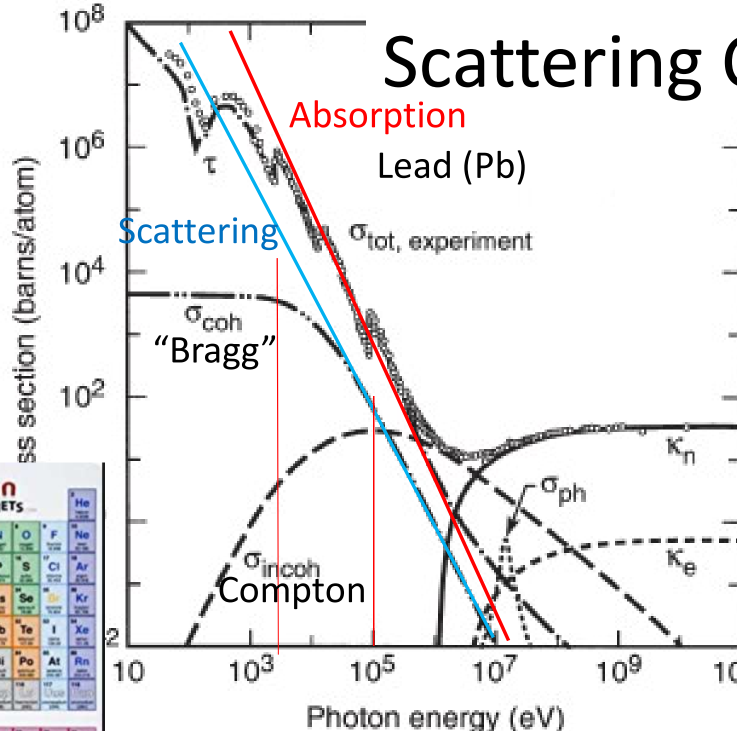
Scattering Cross-sections

Figures: the X-ray data booklet
http://xdb.lbl.gov



. *Total photon cross section σ_{tot} in lead, as a function of energy. See Fig. 3-1. (From Ref. 3; figure courtesy of J. H. Hubbell.)*

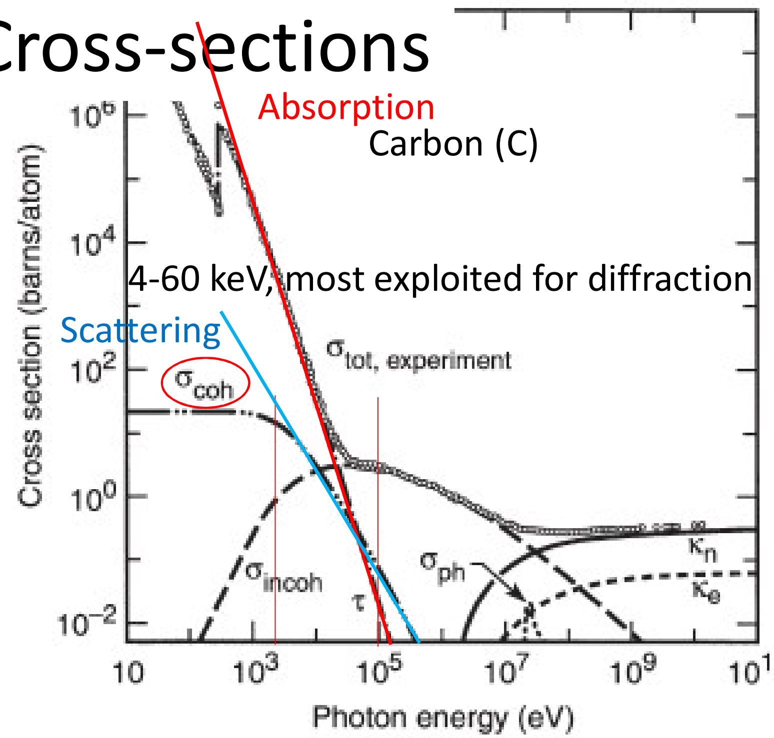
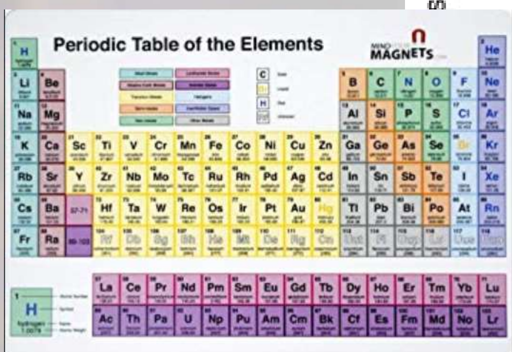


Fig. 3-1. *Total photon cross section σ_{tot} in carbon, as a function of energy, showing the contributions of different processes: τ, atomic photo-effect (electron ejection, photon absorption); σ_{coh}, coherent scattering (Rayleigh scattering—atom neither ionized nor excited); σ_{incoh}, incoherent scattering (Compton scattering off an electron); κ_n, pair production, nuclear field; κ_e, pair production, electron field; σ_{ph}, photonuclear absorption (nuclear absorption, usually followed by emission of a neutron or other particle). (From Ref. 3; figure*



