{nucleus} + \gamma$ Bremsstrahlung characteristic

10^4 keV

e^- not energetic enough to produce new particles, unlike LHC

project:

Sc-2

How to compute these things:

Kepler: you have done it! How to put E, B fields in QM

We did this in 115B

$\vec{p} \rightarrow \vec{p} - e/c\,\vec{A}$

$\vec{p} \cdot \vec{A}$ when squared

$\vec{A} \Rightarrow a^+ + a$ creation/annihilation operators for photons

Basic point: Different from QM you have done so far

Fixed, known # of particle $\psi(\vec{r})$ or $\psi(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_N)$

↑ this is all we really did in 115

Now need to make provision for # particles changing!!

$\psi(\vec{r}_1) \rightarrow \psi(\vec{r}_1, \vec{r}_2)$

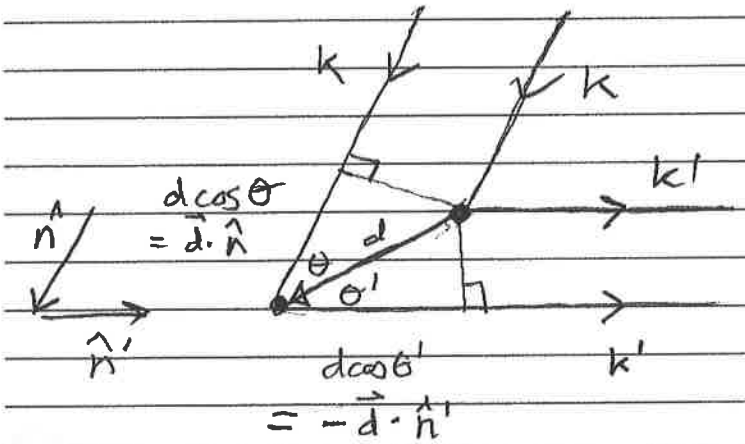
Quantum Field Theory

project:
P3

Van Laue Formulation

Instead of thinking of planes of atoms, consider crystal as ideal set of atoms at $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$

Consider two such scatterers



$$d\cos\theta + d\cos\theta' = \vec{d}\cdot(\hat{n} - \hat{n}') = m\lambda$$

$$\vec{d}\cdot(\vec{k} - \vec{k}') = 2\pi m$$

$$\left(\vec{k} = \frac{2\pi}{\lambda}\hat{n} \quad \vec{k}' = \frac{2\pi}{\lambda}\hat{n}'\right)$$

But $\{\vec{d}\}$ are nothing more than $\{\vec{R}\}$

Hence $\vec{R}\cdot(\vec{k} - \vec{k}') = 2\pi m$

$$\Rightarrow \quad e^{i(\vec{k}-\vec{k}')\cdot\vec{R}} = 1$$

$\Delta\vec{k}$ = Reciprocal lattice vector

project:

D4

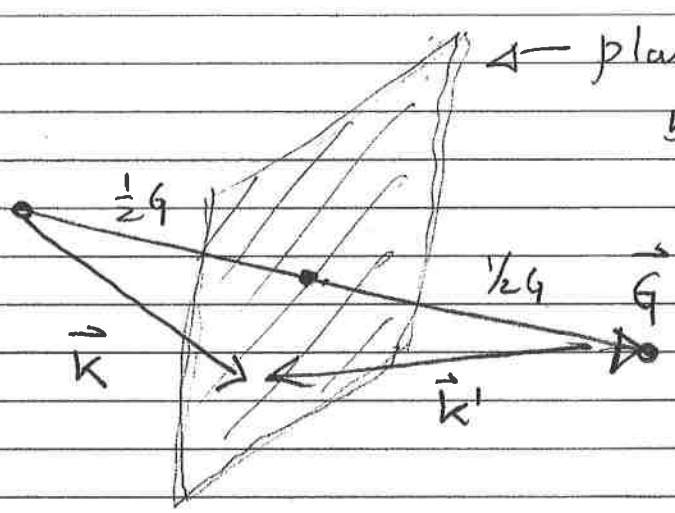
$|\vec{k}'| = |\vec{k}|$ $\quad \vec{k}' = \vec{k} - \vec{G}$ (or $\vec{k} + \vec{G}$, sign irrelevant)

