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” X-ray Physics”

Cheiron School 2009

X-ray photons and matter

1. ***Scattering***

   classical physics

2. ***Absorption***

   Quantum physics

Electromagnetic radiation

$$\text{mass} \cdot \text{acceleration} = \text{force=charge} \cdot \text{field}$$

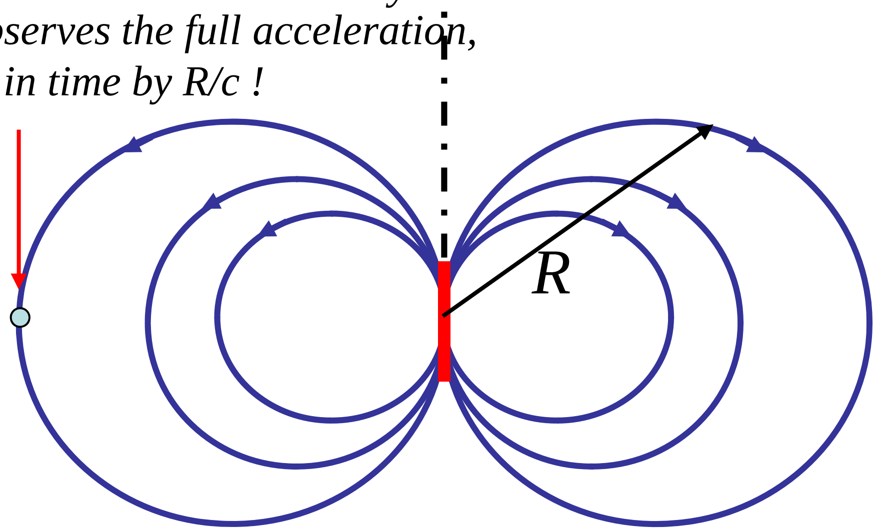
$$m \cdot acc = [-e]E_{in}(t - R/c) = [-e]E_0 e^{-i\omega(t-R/c)}$$

$$= [-e]E_0 e^{-i\,\omega t} \cdot e^{i(\omega/c)R}$$

$$= [-e]E_{in}(t) \cdot e^{ikR}$$

Along this line one does not observe any acceleration

Here one observes the full acceleration, but delayed in time by R/c !



$$\frac{E_{rad}(t)}{E_{in}(t)} = -r_0 \frac{e^{ikR}}{R} \;;$$

$$r_0 = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{mc^2} = 2.82 \cdot 10^{-5}\, Ang$$

Radiation from a dipole-antenna

due to the oscillating charge in the antenna

Guess that

$$E_{rad}(R) \propto \frac{1}{R} \quad \Rightarrow \quad E_{rad}^2 \propto \frac{1}{R^2} \propto energy - density \quad \Rightarrow \quad radiated\ energy \propto \frac{1}{R^2} \cdot 4\pi\, R^2$$

$$E_{rad} \propto \text{charge} \quad q \quad ; \quad E_{rad}(R,t) \propto observed \quad acceleration\,(t - R/c)$$

$$E_{rad}(R,t) = -\frac{1}{R}\frac{-e}{4\pi\varepsilon_0} \cdot \frac{1}{c^2} \cdot acc(t - R/c) \quad ;$$

To get the dimension right !

$$e \cdot E_{rad}(R,t) = \frac{1}{R}\frac{e^2}{4\pi\varepsilon_0} \cdot \frac{acc}{c^2} \cdot$$

$$\text{Force} \quad = \text{Energy} \; \frac{\text{m/sec}^2}{(\text{m/sec})^2} \quad \text{OK}$$

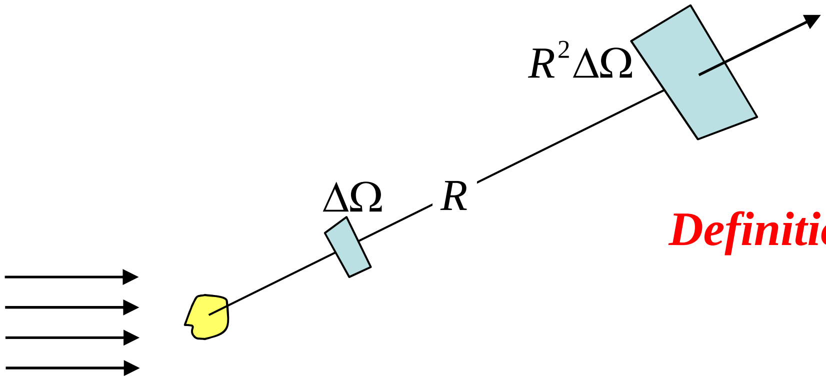
Definition of scattering cross section and flux

$$\frac{d\sigma}{d\Omega} \qquad \phi$$

Particle flux $\phi = \dfrac{ph/\sec}{cm^2}$

Power flux $\phi = \dfrac{energy/\sec}{cm^2}$

$energy/\sec = E \cdot photons/\sec \quad \Rightarrow \quad$ Power flux $= E \cdot$ Particle flux

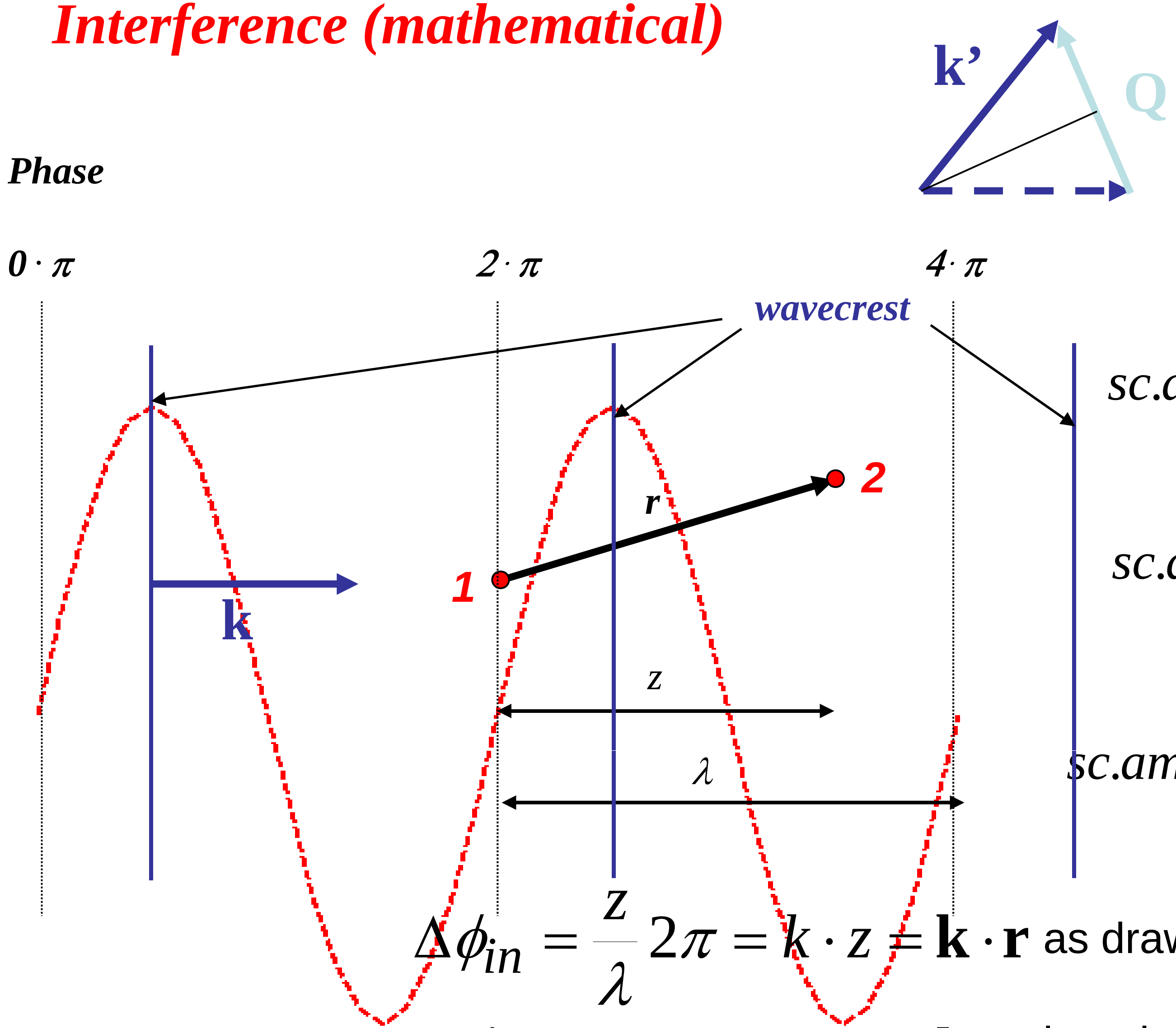


$$I_{scat} = R^2 \Delta\Omega \cdot \phi_{out}$$

Definition $\quad I_{scat} = \phi_{in} \Delta\Omega \dfrac{d\sigma}{d\Omega}$

$$\left(\frac{d\sigma}{d\Omega}\right)_{1electron} = \frac{\phi_{out} R^2}{\phi_{in}} = \frac{\left|E_{rad}\right|^2 R^2}{\left|E_{in}\right|^2} = r_0^2$$

Interference (mathematical)



$$sc.ampl. = r_0 (1 + e^{i\mathbf{Q}\cdot\mathbf{r}})$$

1,2 … many

$$sc.ampl. = r_0 \sum_j e^{i\mathbf{Q}\cdot\mathbf{r}_j}$$

many

$$sc.ampl. = r_0 \int \rho(\mathbf{r})\, e^{i\mathbf{Q}\cdot\mathbf{r}}\, d\mathbf{r}$$

Number density

$\Delta\phi_{in} = \frac{z}{\lambda} 2\pi = k \cdot z = \mathbf{k}\cdot\mathbf{r}$ as drawn #2 is behind #1 for "in"

