Methoden moderner Röntgenphysik II: Streuung und Abbildung

Lecture 4	Vorlesung zum Haupt- oder Masterstudiengang Physik, SoSe 2017 G. Grübel, A. Philippi-Kobs, O. Seeck, T. Schneider, L. Frenzel, M. Martins, W. Wurth		
Location	Lecture hall AP, Physics, Jungiusstraße		
Date	Tuesday	12:30 - 14:00	(starting 4.4.)
	Thursday	8:30 - 10:00	(until 13.7.)

Part II

Magnetism – Magnetic Thin Films

by André Philippi-Kobs (AP)

[23.5.] Magnetic small angle scattering of magnetic domain patterns

- Introduction of magnetism in thin films
- Resonant scattering & X-ray magnetic circular dichroism (XMCD),

[30.5.] Imaging of magnetic domains

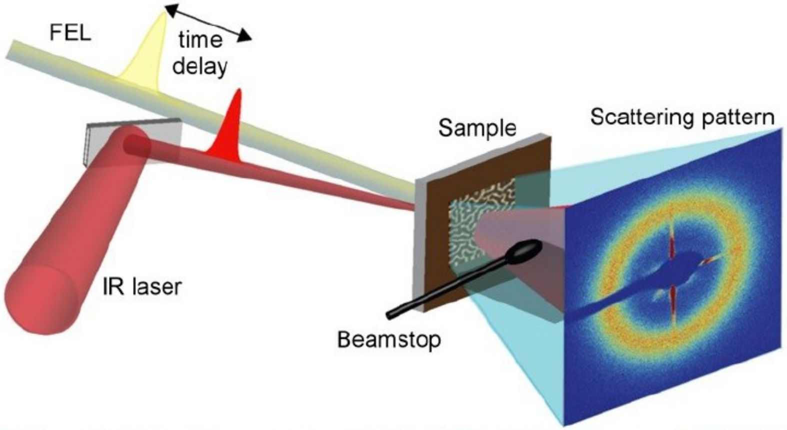
- Fourier transform holography (FTH)
- Scanning transmission X-ray microscopy (STXM)
- Coherent diffraction imaging (CDI), Ptychography

[1.6.] Femtomagnetism

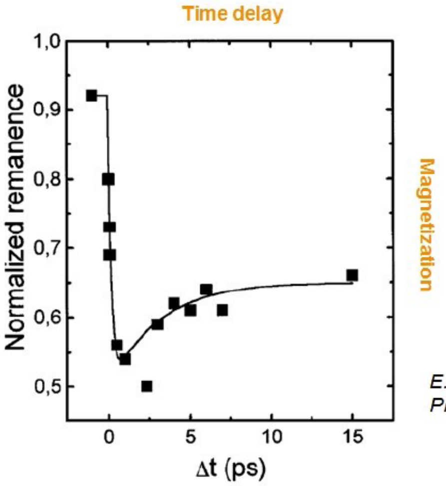
- Introduction of ultrafast magnetization dynamics
- Pump-probe experiments of nano-scale magnetic domain patterns

[13.6.] Related aspects

- Determination of coherence via magnetic domain patterns
- Magnetic XRD of antiferromagnets and chiral systems
- Further electronic inhomogeneities probed by X-rays (charge density wave; Abrikosov vortices in superconductors)



B. Pfau et al., Nature Communications, Vol. 3, 11; DOI:doi:10.1038/ncomms2108 (2012)
L.Müller et al., Rev. Sci. Instrum. 84, 013906 (2013)



Time-resolved MOKE (Ni 120 fs)

E. Beaurepaire et al., PRL 76 (1996) 4250

Methoden moderner Röntgenphysik II: Streuung und Abbildung

Part I:

Basics of X-ray Physics

by Gerhard Grübel (GG)

Introduction
Overview, Introduction to X-ray Scattering

X-ray Scattering Primer
Elements of X-ray Scattering

Sources of X-rays, Synchrotron Radiation
Laboratory Sources, Accelerator Bases Sources

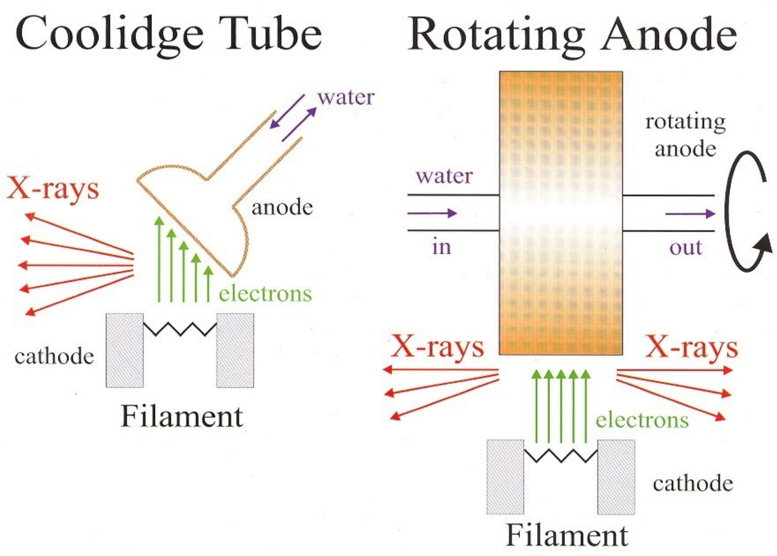
Reflection and Refraction from Interfaces
Snell's Law, Fresnel Equations