$|\vec{k} - \vec{G}| = k$

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

$\vec{k}\cdot\hat{G} = \frac{1}{2}G$

↑ component of $\vec{k}$ along $\hat{G}$ ↑ is 1/2 of length of $\vec{G}$



Laue condition: $\vec{k}$ lies on plane ⊥ to $\vec{G}$ and bisecting $\vec{G}$

"Bragg Plane"

project:

E-1

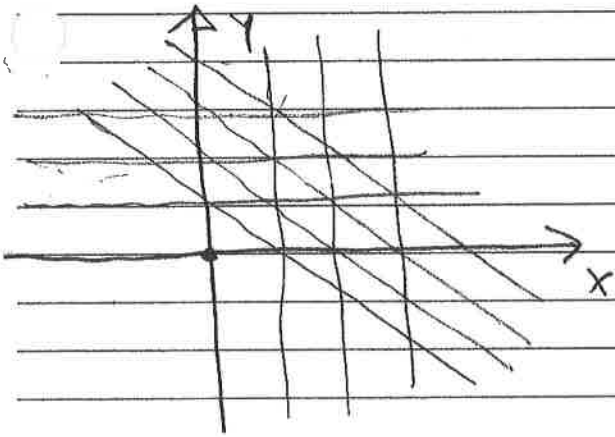
Ewald Construction

Consider an incident x-ray of wave vector $\vec{k}$.

It can give a Bragg peak if its tip lies on a Bragg plane.

Most likely this will not happen: Suppose you have a collection of 2D planes and pick some vector $\vec{k}$. What chance does its tip have of lying in a plane? Very small!

Easier to picture in lower d



I give you a (infinite) collection of lines. Put tail of arrow at origin, and what is chance head will lie in line?

very unlikely: lines are 1d objects in 2d world.

PROBLEM:

⇒ Expect NO BRAGG PEAKS!

project:

E-2

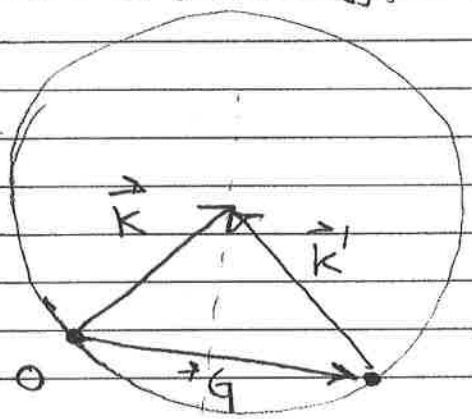
Soln: Allow many $\vec{k}$ either by allowing $|\vec{k}|$ or direction of $\vec{k}$ to vary

Laue Method / Ewald Construction

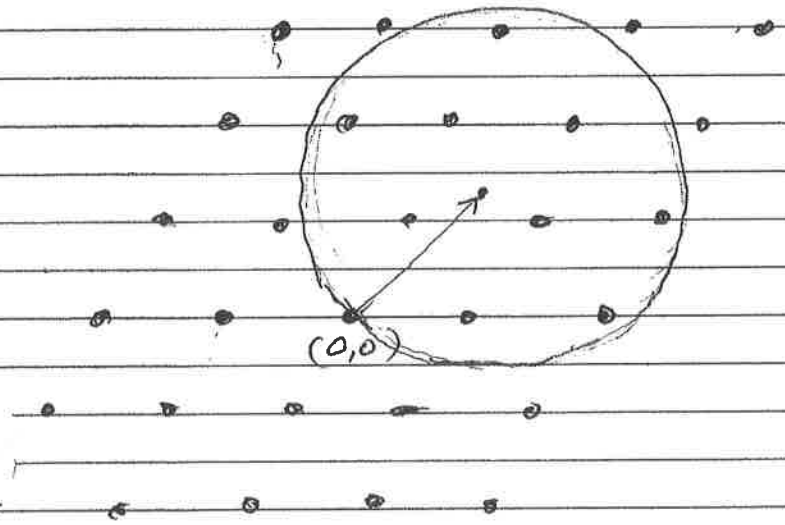
Given incident $\vec{k}$.
Draw sphere centered at tip of $\vec{k}$ (so that it passes through origin)