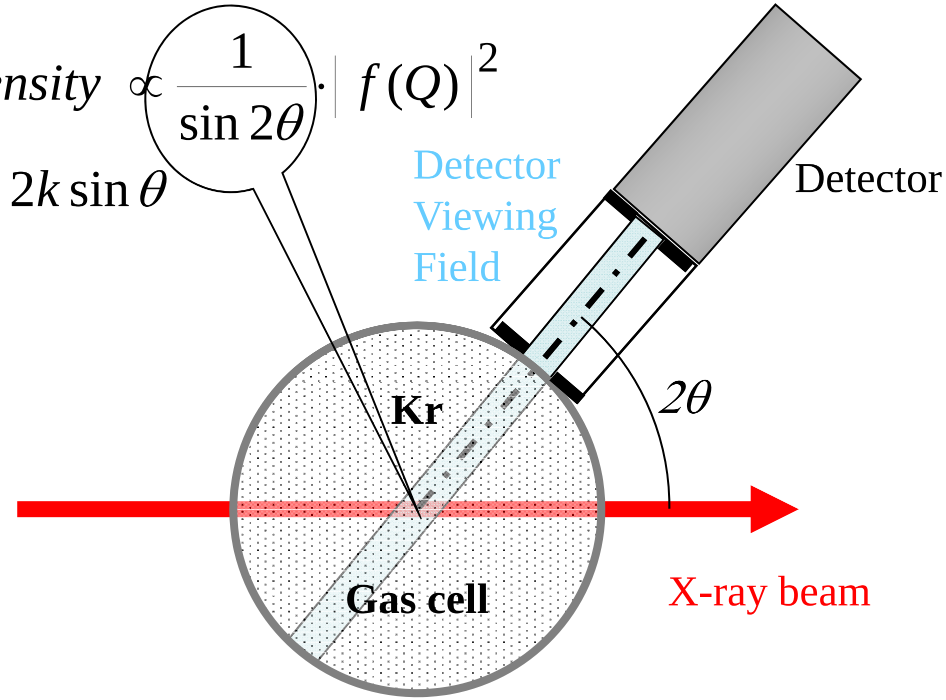
$\Delta\phi_{out} = -\mathbf{k}'\cdot\mathbf{r}$ but ahead for "out" , therefore " – "

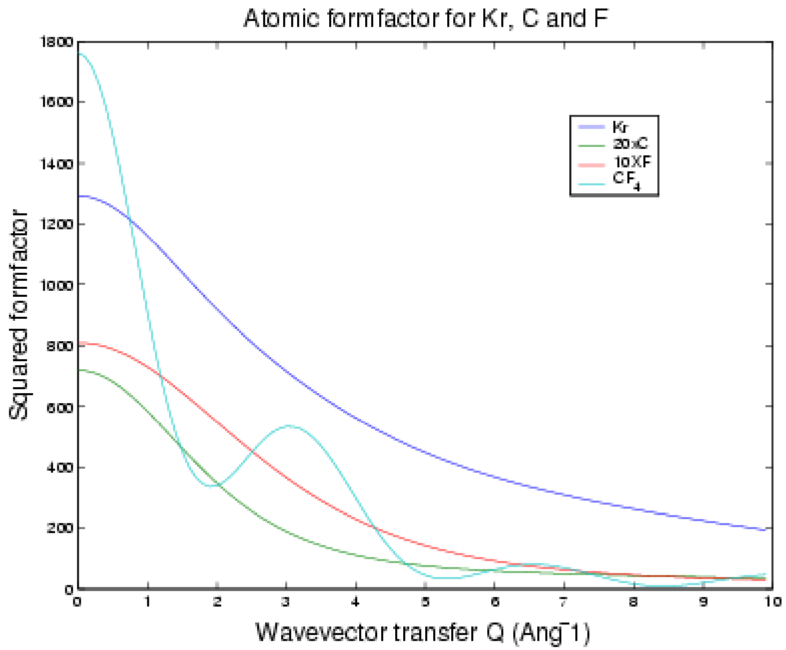
$$\Delta\phi_{res} = (\mathbf{k} - \mathbf{k}')\cdot\mathbf{r} = \mathbf{Q}\cdot\mathbf{r}$$

Measuring atomic and molecular formfactors from gas scattering

$$Intensity \propto \frac{1}{\sin 2\theta} \cdot \left| f(Q) \right|^2$$

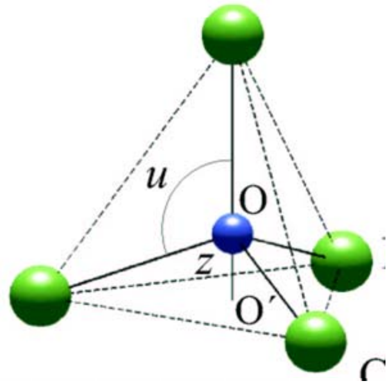
$$Q \equiv 2k \sin\theta$$



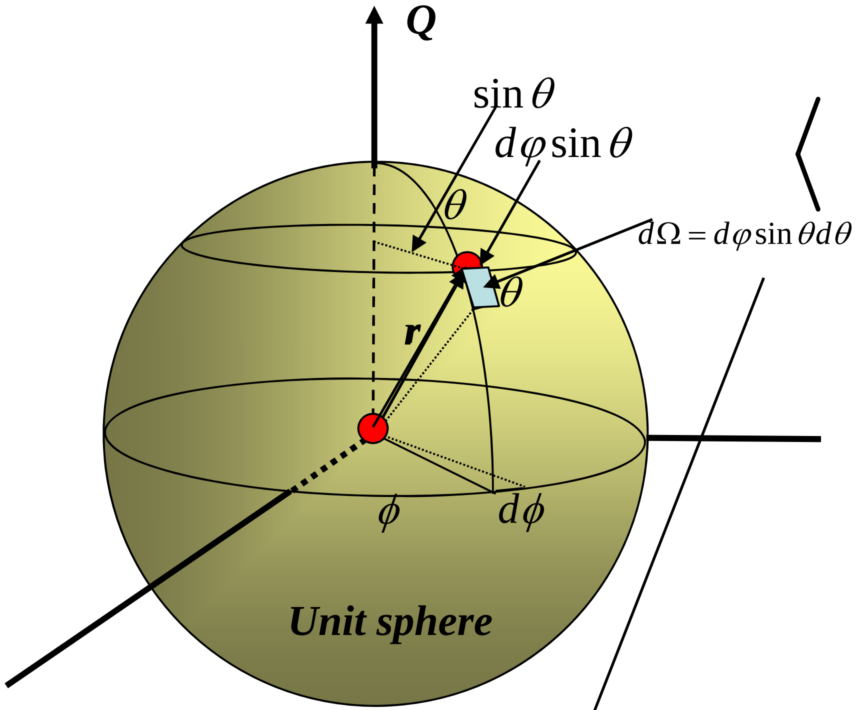


$$f_{atom} \equiv \int \rho_{el}(\mathbf{r}) \cdot e^{i\mathbf{Q}\cdot\mathbf{r}} d\mathbf{r}$$

$$f_{mol} = \sum_j f_j \cdot e^{i\mathbf{Q}\cdot\mathbf{r}_j}$$



Home work: Verify (a few points) on curve for CF4 when Q is parallel or antiparallel to a CF4 bond (bond length 1.38 Ang). The CF 4 molecule is a tetraheder as shown. Prove first that OO'=1/3 of the bondlength. *Hint: "Elements of Modern X-Ray physics", Ch.4 p.115.*



$$\left\langle e^{i\mathbf{Q}\cdot\mathbf{r}} \right\rangle_{\substack{\text{orientational}\\ \text{average}}}$$

$$\left\langle e^{i\mathbf{Q}\cdot\mathbf{r}} \right\rangle_{\substack{\text{orientational}\\ \text{average}}} = \frac{\iint e^{iQr\cos\theta}\sin\theta\, d\theta\, d\varphi}{\iint \sin\theta\, d\theta\, d\varphi} = \frac{2\pi(Qr)^{-1}\int_{x=-1}^{+1} e^{ix}dx}{2\pi\cdot 2} = \frac{\sin(Qr)}{Qr}$$

$$A_2 = f_1 e^{i\mathbf{Q}\cdot\mathbf{r}_1} + f_2 e^{i\mathbf{Q}\cdot\mathbf{r}_2} \quad ; \quad I_2 \propto A_2 \cdot A_2^*$$

$$I_2 = \{ f_1 e^{i\mathbf{Q}\cdot\mathbf{r}_1} + f_2 e^{i\mathbf{Q}\cdot\mathbf{r}_2} \} \cdot \{ f_1 e^{-i\mathbf{Q}\cdot\mathbf{r}_1} + f_2 e^{-i\mathbf{Q}\cdot\mathbf{r}_2} \}$$

$$= f_1^{\,2} + f_2^{\,2} + f_1 f_2 e^{i\mathbf{Q}\cdot(\mathbf{r}_1-\mathbf{r}_2)} + f_1 f_2 e^{-i\mathbf{Q}\cdot(\mathbf{r}_1-\mathbf{r}_2)}$$

$$\langle I_2 \rangle_{orient.average} = f_1^{\,2} + f_2^{\,2} + 2 f_1 f_2 \frac{\sin(Q\,r_{12})}{Q\,r_{12}}$$

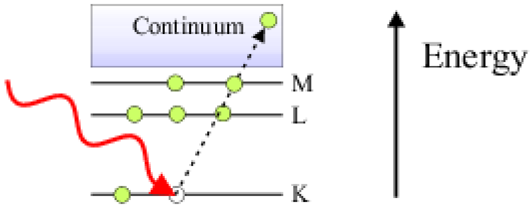
1,2 … many

$$\langle I \rangle_{orient.average} = \sum_i f_i^{\,2} + 2\sum_{i>j} f_i f_j \frac{\sin(Q\,r_{ij})}{Q\,r_{ij}}$$

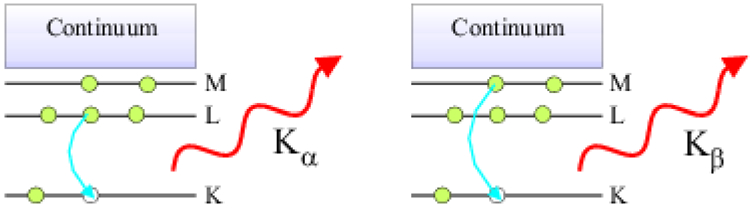
Student : *look at the CF_4 molecule as an example, and compare orientational average with* **Q** *parallel to a C-F bond*