Rule of thumb

absorption ~Z^4

Elastic scattering ("Bragg") ~Z^2

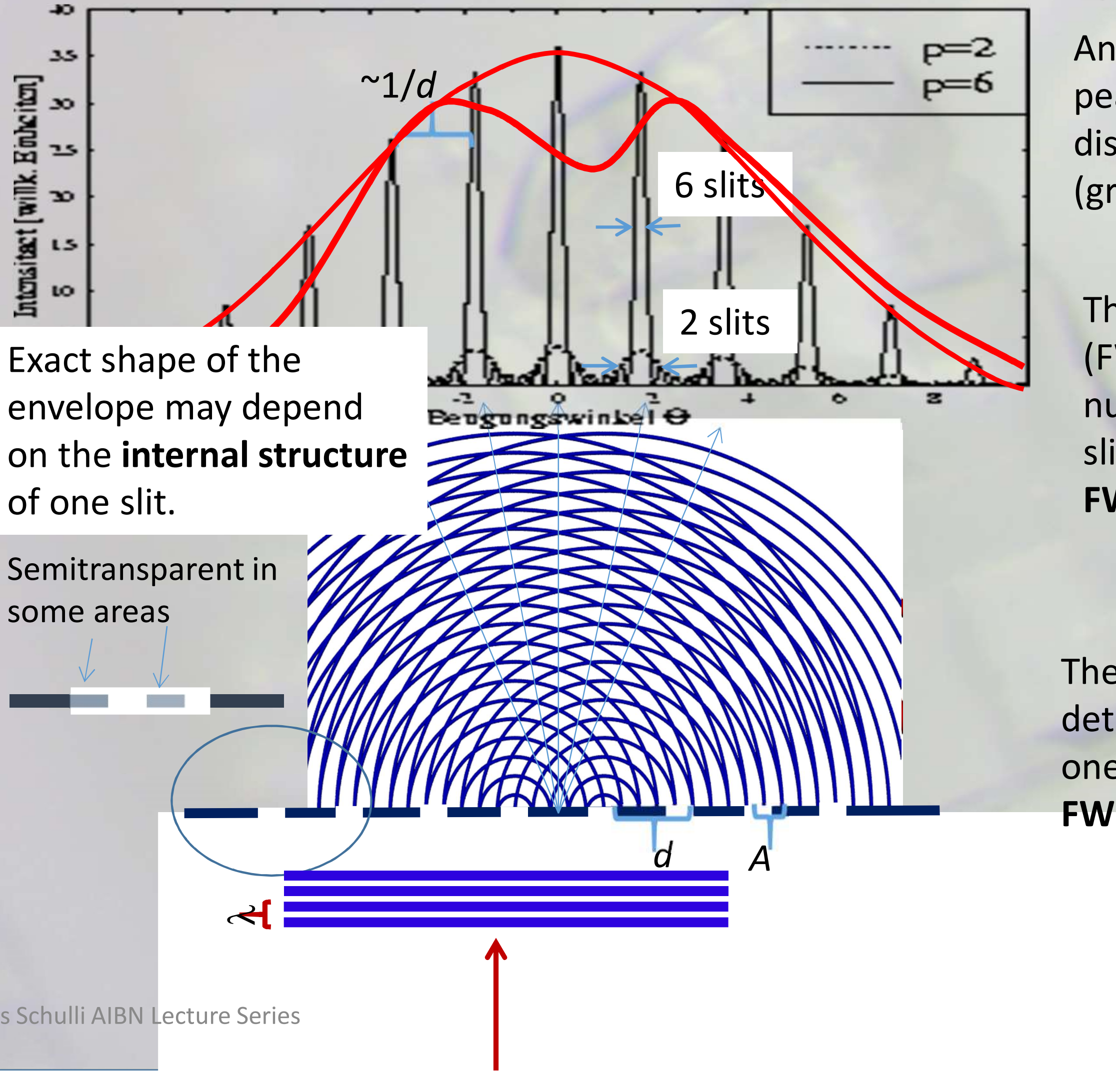
In your experiment it is not only your "sample" that scatters !

Elastic scattering and interference phenomena

Phenomenological approach through light – grating interaction

Plane wave:

Diffraction from a periodic grating



Exact shape of the envelope may depend on the **internal structure** of one slit.

Semitransparent in some areas

Angular distance of the peaks<->determines distances of the slits (grating parameter)

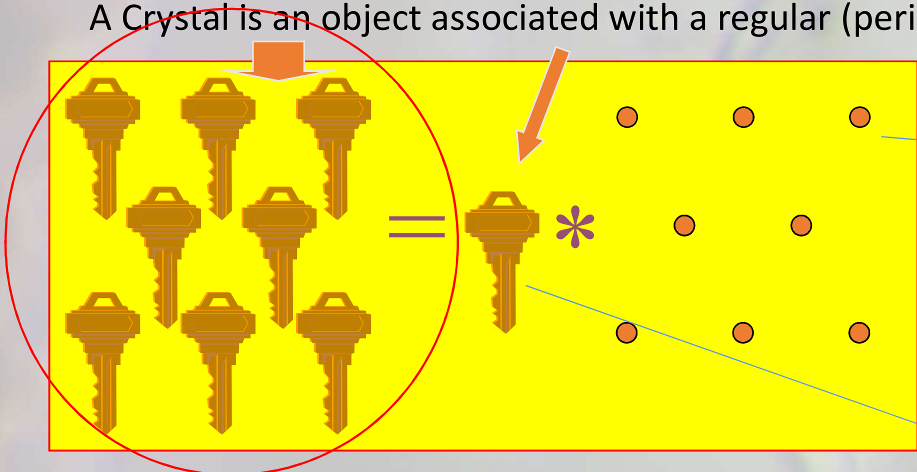
The width of the peaks (FWHM) depends on the number *p* of illuminated slits
FWHM~*1/p*

The **envelope** of the peaks determines the **width *A*** of one slit.
FWHM~*1/A*

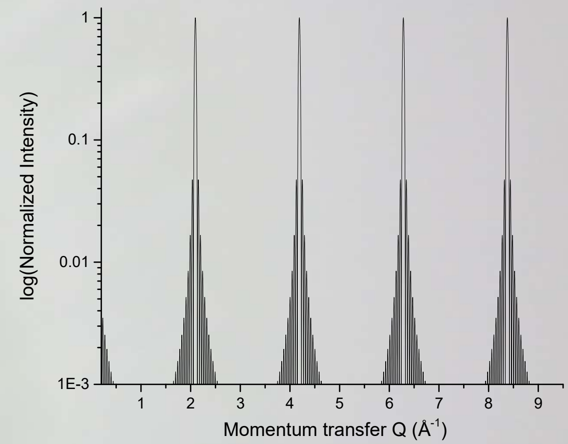
"Crystallography"= study of periodic objects

But in the end, what we are interested in may well be "the object"

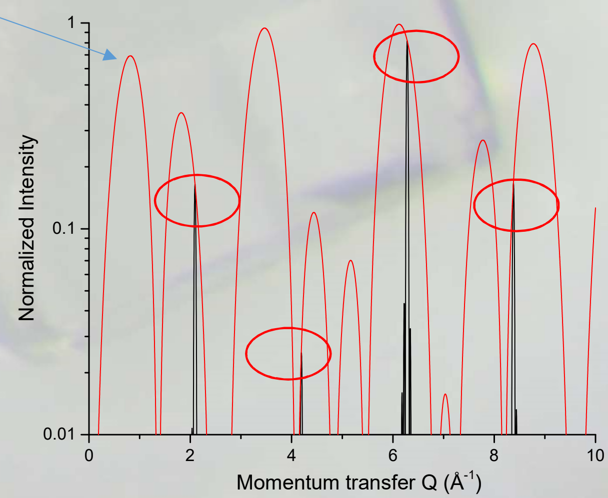
A Crystal is an object associated with a regular (periodic or non-periodic) grating, defining its repetition