Will get Bragg peak if a $\vec{G}$ lies on sphere

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



Can again see that it is unlikely there will be such a $\vec{G}$



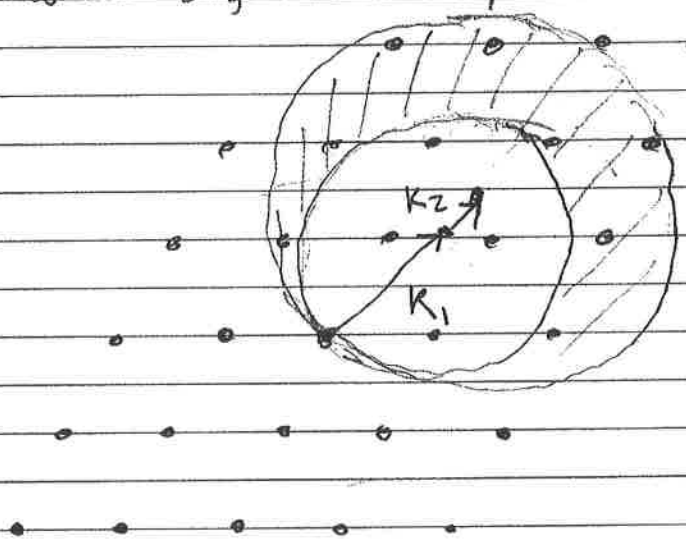
← ~~typical~~ collection of $\vec{G} = n_1\vec{b}_1 + n_2\vec{b}_2$

typical $\vec{k}$ will not intersect any $\vec{G}$.

project:
E3

Use non monochromatic Beam $k_1 < k < k_2$

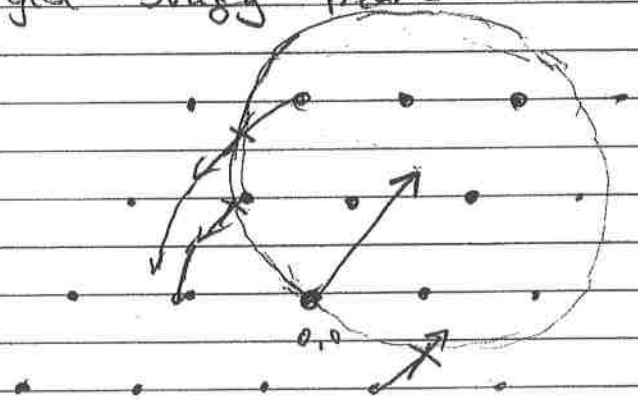
(such as produced by Bremsstrahlung)



Now have 3d space in which to find $\vec{G}$ and there will be non zero probability

Rotating crystal method: Fixed $|\vec{k}|$, but crystal orientation is changed

As $\{\vec{a}_i\}$ are rotated the $\{\vec{b}_i\}$ also trace paths in reciprocal space. Those paths will hit Bragg sphere and give Bragg peaks



Characterization: X-ray

Scattering Techniques

incoming	outgoing	techniques
electron	electron	Auger electron spectroscopy (AES) electron diffraction low energy electron diffraction (LEED) reflection high-energy electron diffraction (RHEED) Scanning electron microscopy (SEM) Transmission electron microscopy (TEM)
ion	ion	Rutherford backscattering (RBS) Channeling
ion	target ion	secondary ion mass spectroscopy (SIMS)
x-ray	x-ray	x-ray fluorescence spectroscopy (XFS) x-ray diffraction
neutron	neutron	neutron diffraction
x-ray	electron	x-ray photoelectron spectroscopy (XPS)
UV	electron	UV photoelectron spectroscopy (UPS)
electron	x-ray	electron microprobe (EM) x-ray microanalysis
photon	electron	photoemission
electron	photon	inverse photoemission