Absorption

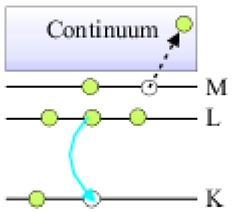
(a) Photoelectric absorption

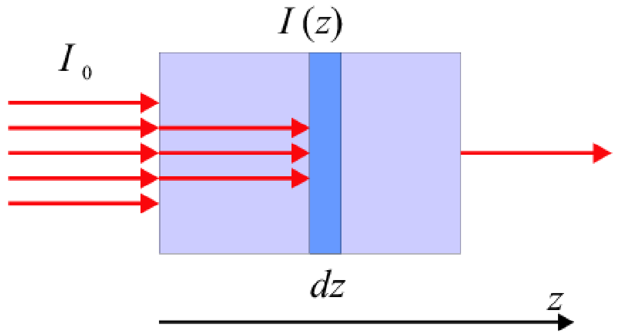


(b) Fluorescent X-ray emission



(c) Auger electron emission





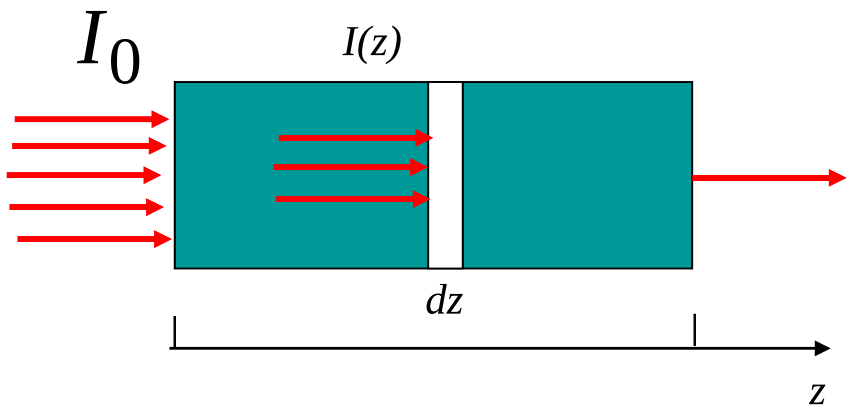
$$-dI = I(z)\cdot dz \cdot \mu \quad \Rightarrow$$

$$I(z) = I_0 \cdot e^{-\mu z}$$

μ(atomic number Z, photon energy $\hbar\omega$)

$$\mu(Z,\hbar\omega) \propto Z^4 \left(\frac{1}{\hbar\omega}\right)^3$$

X-ray absorption



$$-dI = \mu \cdot I(z)dz \quad \Rightarrow \quad I(z) = I_0 \cdot e^{-\mu z}$$

$$\mu^{-1} \text{ - the absorption length}: \quad \mu = \frac{\rho_m N_{Av}}{A}$$

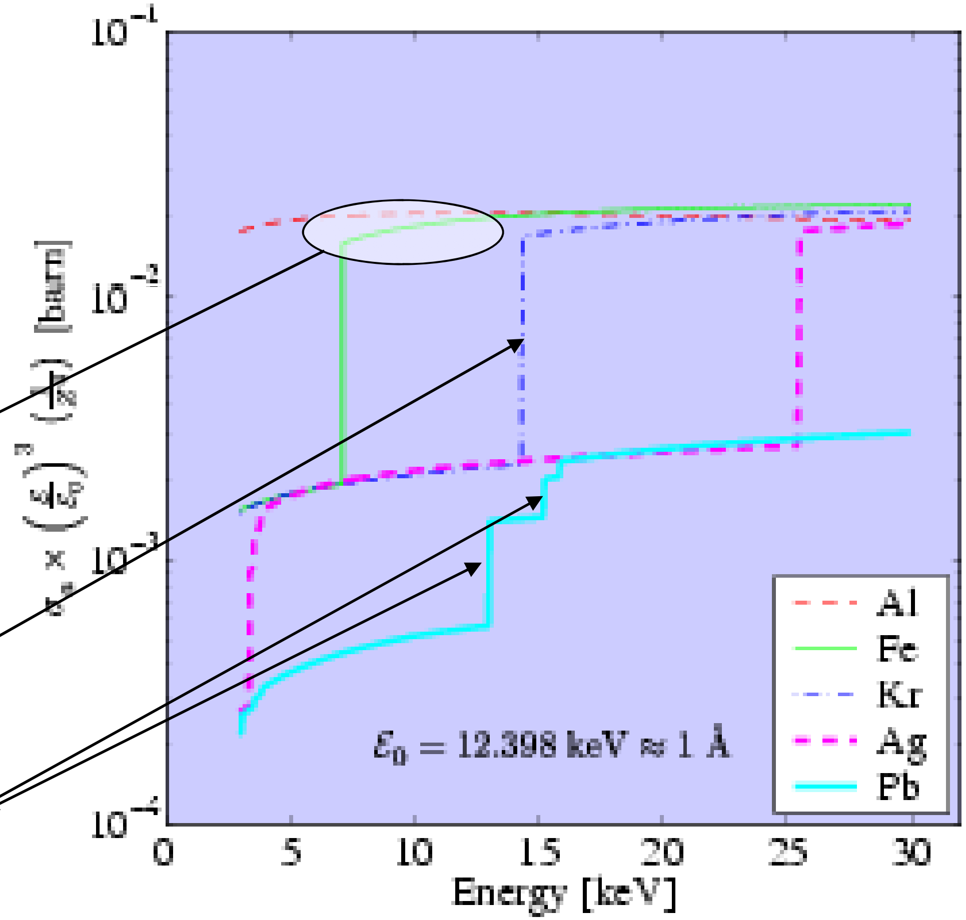
Easy to measure μ and thereby σ

Fine structure occurs here in solids and liquids
It is called EXAFS and contains information
about distances to near neighbors .

K-edge for Kr is at 14.435 keV

L-edges for Pb

$$\sigma_{abs}(Z, \hbar\omega)$$

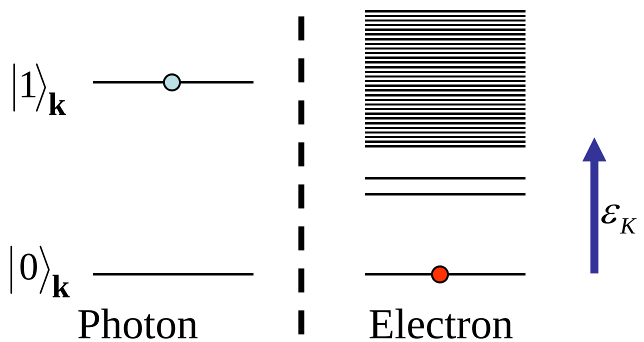


N_{Av} atoms in A gram $\Rightarrow$ N_{Av}/A in 1 gram $\Rightarrow$ $\rho_m (N_{Av}/A)$ in 1 cm^3

$\rho_m (N_{Av}/A) dz$ in 1 cm^2 area of the thin slice

X-ray photon and electron in atom

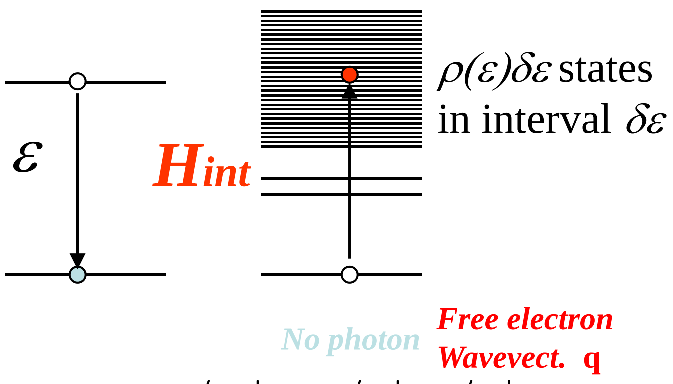
Initial state $|i\rangle$



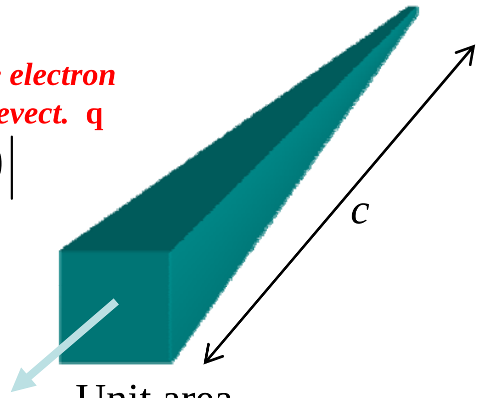
One photon with wavevector $\mathbf{k}$; $|1\rangle_{\mathbf{k}}$

Electron in K-shell $\psi_{1s}(\mathrm{r})$; $|g\rangle$

With interaction between photon-field and electron transitions may occur



Final state $\langle f| =_{\mathbf{k}} \langle 0| \cdot_{\mathbf{q}} \langle 0|$



Reaction rate Fermi's "golden Rule"

$$W = \frac{2\pi}{\hbar} |M_{if}|^2 \rho(\varepsilon) = \sigma_{abs} \cdot \phi$$

$$= \sigma_{abs} \cdot (c/V)$$

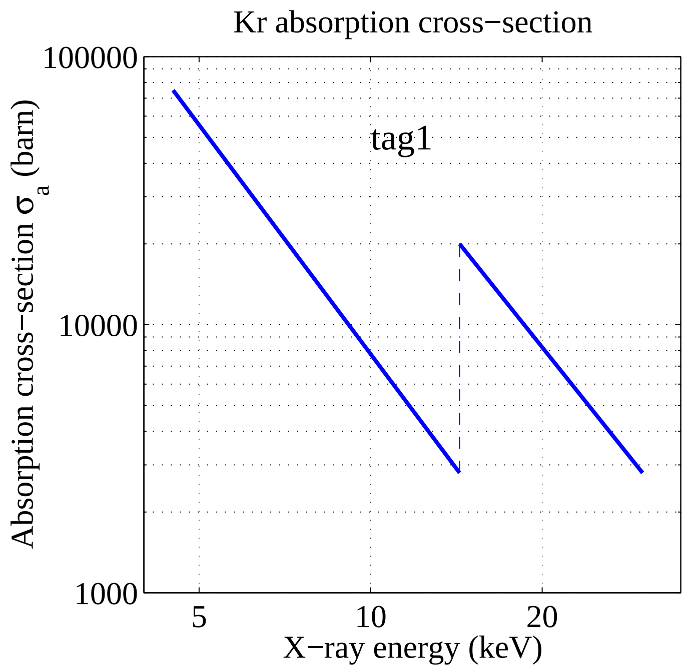
$$M_{if} = \langle f | H_{\text{int}} | i \rangle$$