Grating Leads to regular "Bragg" peaks



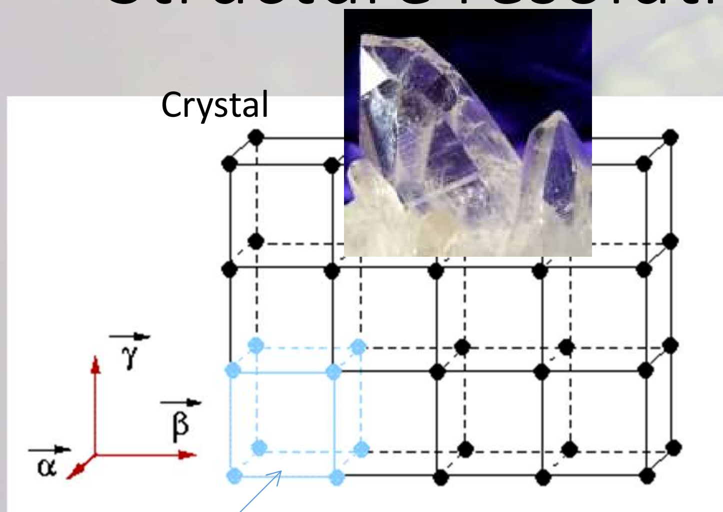
"Object" leads to a structure that determines the height of the peaks



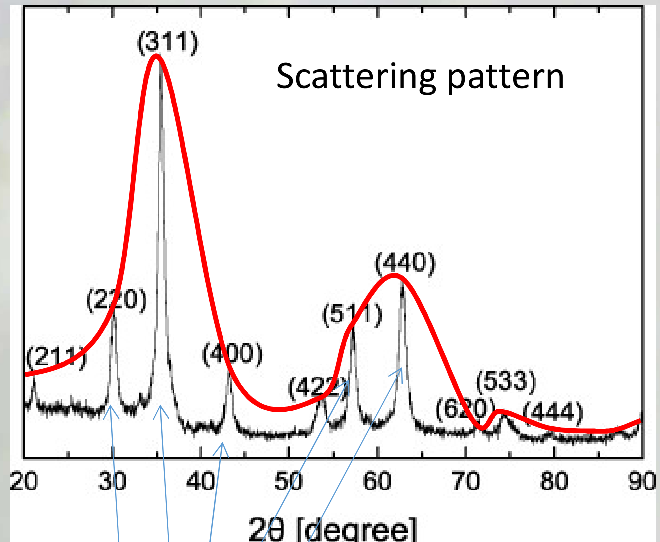
Crystallography: We can only sample the read curve in distinct points, but a precise knowledge of the red curve is required to resolve an image of the "object"

Why using a crystal ?

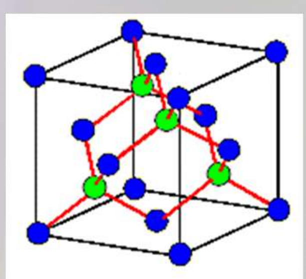
Structure resolution by diffraction



“Unit cell” (smallest repetitive building block)



“Bragg-peaks” corresponding to different net planes)

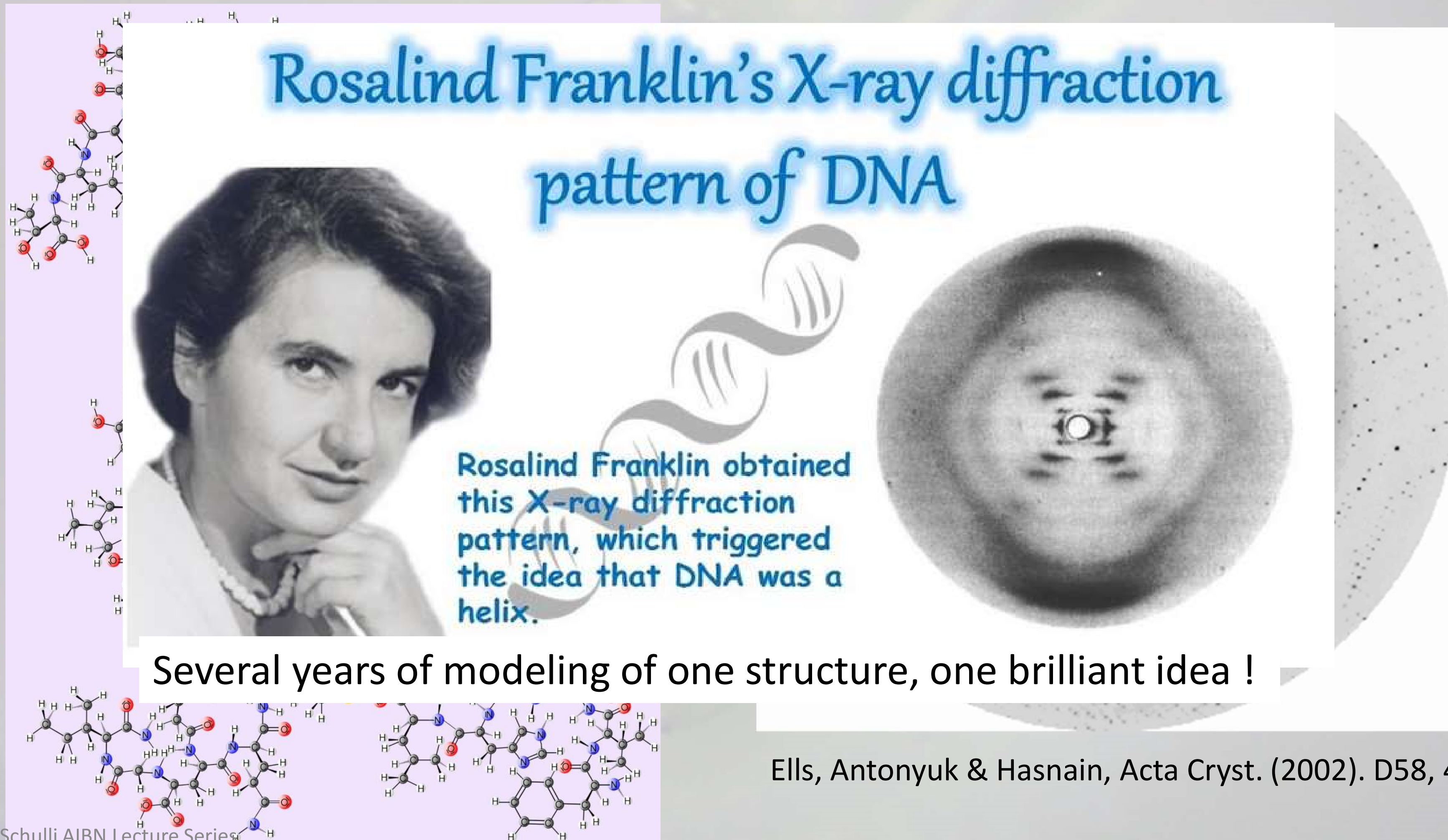


Envelope->

Information about the atomic arrangement inside the unit cell.