X-Ray: Generation

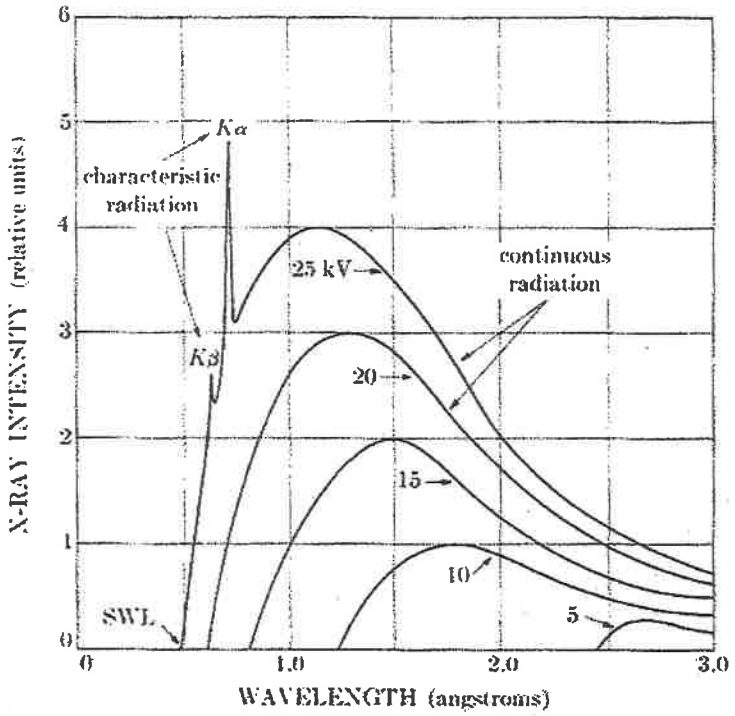
Accelerated electrons hitting an anode (Wilhelm Röntgen, 1895)

X ray

.01 – 10 nm } match atomic spacing in crystal

120eV → 120 keV

why X ray
↳ unknown form of radiation



X-ray spectrum of molybdenum as a function of applied voltage (schematic).
Line widths not to scale.

1901 Nobel Prize in Physics

high velocity electron

anode

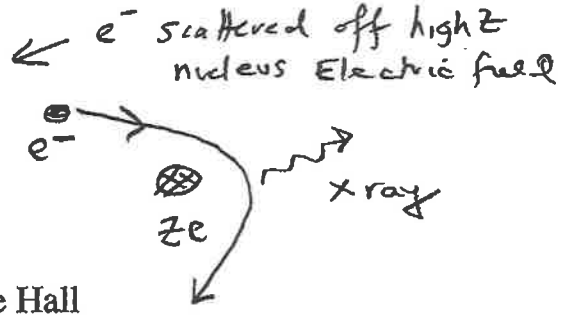
Tungsten
Molybdenum
Rhenium
Copper
cobalt

Continuous spectrum: Bremsstrahlung

λ_{min} (Å)=12.39/V_o (kV)