Flux ϕ =density* c = (1/V)* c

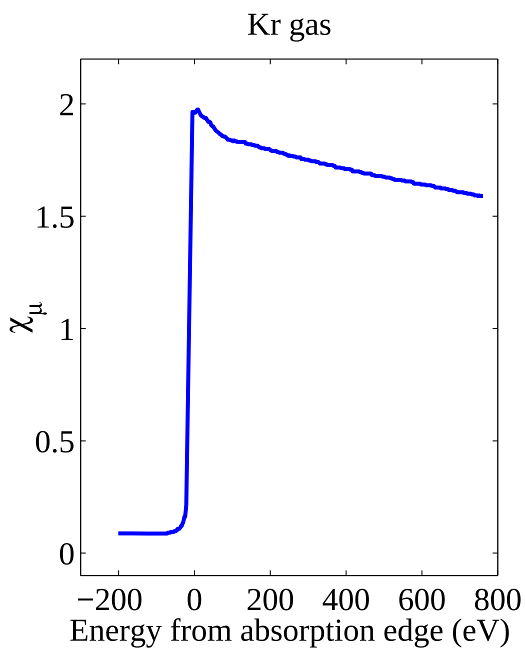
Flux $\Phi : \; c \cdot |\psi|^2$ Intensity = Flux · Area $I_{\substack{scattered \\ thru\ \Delta\Omega}} = \Phi_{in} \cdot \Delta\Omega \cdot \frac{d\sigma}{d\Omega}$

$$W_{absorption} = \Phi_{in} \cdot \sigma_{abs}$$

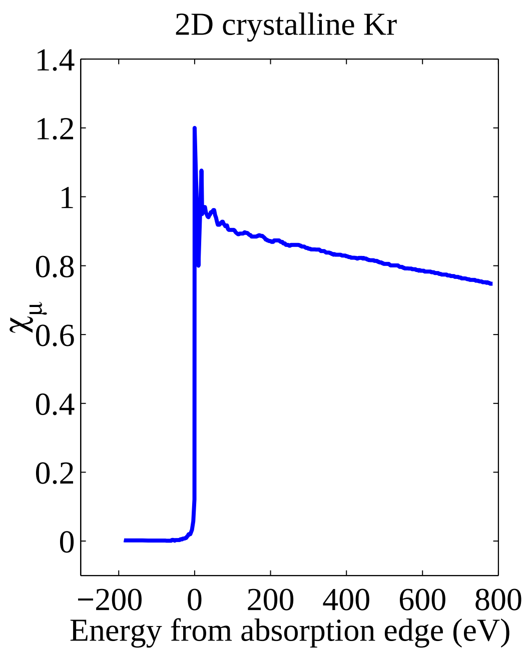
If $\varepsilon < \varepsilon_K$ a K-electron cannot be expelled --> the K-edge in $\sigma_{abs}(\varepsilon = \hbar\omega)$



Kr absorption cross−section
100000
10000
1000
tag1
5
10
20
X−ray energy (keV)
Absorption cross−section σ_a (barn)



Kr gas
2
1.5
1
0.5
0
χ_μ
−200
0
200
400
600
800
Energy from absorption edge (eV)



2D crystalline Kr
1.4
1.2
1
0.8
0.6
0.4
0.2
0
χ_μ
−200
0
200
400
600
800
Energy from absorption edge (eV)

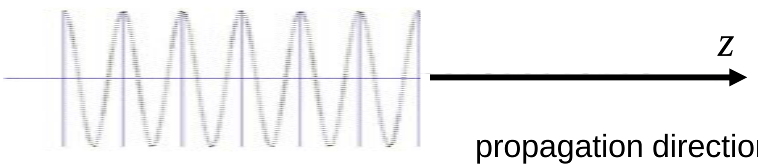
Reflection and refraction

How is the index of refraction related

to the 2 basic processes

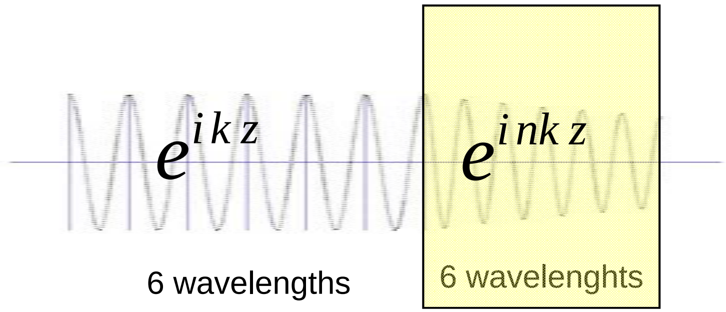
1. ***scattering***

2. ***absorption***



propagation direction

plane wave



6 wavelengths

hitting an interface head-on

1. The wavelength changes from λ to λ/n
   wavenumber changes from k to nk

2 The amplitude decays exp{-(μ/2) z }
   Intensity decays exp{- μz}

$$n = 1 - \delta + i\beta$$

$$inkz = i(1-\delta)kz - k\beta z \quad \Rightarrow k\beta = \mu / 2$$

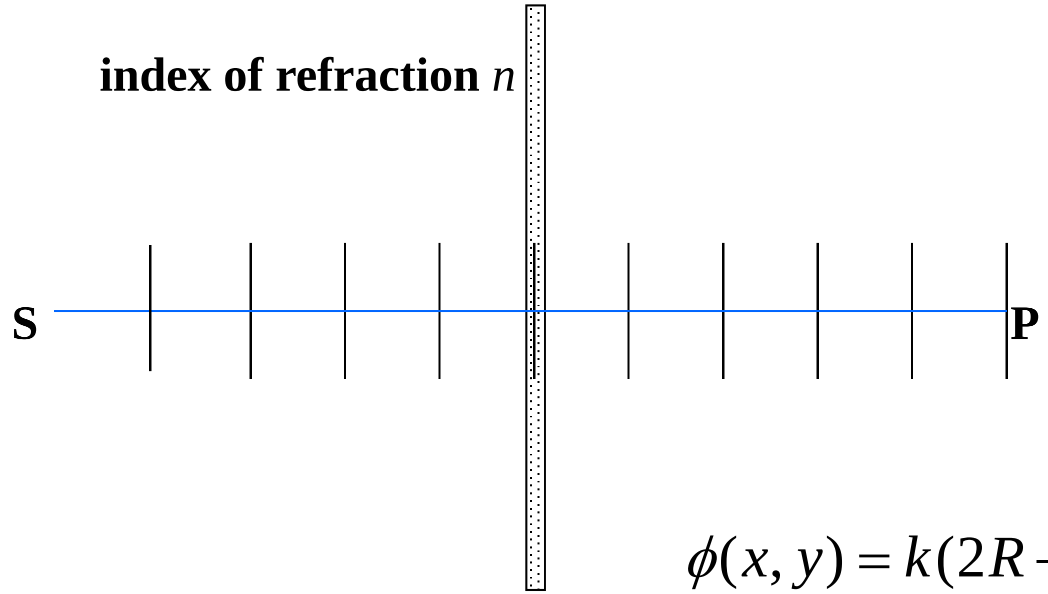
i.e. absorption

to be proven

$$\delta = \frac{2\pi}{k^2} r_0 \rho_{el}$$

i.e. scattering

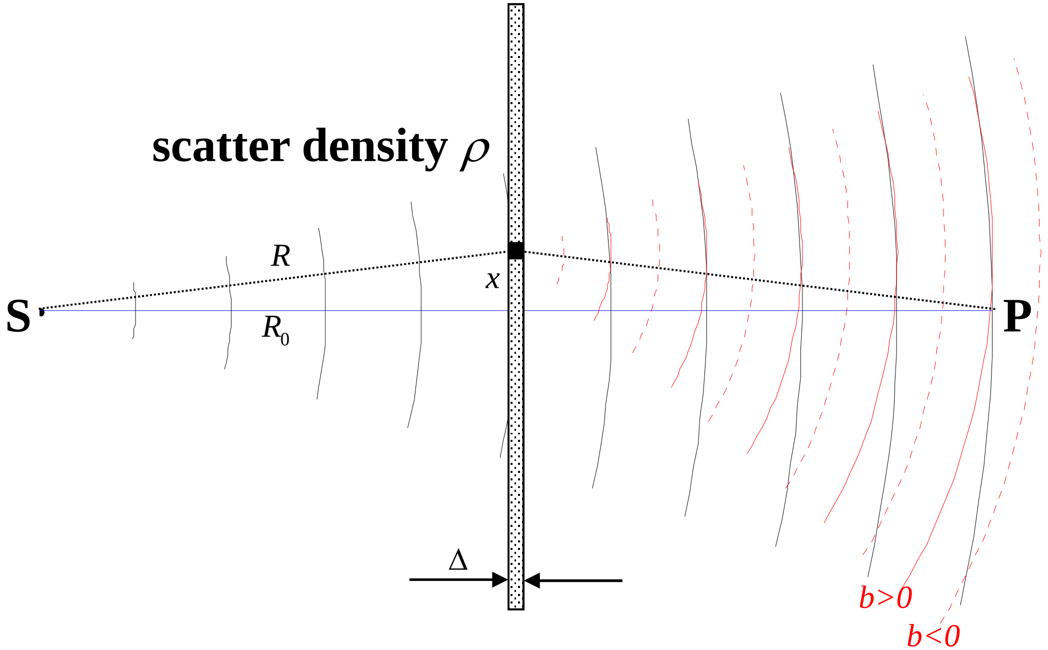
Index of refraction vs. scattering



$$\psi_{tot}^{P} = \psi_0^{P} e^{i(nk-k)\Delta}$$

$$\cong \psi_0^{P}\left[1 + i(n-1)k\Delta\right]$$

$$\phi(x,y) = k(2R - R_0) \cong k(x^2+y^2)/R_0$$



$$\psi_{tot}^{P} = \psi_0^{P} + \int d\psi_s^{P}$$

$$d\psi_s^{P} = \frac{e^{ikR_0}}{R_0}$$ incident wave

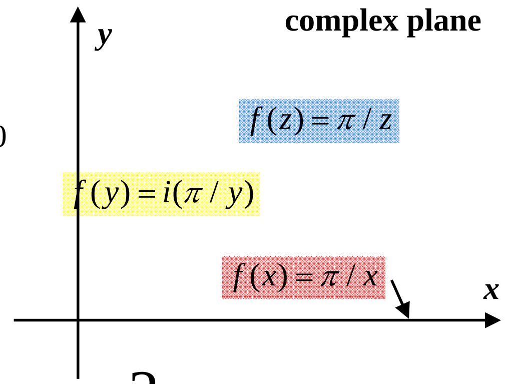
$\rho\Delta dxdy$ number of scatterer

$$b\frac{e^{ikR_0}}{R_0}$$ scattered wave

$e^{i\phi(x,y)}$ apart from phase factor

$$I = \int_{-\infty}^{\infty} e^{ik(x^2+y^2)/R_0}\,dxdy$$

$$f(\alpha) = \int_{-\infty}^{\infty} e^{-\alpha(x^2+y^2)}dxdy = \int_{r=0}^{\infty} e^{-\alpha r^2}\pi dr^2 = \frac{\pi}{\alpha} \quad ; \quad \alpha > 0$$