The envelope that contains all the information on the detailed distribution of electron density inside a unit cell can only be sampled at certain discrete positions, the Bragg peaks that correspond to the basic long range periodicities, also called the Fourier components

Reconstruction of complex molecules through their Fourier components

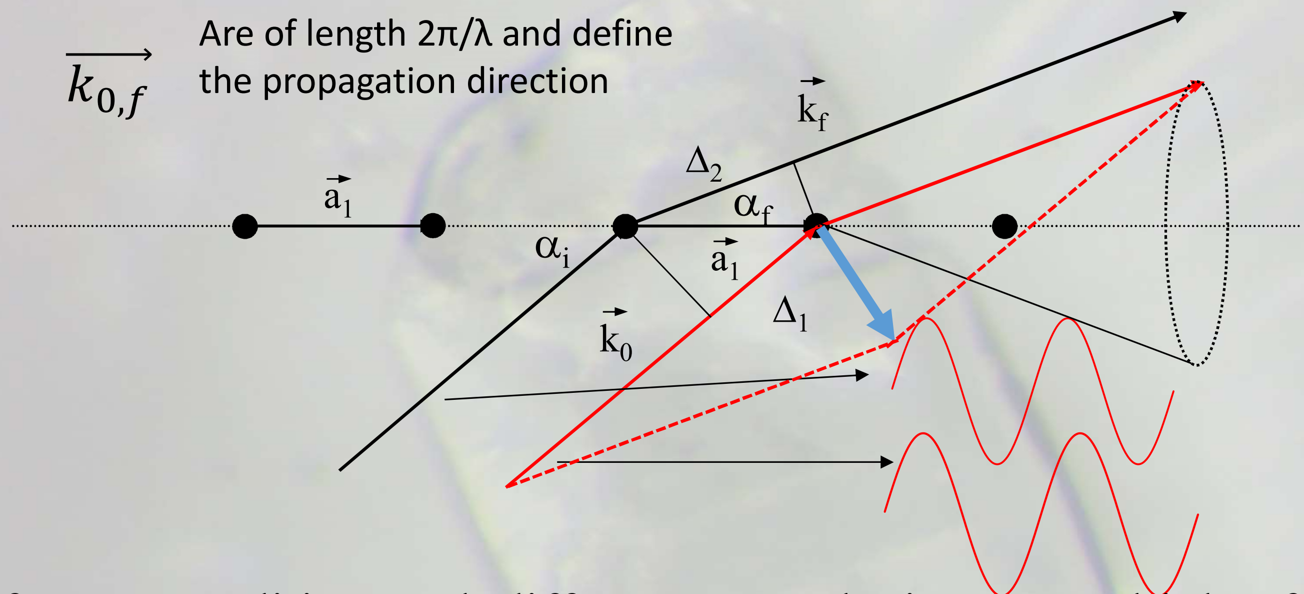


Several years of modeling of one structure, one brilliant idea !

Ells, Antonyuk & Hasnain, Acta Cryst. (2002). D58, 456

Laue construction, scattering from 3D lattices

$\overrightarrow{k_{0,f}}$ Are of length 2π/λ and define the propagation direction

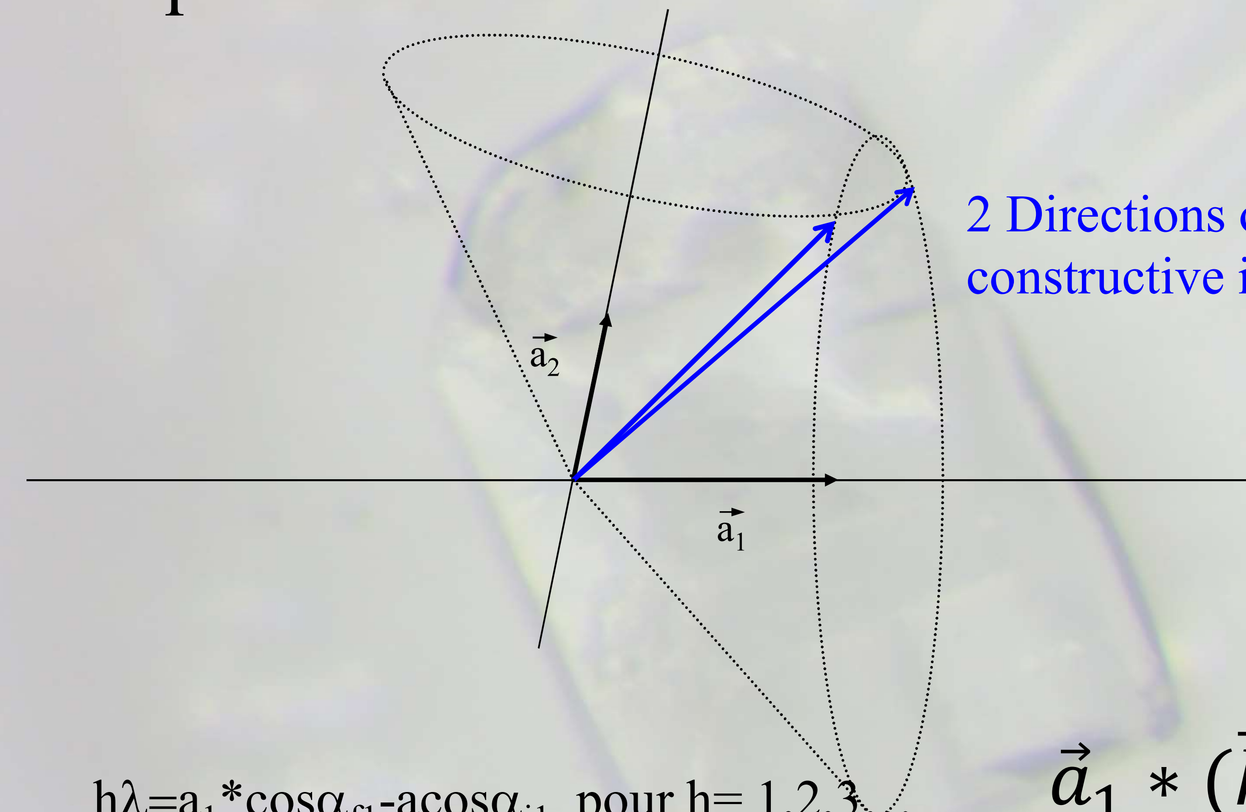


Interference condition: path difference must be integer multiple of λ:

$$h\lambda=\Delta=\Delta_2-\Delta_1=a_1*\cos\alpha_f-a_1\cos\alpha_i \text{ pour } h= 1,2,3\ldots$$

$$\vec{a}_1 * (\underbrace{\vec{k}_f-\vec{k}_0}) = h\lambda$$

Laue equations



2 Directions of constructive interference

$h\lambda = a_1 * \cos\alpha_{f1} - a\cos\alpha_{i1}$ pour h= 1,2,3…

$k\lambda = a_2 * \cos\alpha_{f2} - a\cos\alpha_{i2}$ pour k= 1,2,3…

$$\vec{a}_1 * (\vec{k}_f - \vec{k}_0) = h\lambda$$

$$\vec{a}_2 * (\vec{k}_f - \vec{k}_0) = k\lambda$$

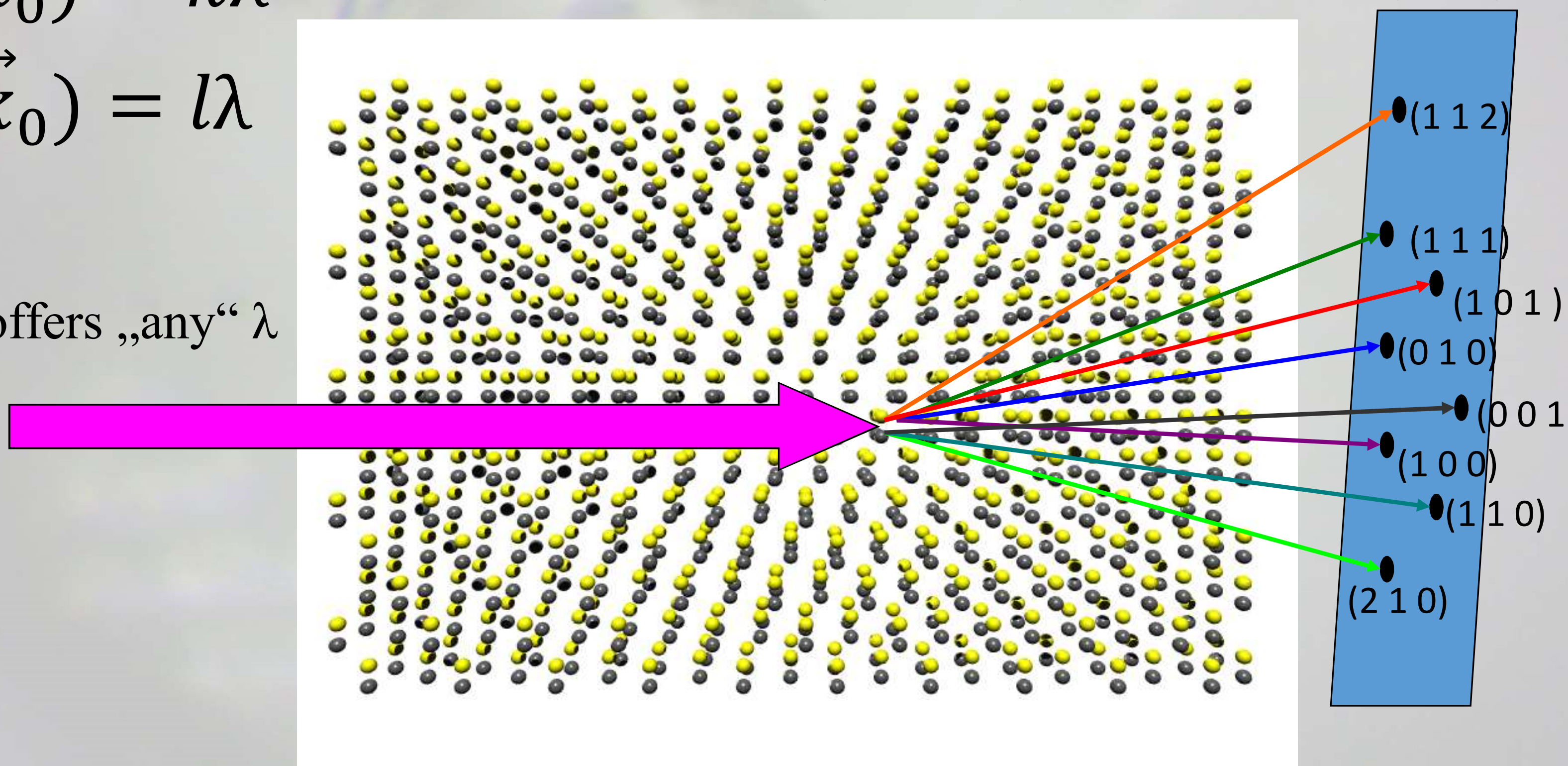
Laue equations

$$\vec{a}_1 * (\vec{k}_f \text{-} \vec{k}_0) = h\lambda$$
$$\vec{a}_2 * (\vec{k}_f \text{-} \vec{k}_0) = k\lambda$$
$$\vec{a}_3 * (\vec{k}_f \text{-} \vec{k}_0) = l\lambda$$

With h,k,l as integers, it may be rare to find a solution for arbitrary $\vec{k}_0$

Laue's solution: use white light (λ as 4th parameter that can adopt "any" value)