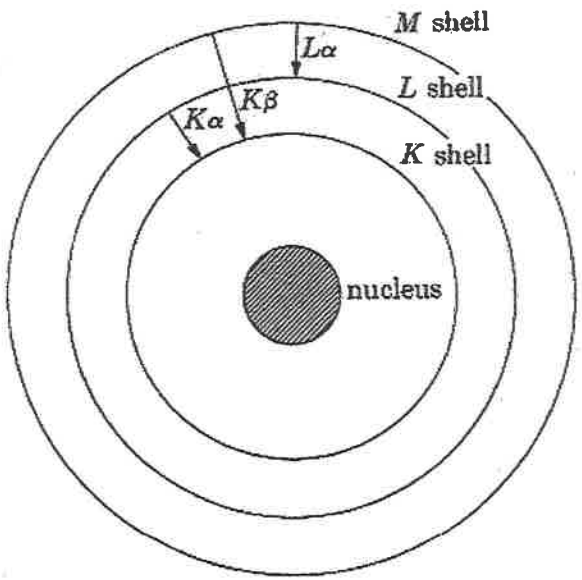
Line spectrum: characteristic x-ray

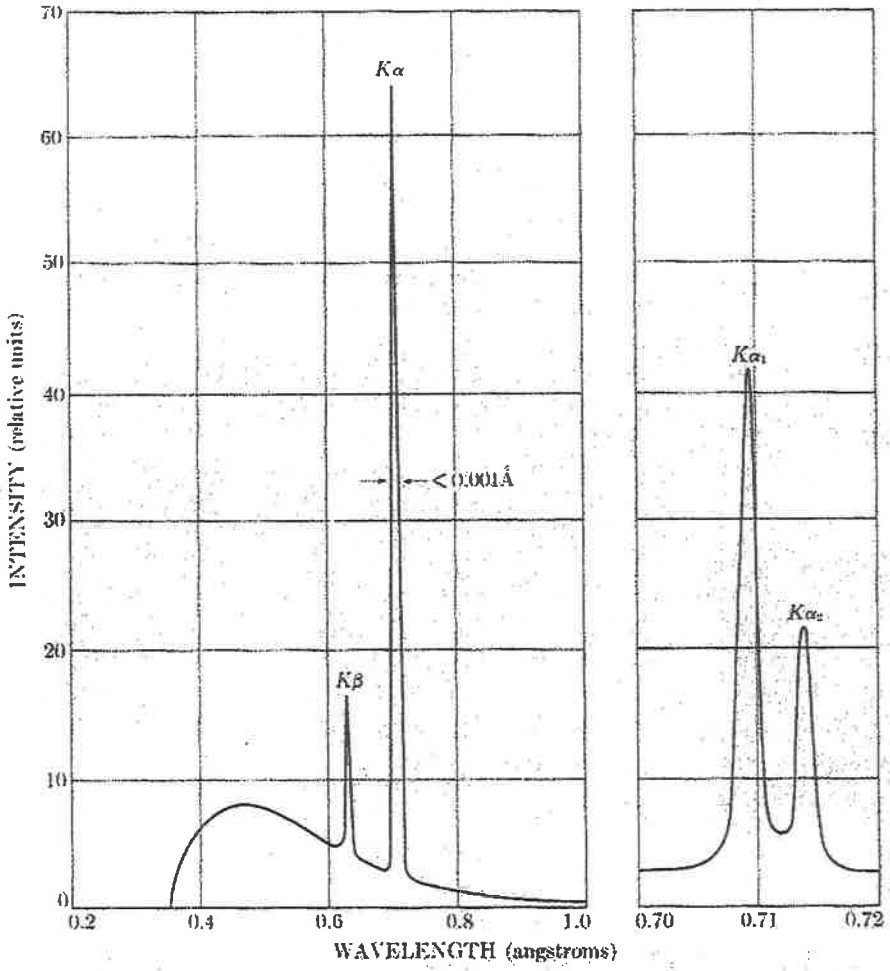
Ref: Elements of x-ray diffraction, B. D. Cullity, 3rd Ed. Prentice Hall



efficiency ~ 1%

Line Spectrum





Spectrum of Mo at 35 kV (schematic). Line widths not to scale. Resolved $K\alpha$ doublet is shown on an expanded wavelength scale at right.

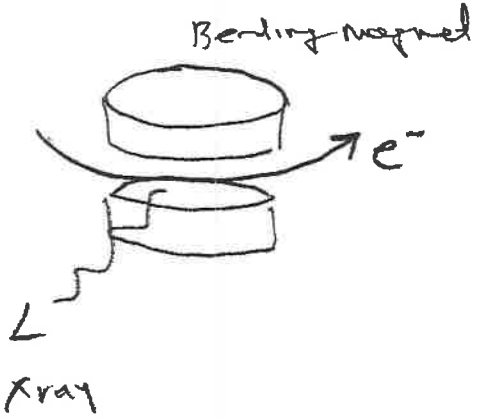
Characteristic x-ray:
unique to element

Incident e^- Knocks e^- out of orbit of inner shell. outer shell e^- drops to fill.

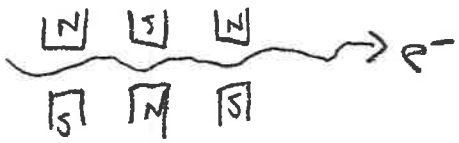
Cu Lines

		Siegbahn Notation	Designation	Energy in keV	Absorption Edge in keV
					8.98029 (K)
K X-Rays	Kβ	$K\beta_5$	$KM_{IV,V}$	8.9770	
		$K\beta_{1,3}$	$KM_{II,III}$	8.90529	
		$K\beta_3$	KM_{II}	8.9029	
	Kα	$K\alpha_1$	KL_{III}	8.04778	
		$K\alpha_2$	KL_{II}	8.02783	
L X-Rays	Lβ	$L\beta_{3,4}$	$L_IM_{II,III}$	1.0228	0.95268(L_{II})
		$L\beta_1$	$L_{II}M_{IV}$	0.9498	
	Lα				0.93306(L_{III})
		$L_{\alpha 1,2}$	$L_{III}M_{IV,V}$	0.9297	
		$L\eta$	$L_{II}M_I$	0.832	
		L_l	$L_{III}M_I$	0.8111	