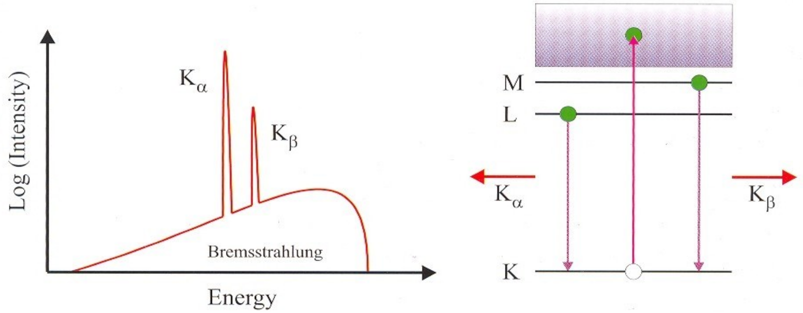
Kinematical Diffraction (I)
Diffraction from an Atom, a Molecule, from Liquids, Glasses, …

Kinematical Diffraction (II)
Diffraction from a Crystal, Reciprocal Lattice, Structure Factor, …

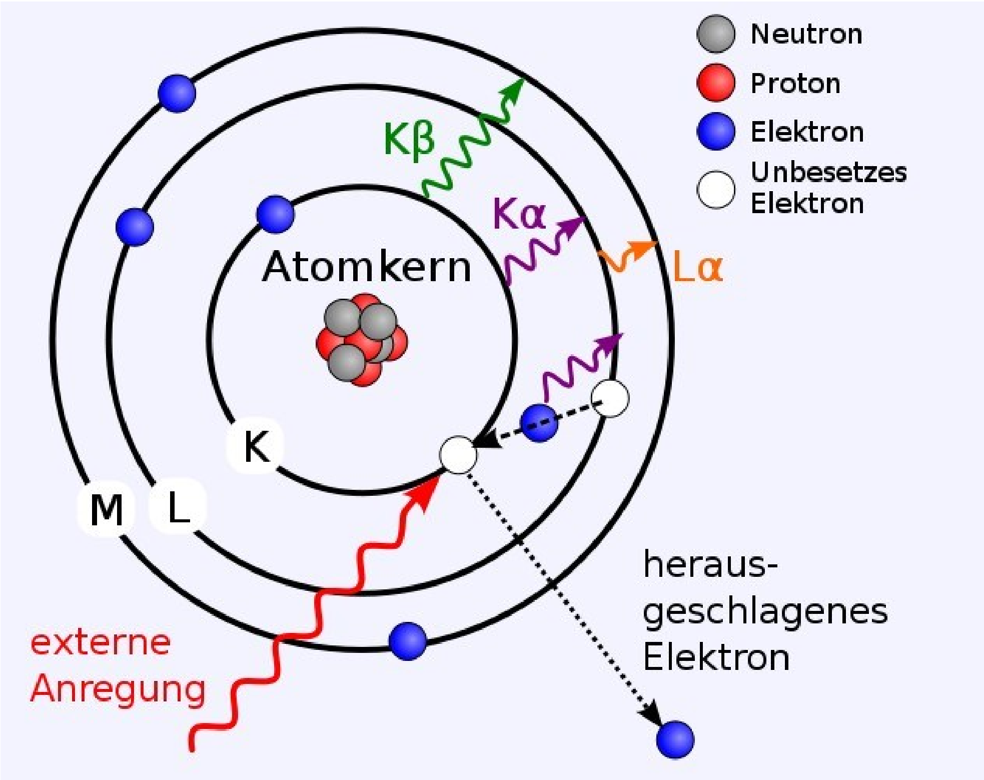
Source of X-Rays