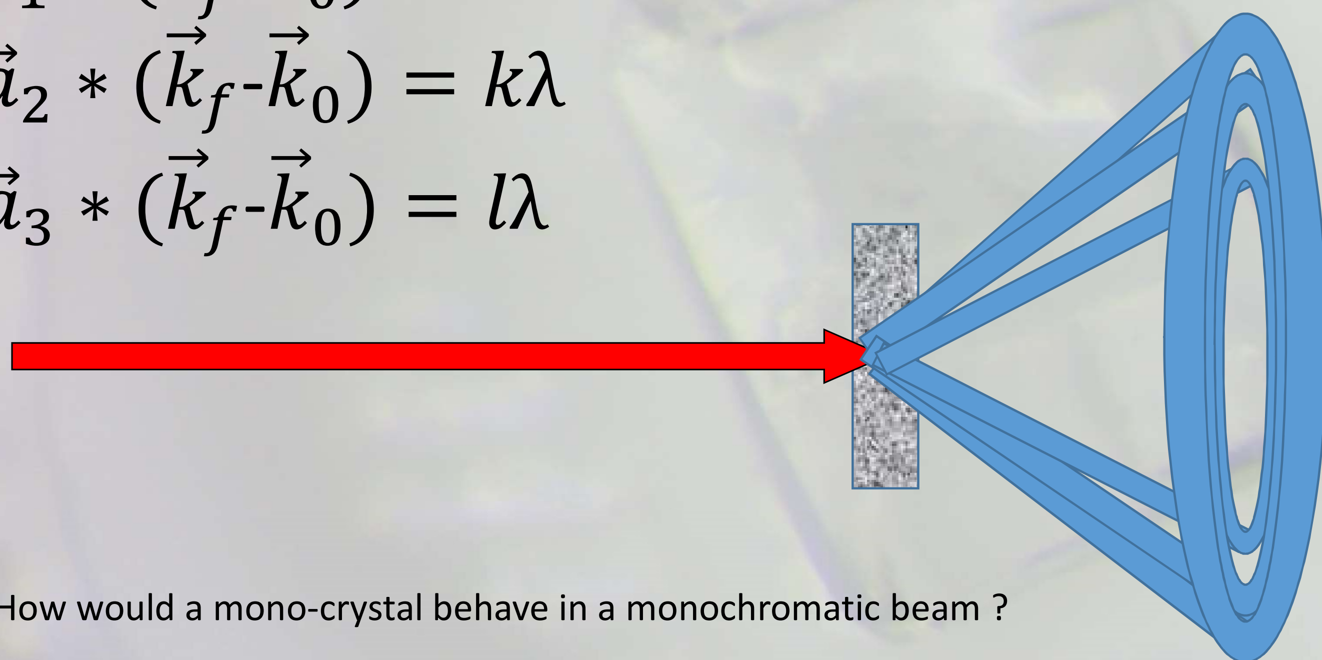
White beam offers „any“ λ



Just to throw it in….

And what about powder diffraction ?
Wavelength λ is fixed this time (monochromatic beam),
but we offer all directions of
In the form of crystallite orientations $\overrightarrow{k_0}$

$$\vec{a}_1 * (\vec{k}_f\text{-}\vec{k}_0) = h\lambda$$
$$\vec{a}_2 * (\vec{k}_f\text{-}\vec{k}_0) = k\lambda$$
$$\vec{a}_3 * (\vec{k}_f\text{-}\vec{k}_0) = l\lambda$$



We lose 1 parameter (λ) and we “win” 2 with free choice of $\overrightarrow{k_0}$,
-> the “solution” is no longuer a “point” but becomes a (ring shaped) line

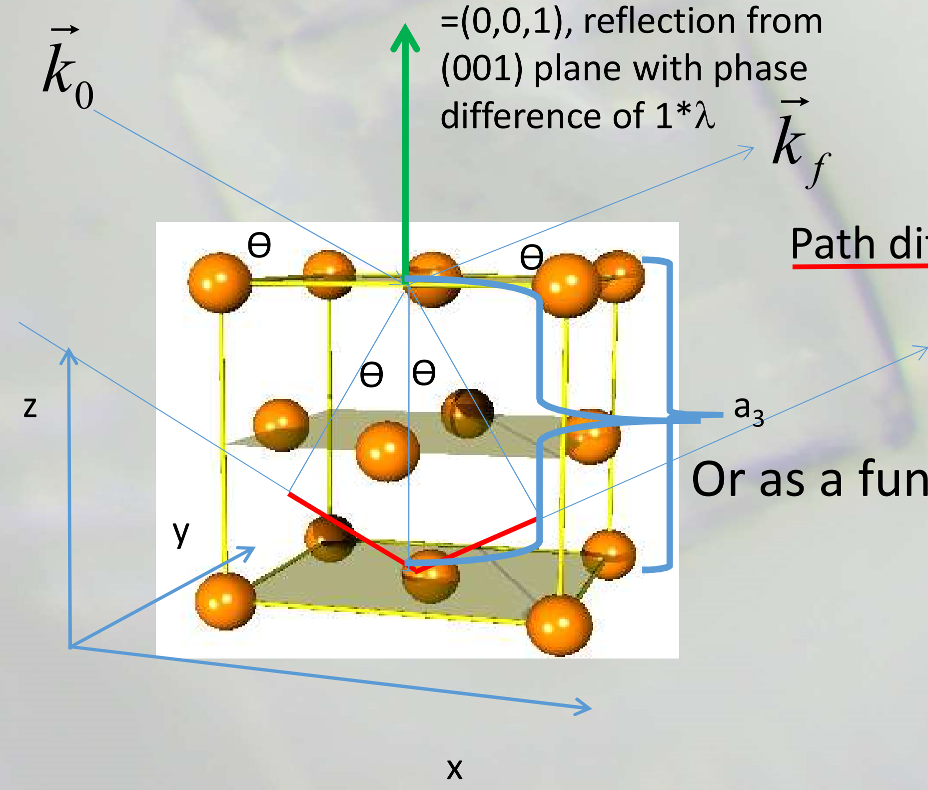
How would a mono-crystal behave in a monochromatic beam ?

In this notation $\overrightarrow{k_f}$ and $\overrightarrow{k_0}$ are vectors of length 2π/λ

Bragg description of diffraction

Laue: diffraction is 3D interference from point lattice

William (Laurence+Henry) Bragg: diffraction is interfering reflection from net planes of the Crystal (1913). Their approach focused on monochromatic “characteristic” x-rays