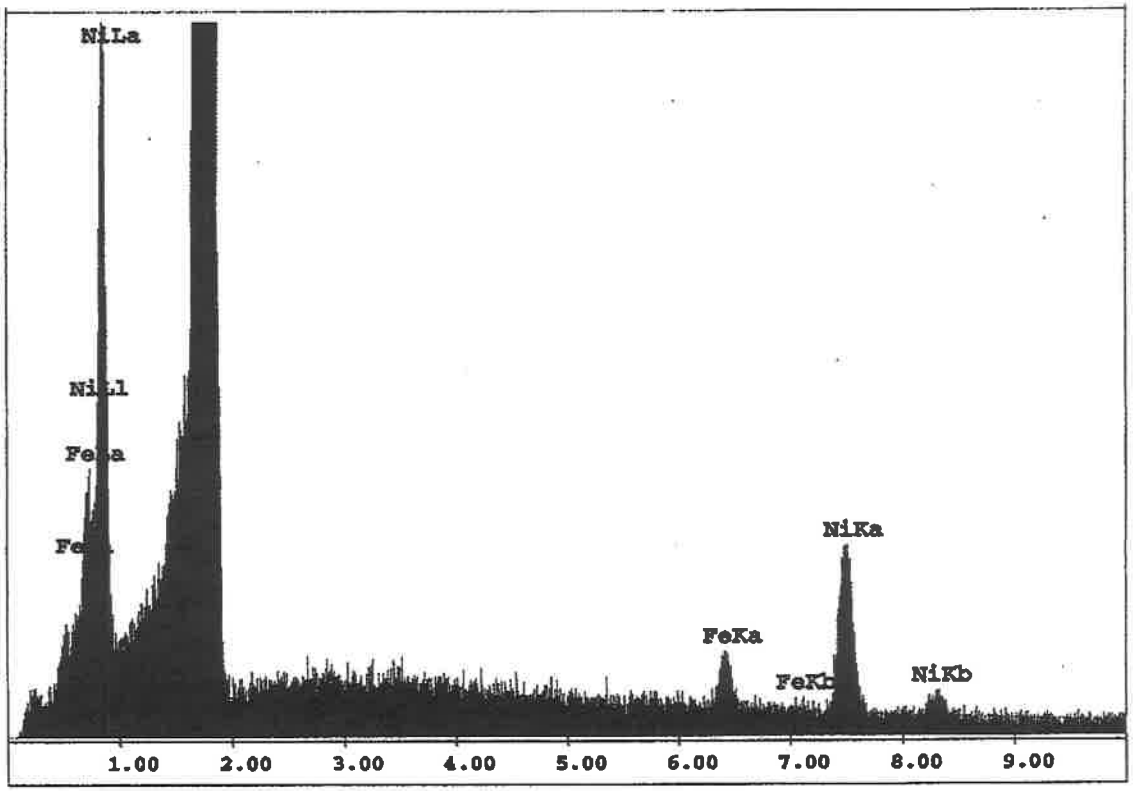
Nowadays synchrotron radiation (like Bremsstrahlung)



undulator or wiggler



EDX



EDAX PhiRhoZ Quantification (Standardless)
Element Normalized
SEC Table : Default

Element	Wt %	At %	K-Ratio	Z	A	F
FeK	15.47	16.14	0.1813	0.9876	0.9885	1.2000
NiK	84.53	83.86	0.8192	1.0022	0.9671	1.0000
Total	100.00	100.00				

Element	Net Inte.	Bkgd Inte.	Inte. Error	P/B
FeK	2.50	1.55	5.47	1.61
NiK	8.07	1.39	2.36	5.82