If α complex, OK by anayltic continuation. Here $\alpha = -i\,k / R_0$

$$I = \frac{\pi}{(-i)(k/R_0)} = i\frac{2\pi}{k}\frac{R_0}{2}$$

so $$\int d\psi_s^P = \frac{e^{ik\,2R_0}}{R_0^2}\cdot b\rho\Delta\cdot i\frac{2\pi}{k}\frac{R_0}{2} = \psi_0^P b\rho\Delta\cdot i\frac{2\pi}{k}$$

$$\psi_{tot}^P = \psi_0^P\left[1 + b\rho\Delta\cdot i\frac{2\pi}{k}\right] \Rightarrow \quad b\rho\frac{2\pi}{k^2} = (n-1)$$

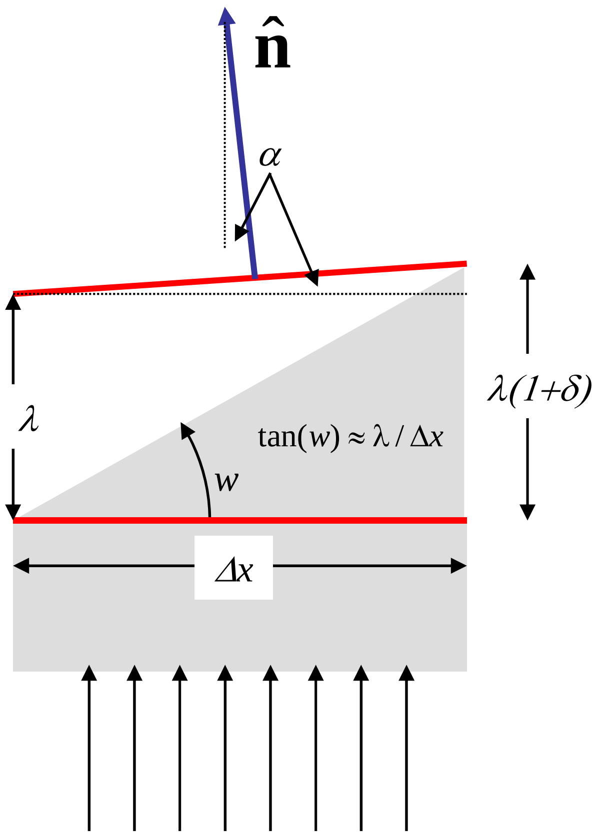
$$= \psi_0^P\left[1 + i(n-1)k\Delta\right]$$

$n > 1 \quad \Rightarrow b > 0$ scatter in-phase

$n < 1 \quad \Rightarrow b < 0$ scatter out-of-phase

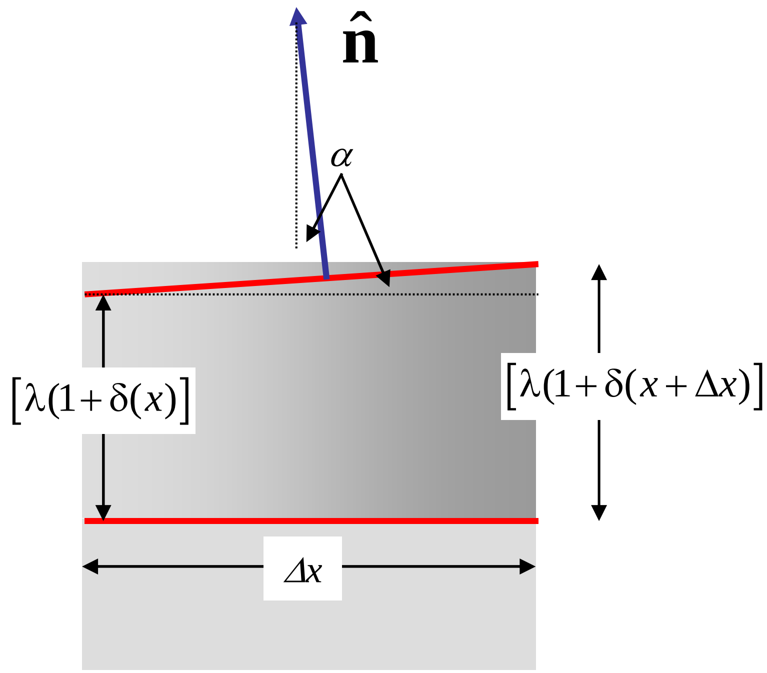
X-rays: $\quad n < 1 \quad \Rightarrow b = -r_0 \quad ; \quad \delta = \frac{2\pi}{k^2} r_0 \rho_{el}$

Homogenous wedge



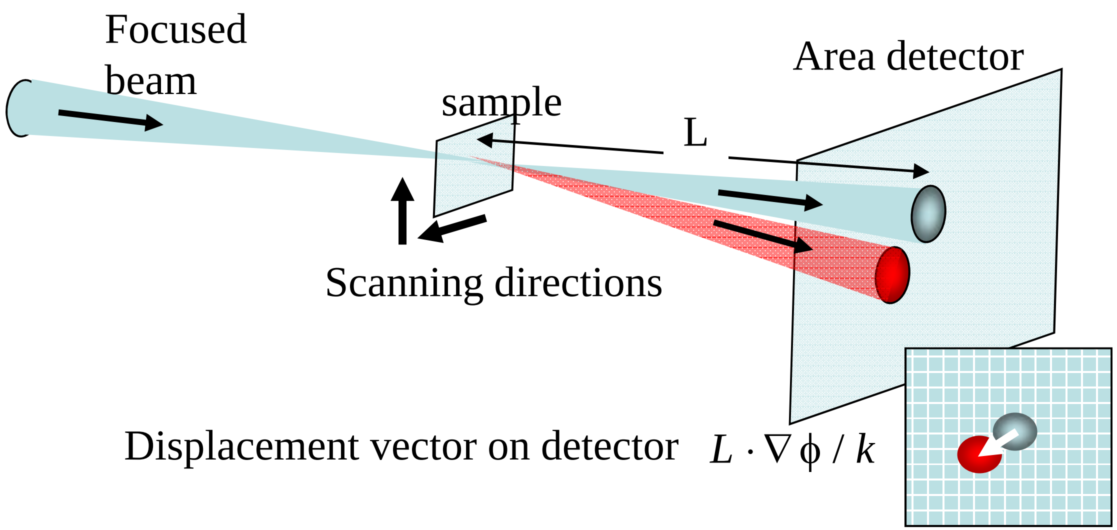
$$\alpha = \left[\lambda(1+\delta)-\lambda\right] / \Delta x = \delta(\lambda / \Delta x) = \delta \cdot \tan(w)$$

Inhomogenous plate



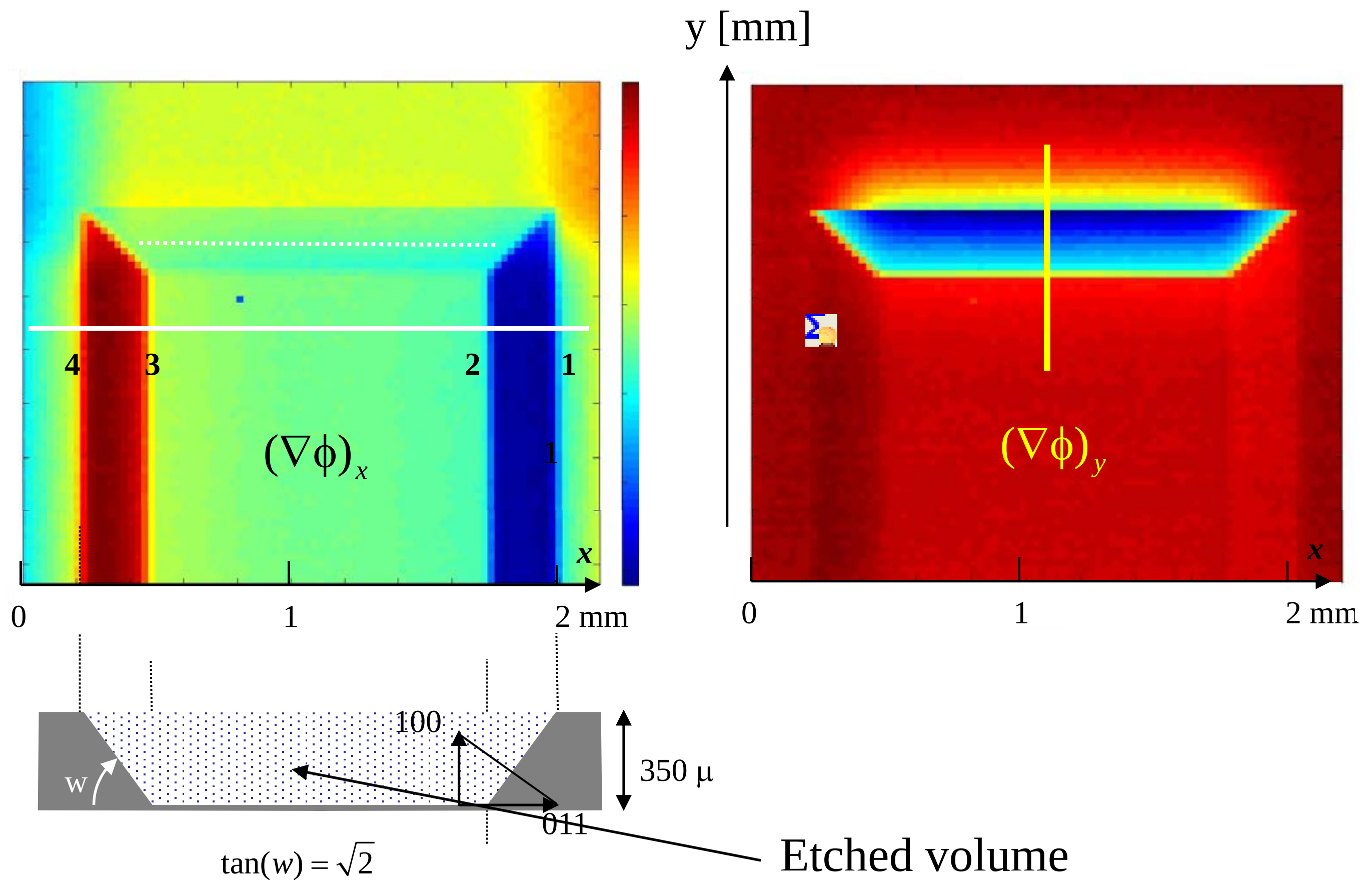
$$\alpha = \lambda\, \Delta x\, \delta'(x) / \Delta x = \lambda \cdot \delta'(x)$$