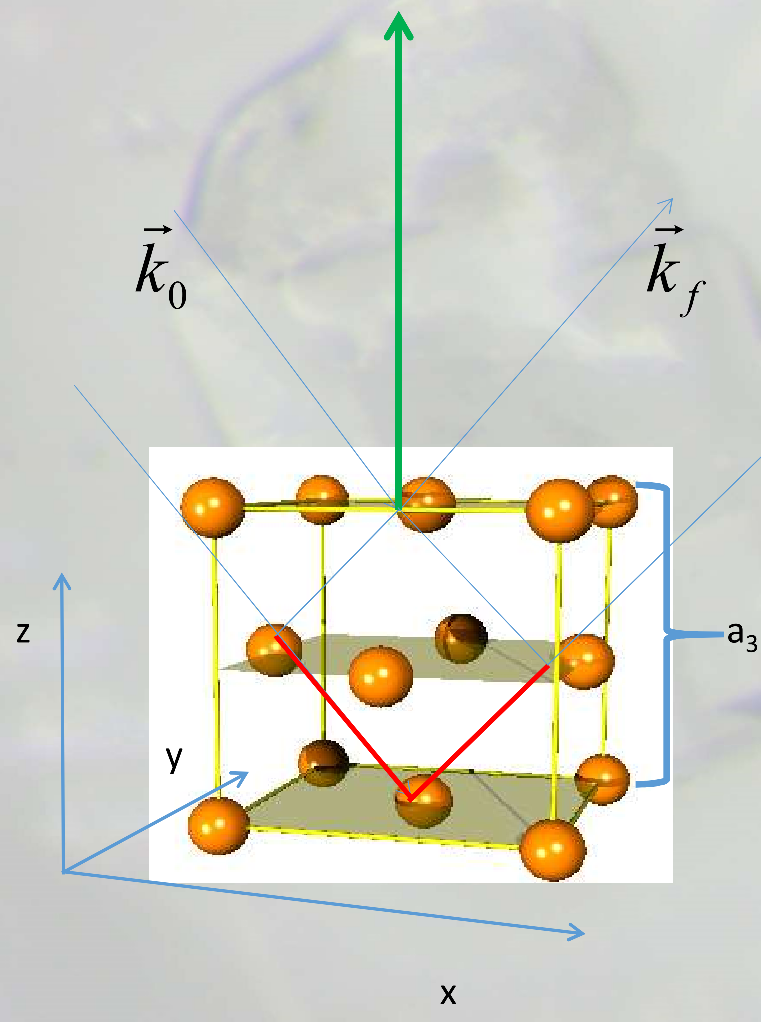


Path difference 2*a_3*sinϴ:= 1*λ,

Or as a function of lattice spacing d=a_3 :

$$\sin(\theta) = \frac{\lambda}{2d}$$

=(0,0,2), reflection from (001) plane with phase difference of 2*λ
h=k=0, l=2 in the Laue equations



Increase angle up to

Phase difference $2*a_3*\sin\Theta := 2*\lambda$
leading to Braggs law

$$\sin\Theta = (n*\lambda)/(2*d)$$

with n=1,2,3,….

=(0,0,2), reflection from (002) plane with phase difference of 1*λ

For better convenience:

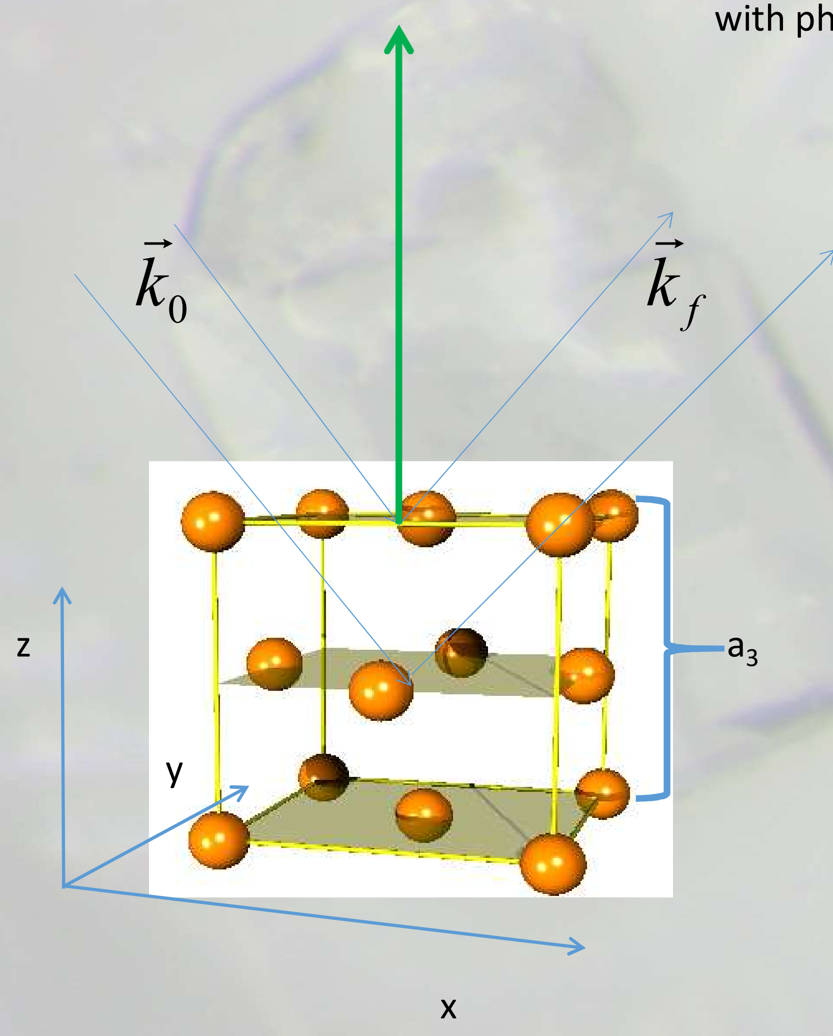
$sin\theta_{hkl}$=(n∗λ)/(2∗ d_{hkl})

In our indexing terminology skips the "n"

$sin\theta_{hkl}$=(λ)/(2∗ d_{hkl})

For the cubic case:

$$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$$



Phase difference: λ

Definition of the net planes (Miller, 1801–1880)

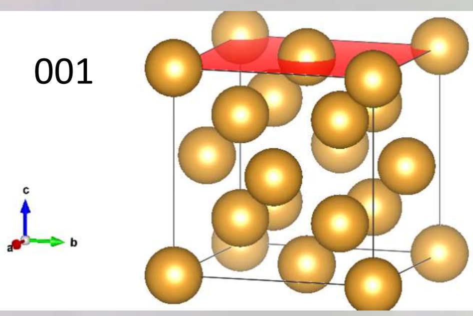
(hkl) netplane is defined as the plane that intersects the real space unit cell axis in the points

$$\frac{1}{h}\vec{a}_1, \frac{1}{k}\vec{a}_2, \frac{1}{l}\vec{a}_3$$

The higher the indexation, the closer the netplanes are spaced

René Just Haüy formulates the law of rational indices (1781): *For the given crystal species it is always possible to choose three vectors, **a, b** and **c** so that all the natural faces of this crystal cut the lengths proportional to the three integer numbers*

001



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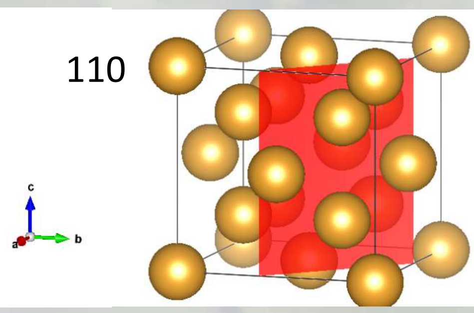