Absorption/Filtering

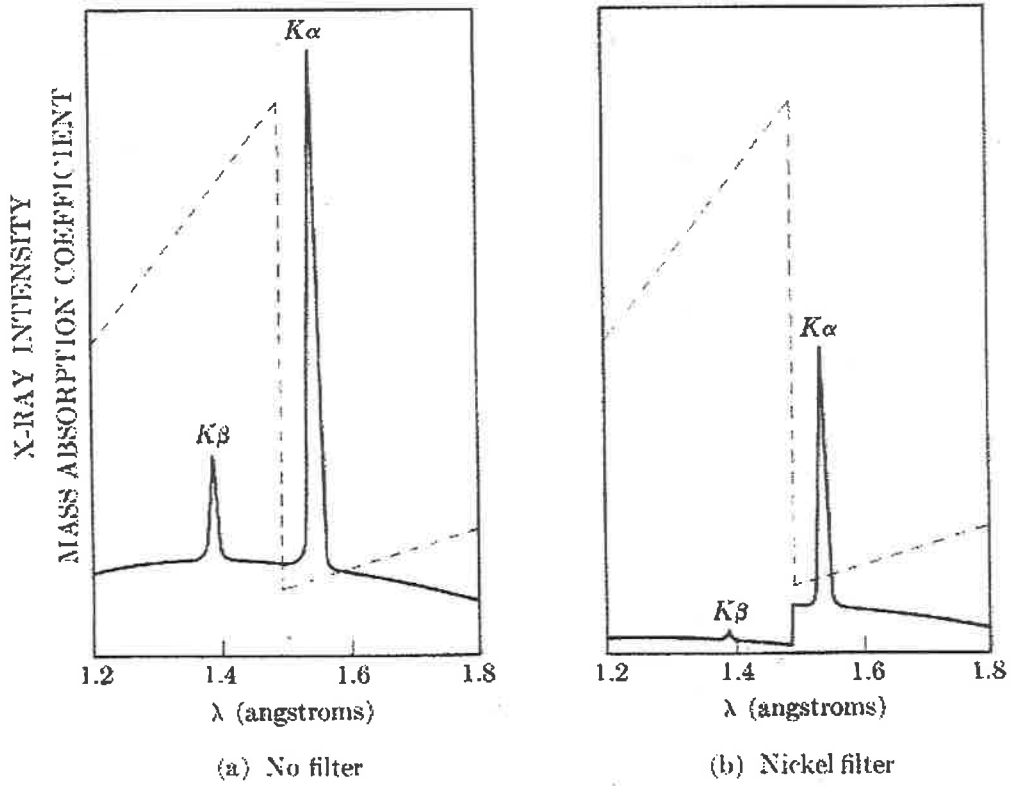
$$I_x = I_o e^{-(\mu/\rho)\rho x}$$

$\mu/\rho = k\lambda^3 Z^3$ Mass absorption coefficient

μ– Absorption coefficient (cm^{-1})