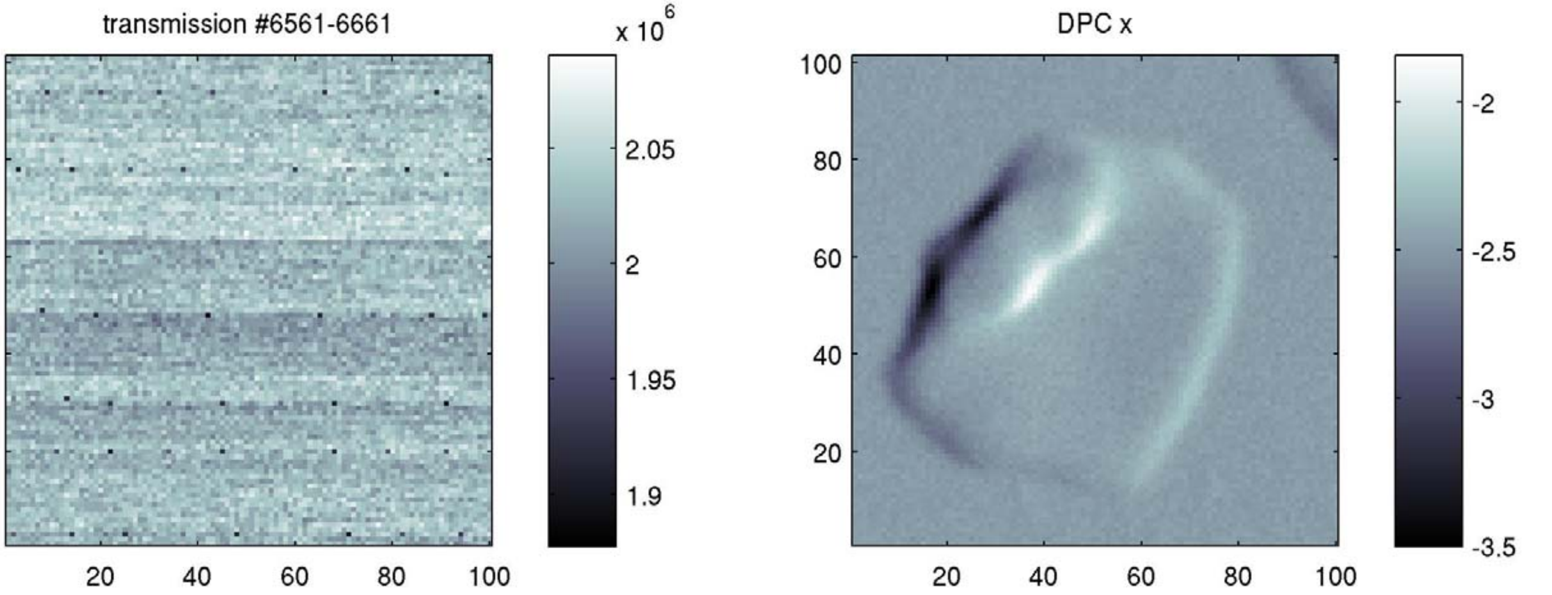
$\delta \approx 10^{-5}$ so the refraction effect is small


Focused
beam
sample
L
Area detector
Scanning directions
Displacement vector on detector $L \cdot \nabla \phi / k$

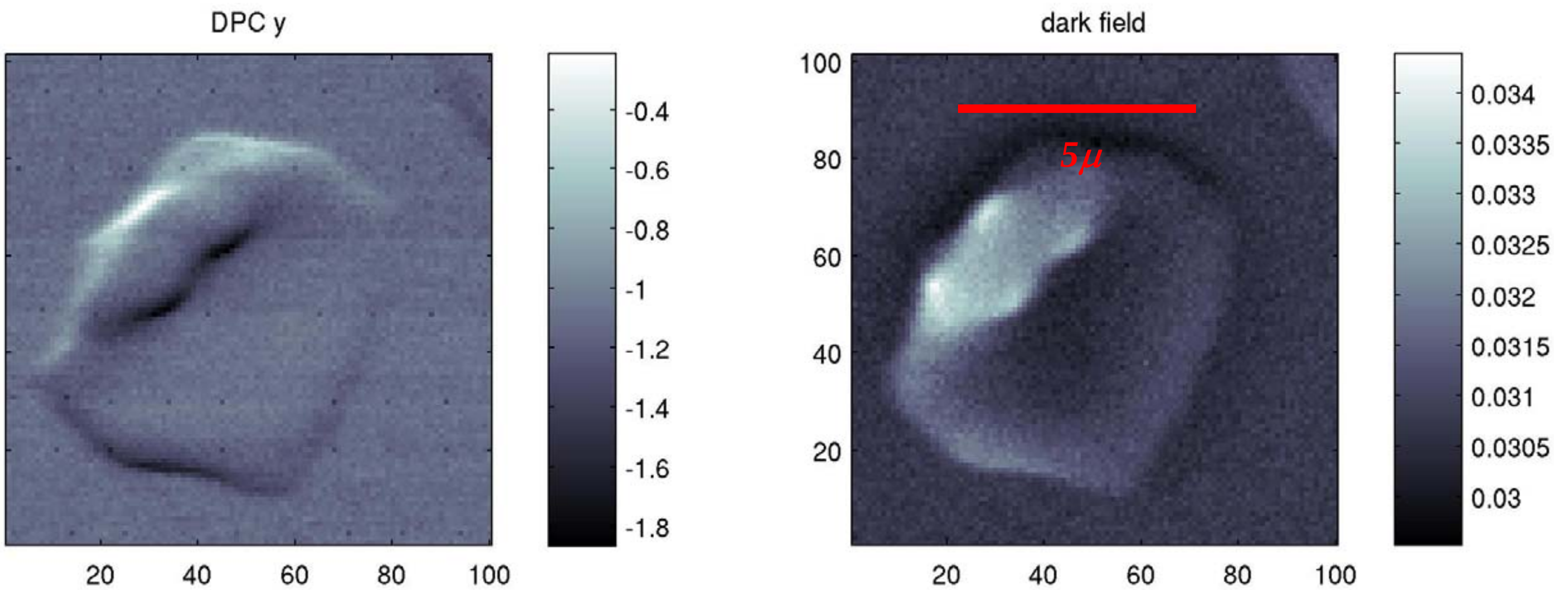
Example : The "invisible" substrate

Si single crystal wafer, perfect. All scattering condensed in Bragg points.
Make a thin area (thickness ca. 10 μ) in a 300 μ thick wafer by etching





nergy 6200 eV



Grazing incidence

Incident, reflected and transmitted plane waves have index *I, R, and T*

General wavevectors are shown below, BUT

(i) z-component >0 for I and T, and <0 for R

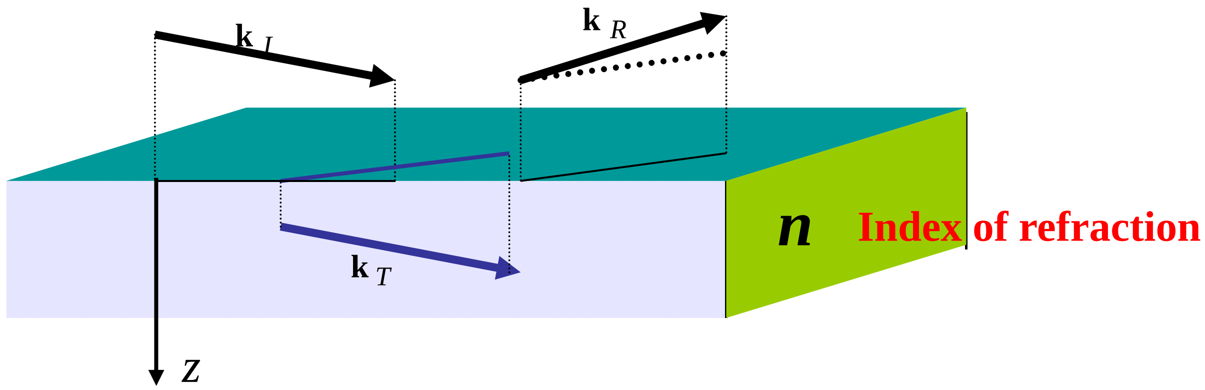
(ii) In-plane components must be all identical by continuity condition

(iii) Common in-plane direction is denoted x.

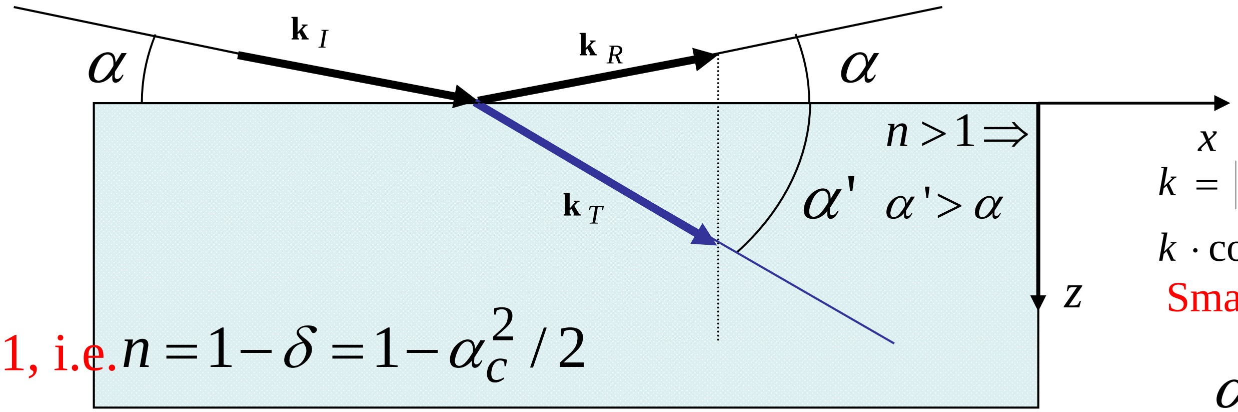
$$e^{i\mathbf{k}\cdot\mathbf{r}} = e^{i\mathbf{k}_{xy}\cdot\mathbf{r}_{xy}} \cdot e^{ik_z z}$$