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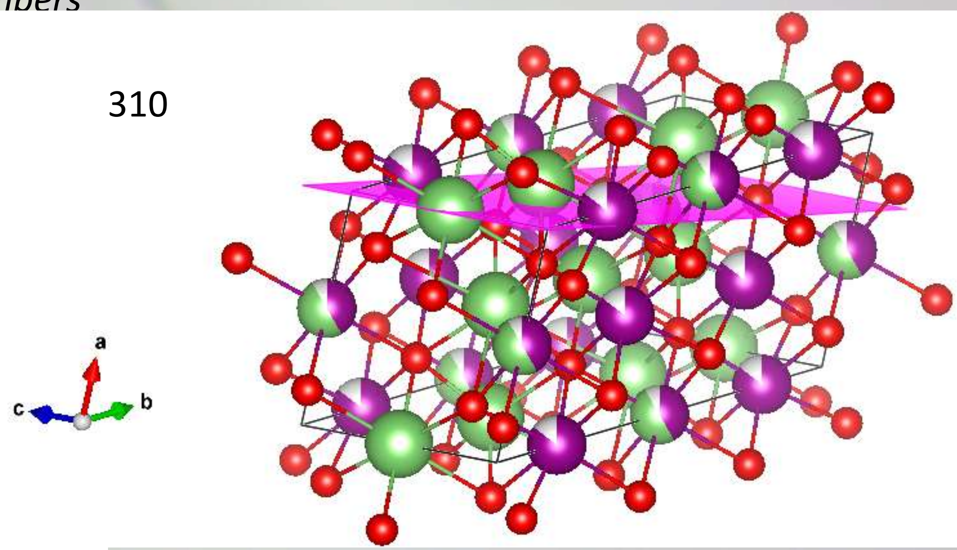

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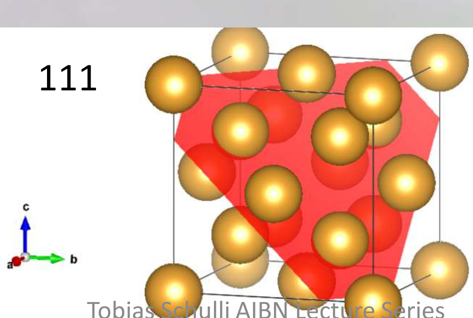

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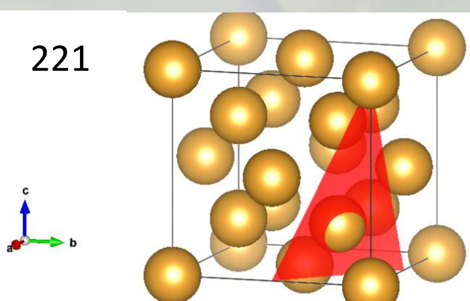


Low index: fundamental structure (unit cell)
High index: structural details

Scattering of x-rays by electrons

Why electrons (and not protons, or other nuclei) ?

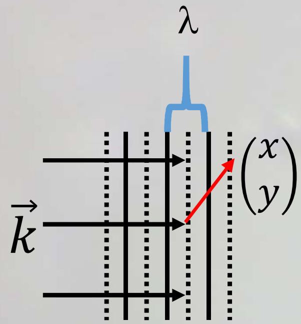
Larmors formula for the power irradiated by an accelerated charge: $P = \frac{2}{3}\frac{e^2}{c^3}\left|\dot{\vec{v}}\right|^2$

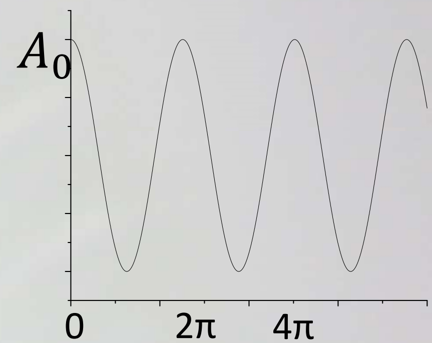
$\left|\dot{\vec{v}}\right| = \frac{F}{m}$, with $F \sim e$ (elementary charge)

For a hydrogen atoms:
Light as an electromagnetic field accelerates e- and p+ with the same force (as equal elementary charges), however the higher mass of protons leads to 1836 times weaker acceleration $\left|\dot{\vec{v}}\right|$, and thus 1836^2=3.4*10^6 times weaker irradiated power: $P_{Proton} = 2.97 * 10^{-7} P_{electron}$

It is thus the electrons in a material that are essentially responsible for the scattering of X-rays as electromagnetic waves

Propagating plane wave





Oscillating field at a fix point x: $A_x(t) = A_0 \cos(2\pi f t)$

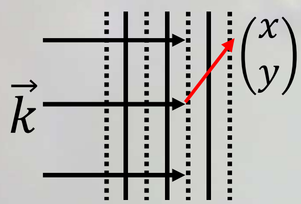
$= A_0 \cos(\omega t)$, *with* ω=2*πf*

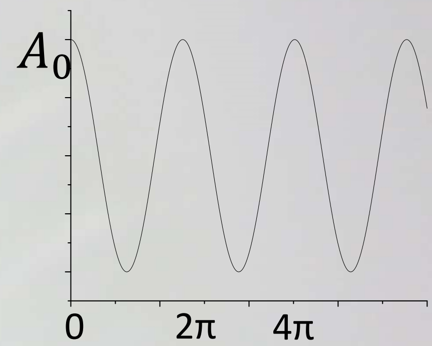
Same wave frozen in time: $A_t(x) = A_0 \cos(\frac{2\pi x}{\lambda})$ $\qquad k = \frac{2\pi}{\lambda}$

Oscillation in space and time: $A(x,t) = A_0 \cos(\omega t + kx)$

Oscillation in space and time: $A(x,y,t) = A_0 \cos\left(\omega t + \begin{pmatrix} k_x \\ k_y \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}\right) = A_0 \cos\left(\omega t + \vec{k}\vec{r}\right)$

Propagating plane wave





Oscillation in space and time: $A(\vec{r},t) = A_0 \cos\left(\omega t + \vec{k}\vec{r}\right)$

"Equivalent description": $A(\vec{r},t) = A_0\, e^{i(\omega t+\vec{k}\vec{r})} = A_0(\cos\left(\omega t + \vec{k}\vec{r}\right) + i * \sin\left(\omega t + \vec{k}\vec{r}\right))$

Essentially carries advantages for the analytical treatment of wave propagation