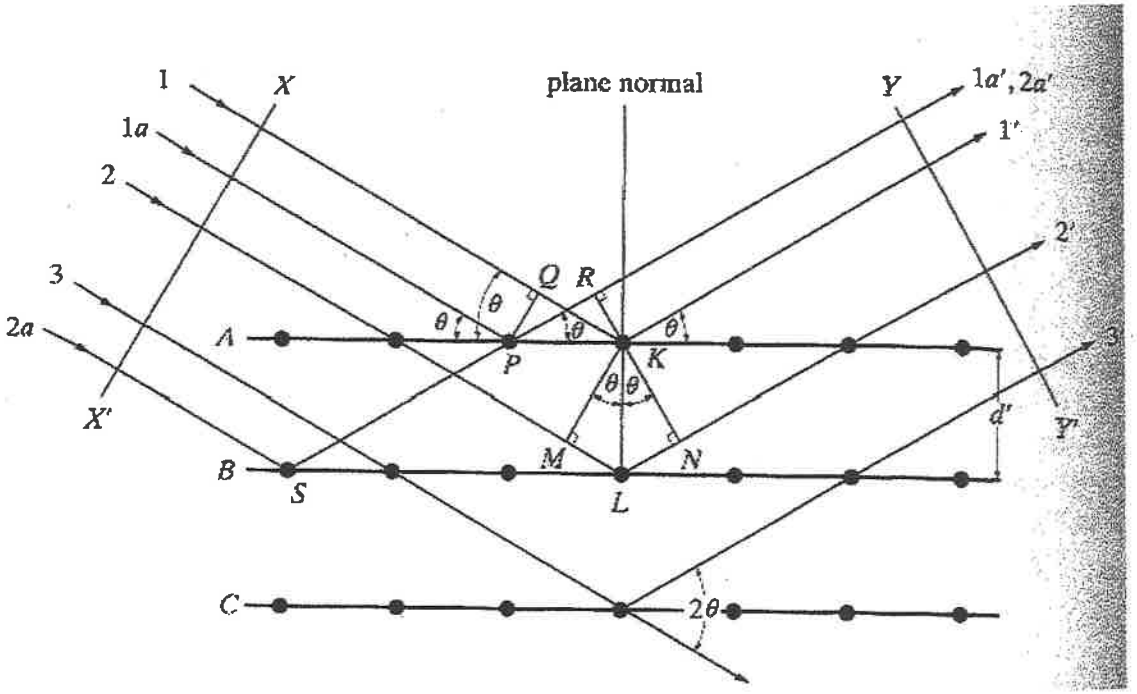
x: thickness

1/μ - One absorption length



Comparison of the spectra of copper radiation (a) before and (b) after passage through a nickel filter (schematic). The dashed line is the mass absorption coefficient of nickel.

Diffraction



Scalar description:

Bragg's Law: $2d\sin\theta = n\lambda$

Vector description:

Laue conditions: $\Delta\mathbf{k} = \mathbf{k}_o - \mathbf{k} = \mathbf{G}$ **- necessary**

q-value: $|\Delta\mathbf{k}| = 4\pi\sin\theta/\lambda$

d-Spacing

Cubic:
$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

Tetragonal:
$$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

Hexagonal:
$$\frac{1}{d^2} = \frac{4}{3}\left(\frac{h^2 + hk + k^2}{a^2}\right) + \frac{l^2}{c^2}$$

Rhombohedral:
$$\frac{1}{d^2} = \frac{(h^2 + k^2 + l^2)\sin^2\alpha + 2(hk + kl + hl)\cos^2\alpha - \cos\alpha)}{a^2(1 - 3\cos^2\alpha + 2\cos^3\alpha)}$$

Orthorhombic:
$$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

Monoclinic:
$$\frac{1}{d^2} = \frac{1}{\sin^2\beta}\left(\frac{h^2}{a^2} + \frac{k^2\sin^2\beta}{b^2} + \frac{l^2}{c^2} - \frac{2hl\cos\beta}{ac}\right)$$

Triclinic:
$$\frac{1}{d^2} = \frac{1}{V^2}(S_{11}h^2 + S_{22}k^2 + S_{33}l^2 + 2S_{12}hk + 2S_{23}kl + 2S_{13}hl)$$

In the equation for triclinic crystals,

V = volume of unit cell (see below),

$S_{11} = b^2c^2\sin^2\alpha$,

$S_{22} = a^2c^2\sin^2\beta$,

$S_{33} = a^2b^2\sin^2\gamma$,

$S_{12} = abc^2(\cos\alpha\cos\beta - \cos\gamma)$,

$S_{23} = a^2bc(\cos\beta\cos\gamma - \cos\alpha)$,

$S_{13} = ab^2c(\cos\gamma\cos\alpha - \cos\beta)$.

Structure Factor

$$F_{hkl} = \sum_{1}^{N} f_n e^{2\pi i(hu_n + kv_n + lw_n)}$$

$$|F| = \frac{\text{amplitude of the wave scattered by all the atoms in a unit cell}}{\text{amplitude of the wave scattered by one electron}}$$

e.g.: fcc lattice, 4 same atoms at (0, 0, 0), (½, ½, 0), (½, 0, ½) and (0, ½, ½).

$F_{hkl} = f[1 + e^{\pi i(h+k)} + e^{\pi i(k+l)} + e^{\pi i(l+k)}] \neq 0$ if h, k, l are all odd or all even

Allowed diffraction:

fcc: all odd or all even

bcc: h+k+l=even