Continuity at $z = 0 \quad \Rightarrow$

$$\mathbf{k}_{I,xy} = \mathbf{k}_{R,xy} = \mathbf{k}_{T,xy}$$



simplification



If $n<1$, i.e. $n = 1 - \delta = 1 - \alpha_c^2 / 2$

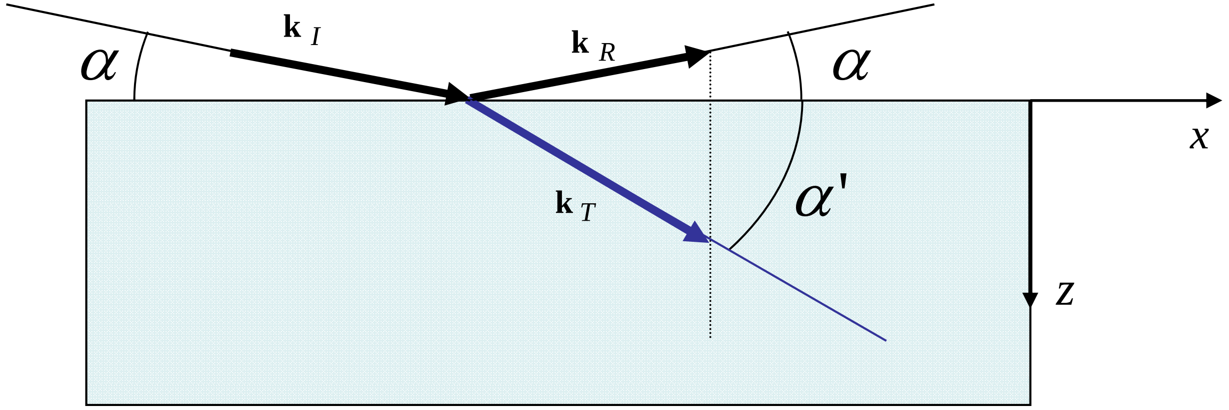
$$k = |\mathbf{k}_I| = |\mathbf{k}_R| \quad ; \quad n \cdot k = |\mathbf{k}_T|$$

$$k \cdot \cos\alpha = n\, k \cos\alpha'$$

Small angles

$$\alpha^2 = \alpha'^2 + \alpha_c^2$$

Amplitudes are denoted $a_I, a_R,$ and a_T



Small angles

$$\alpha^2 = \alpha'^2 + \alpha_c^2$$

Snell's law

$$|\mathbf{k}_I| \sin\alpha \cong k\alpha \text{ etc.}$$

continuity

$$\psi(0,0,0) = a_I + a_R = a_T$$

above below

continuity

$$\left(\frac{\partial\psi}{\partial z}\right)_{z=0} = (ik\alpha)a_I - (ik\alpha)a_R = (i\,n\,k\alpha')a_T$$

above below

$$(a_I - a_R)\alpha = n(a_I + a_R)\alpha' \cong (a_I + a_R)\alpha'$$

Fresnel's law(s)

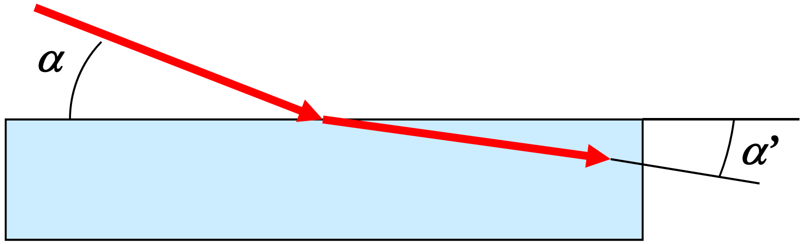
$$\frac{a_R}{a_I} = \frac{(\alpha - \alpha')}{(\alpha + \alpha')} \quad ; \quad \frac{a_T}{a_I} = \frac{2\alpha}{(\alpha + \alpha')}$$

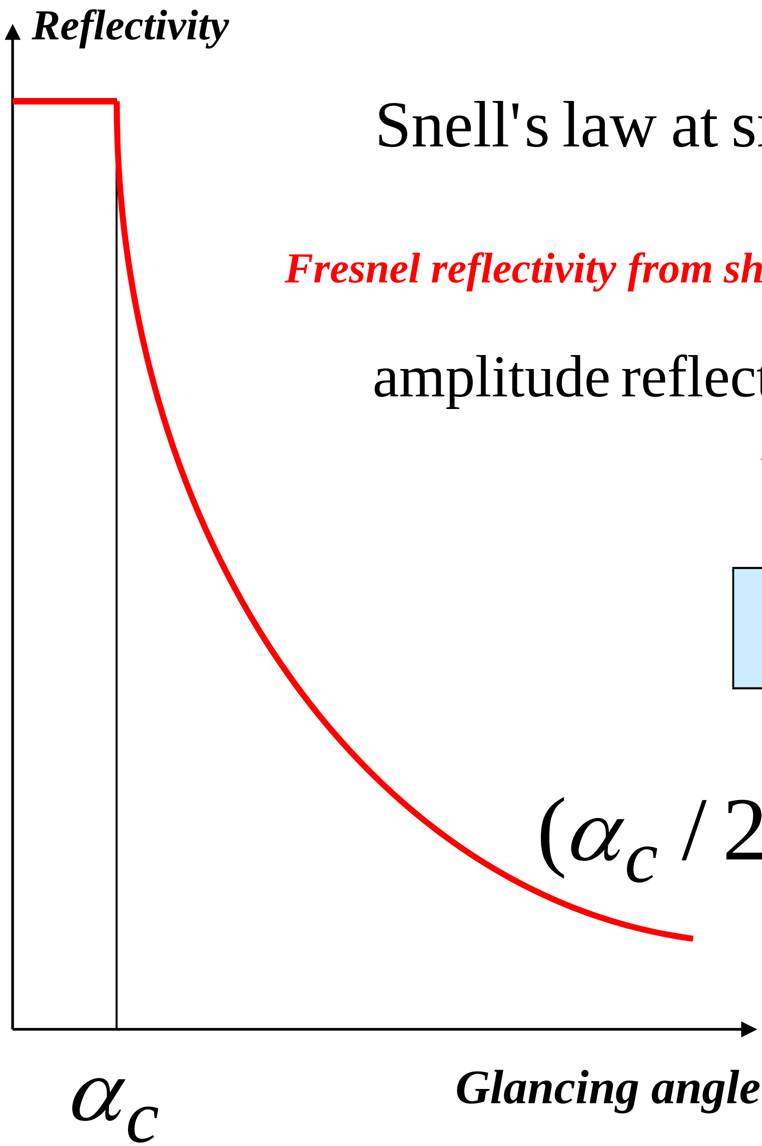
$$\psi = a\,e^{ik_z z} = a\,e^{ik\alpha z} \quad \Rightarrow \quad \left[\frac{\partial\psi}{\partial z}\right]_{z=0} = a\,(ik\alpha)e^{ik\alpha\cdot 0}$$

Snell's law at small angles: $\alpha^2 = \alpha'^2 + \alpha_c^2$

Fresnel reflectivity from sharp interface

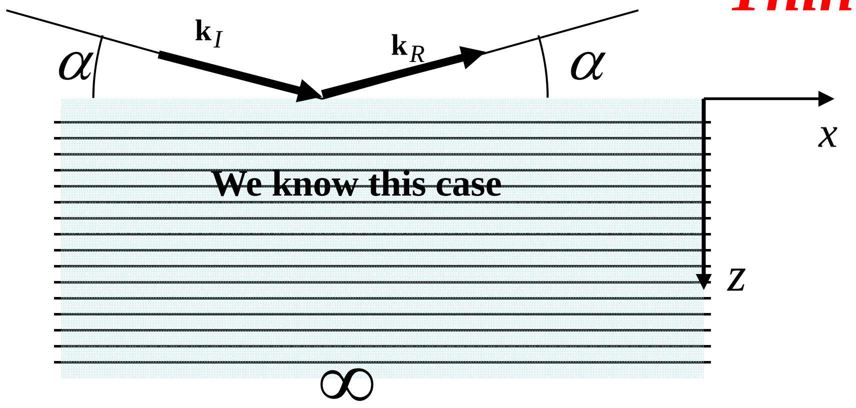
amplitude reflectivity : $r = \dfrac{\alpha - \alpha'}{\alpha + \alpha'}$

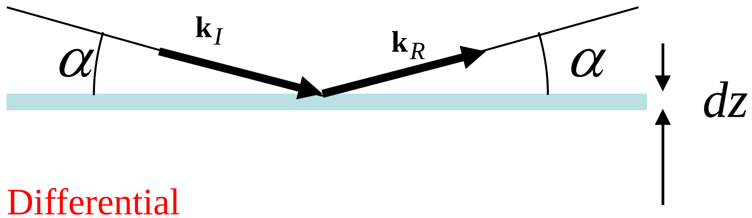




$$\alpha_c = \lambda\sqrt{\rho_{el} \cdot r_0 / \pi} \quad \text{where } r_0 = \frac{e^2}{mc^2} = 2.82 \cdot 10^{-5}\, Ang$$

Thin plate reflectivity





Differential Reflectivity

$$dr \propto \rho \cdot r_o \cdot \frac{dz}{\sin\alpha}$$

Dimension 1/Length

$$dr = c\lambda \cdot \rho \cdot r_o \cdot \frac{dz}{\sin\alpha}$$

dimensionless complex constant, determined by

$$r_F \equiv \frac{a_R}{a_I} \rightarrow \left(\frac{\alpha_c}{2\alpha}\right)^2 \quad \text{for} \quad \alpha >> \alpha_c$$

$$\alpha_c^2 = \pi^{-1}\lambda^2 \cdot \rho_{bulk} \cdot r_o$$

$$r = \int_{z=0}^{\infty} e^{iQz}\, dr = c\,\frac{\lambda \cdot \rho_{bulk} \cdot r_o}{\alpha} \int_{z=0}^{\infty} \frac{\rho(z)}{\rho_{bulk}}\, e^{iQz}\, dz$$

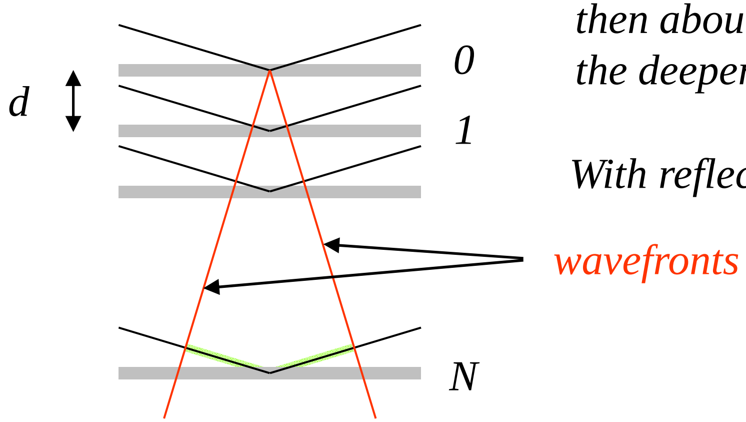
1. $$\frac{\lambda \cdot \rho_{bulk} \cdot r_0}{\alpha} = \frac{\lambda}{\alpha} \cdot \frac{\pi\, \alpha_c^2}{\lambda^2} = \frac{k\, \alpha_c^2}{2\, \alpha}$$

2. With $$\frac{\rho(z)}{\rho_{\text{bulk}}} \equiv f(z); \quad \int_0^{\infty} f(z)\, e^{iQz} dz = \left[f(z) \frac{1}{iQ} e^{iQz} \right]_0^{\infty} - \frac{1}{iQ} \int_0^{\infty} f'(z)\, e^{iQz} dz \equiv i \frac{1}{Q} \phi(Q)$$

(i) $f(z) = stepfunction \;\Rightarrow\; f'(z) = \delta(z)$ and $\phi(Q) = 1$; (ii) $Q = 2k\alpha$

$$r_F = \frac{\alpha_c^2}{4\alpha^2} = c\,\frac{k}{2}\,\frac{\alpha_c^2}{\alpha} \cdot i\, \frac{1}{2k\alpha} \cdot 1 \;\Rightarrow\; c = (-i)$$

The bandwidth from Bragg reflection



Green path length = N 2d sinθ

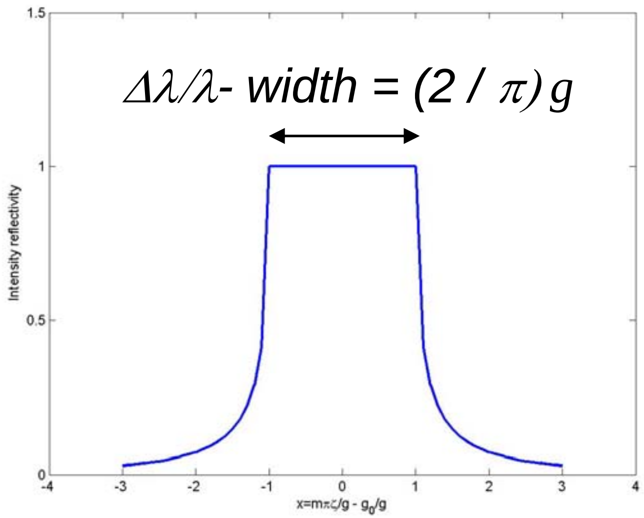
If reflectivity of one layer is 0.01
then about 100 layers will effectively reflect –
the deeper layers are not illuminated

With reflectivity per layer = g → N=1/g

Student problem:
Determine the wavelengthband
from a Si(111) monochromator.
Hint: Si has the diamond structure
with a=5.43 Ång.

$$\Delta\varphi_N(\Delta\lambda) = \frac{N \cdot 2d\sin\theta}{\lambda + \Delta\lambda} \cdot 2\pi - 2\pi N \approx 2\pi N \Delta\lambda / \lambda \approx \pi$$

$$\Rightarrow \quad \frac{\Delta\lambda}{\lambda} = \frac{1}{2N}$$



$$\left(\frac{\Delta\lambda}{\lambda}\right)_{FWHM} \approx \frac{1}{N} \cong g$$

$$r_{thinplate} = (-i)\lambda \frac{d}{\sin\alpha} \cdot r_o \cdot \rho \rightarrow g = 2d^2 r_0 \frac{|F_{hkl}|}{v_c}$$

Unit cell volume

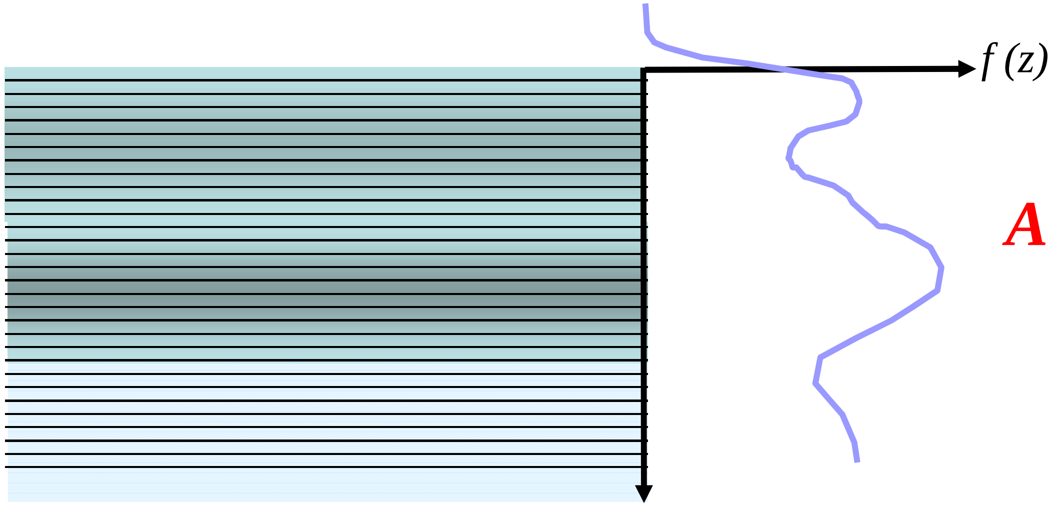
Reflectivity from fuzzy interface

$$r = \int_{z=0}^{\infty} e^{iQz}\, dr(z) = c\frac{\lambda \cdot \rho_{bulk} \cdot r_o}{\alpha} \int_{z=0}^{\infty} \frac{\rho(z)}{\rho_{bulk}} e^{iQz}\, dz = r_F \int_{z=0}^{\infty} f'(z) \cdot e^{iQz}\, dz \equiv \phi(Q) \cdot r_F$$

Thin plate

$f(z)$

$\delta(z)$ for sharp interface

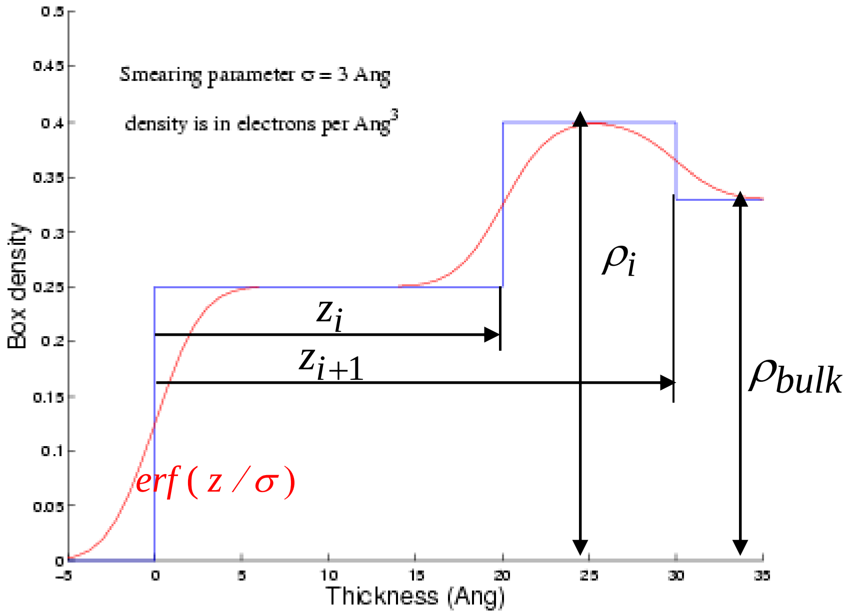


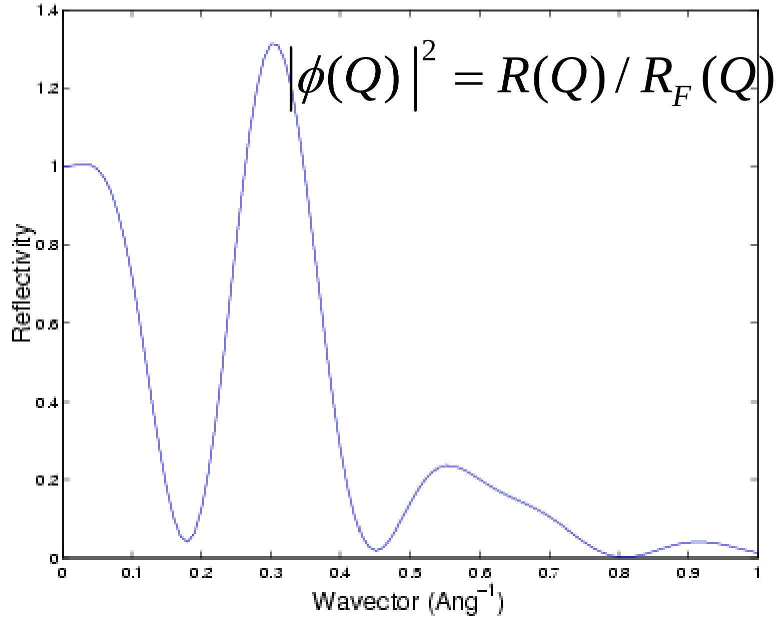
FT(Gaussian)=Gaussian

A $$\int_{z=-\infty}^{\infty} e^{-z^2/2\sigma^2} \cdot e^{iQz}\, dz = e^{-Q^2\sigma^2/2}$$

B $$\int_{z=-\infty}^{\infty} f(z-z_0) \cdot e^{iQz}\, dz = e^{iQz_0} \cdot \int_{z-z_0=-\infty}^{\infty} f(z-z_0) \cdot e^{iQ(z-z_0)}\, d(z-z_0) = e^{iQz_0} \cdot \phi(Q)$$

A and B + box model





$$\phi(Q) = e^{-Q^2\sigma^2/2} \sum_{i=1}^{N} \frac{\rho_{i+1} - \rho_i}{\rho_{bulk}} e^{iQz_i}$$