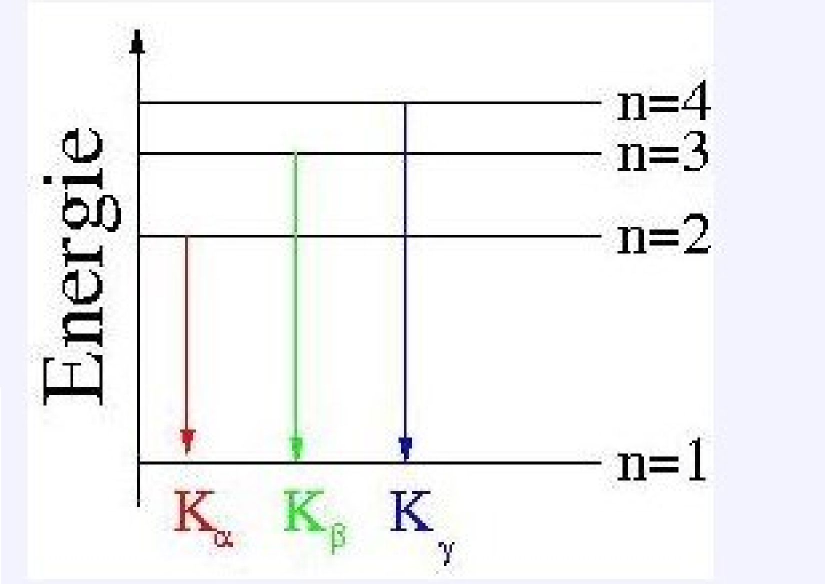
1895	Discovered by W.C. Röntgen
1912	First diffraction experiment (v. Laue)
1912	Coolidge tube (W.D. Coolidge, GE)
1946	Radiation from electrons in a synchrotron, GE, Physical Review, 71,829 (1947)



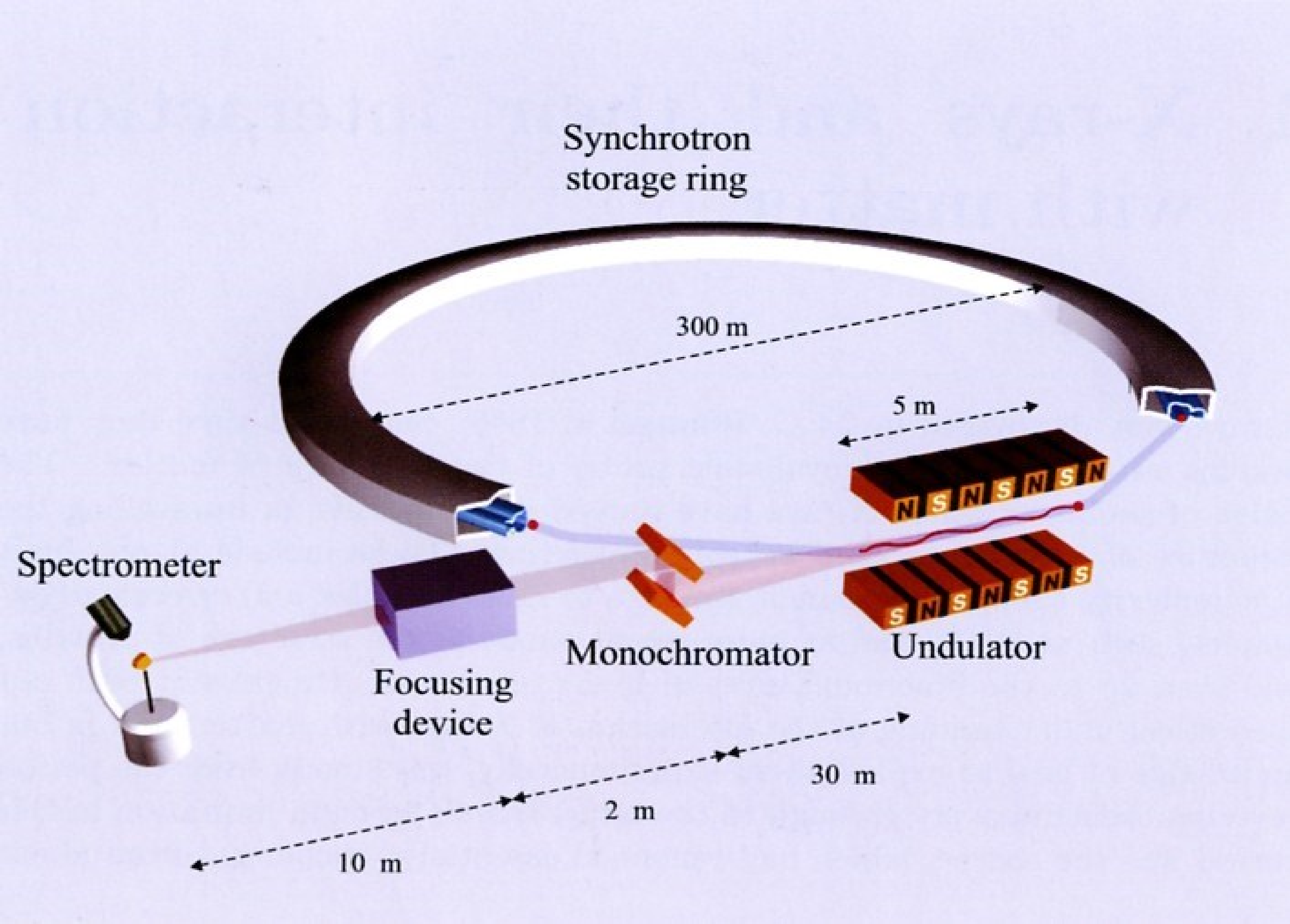


X-Ray Tube

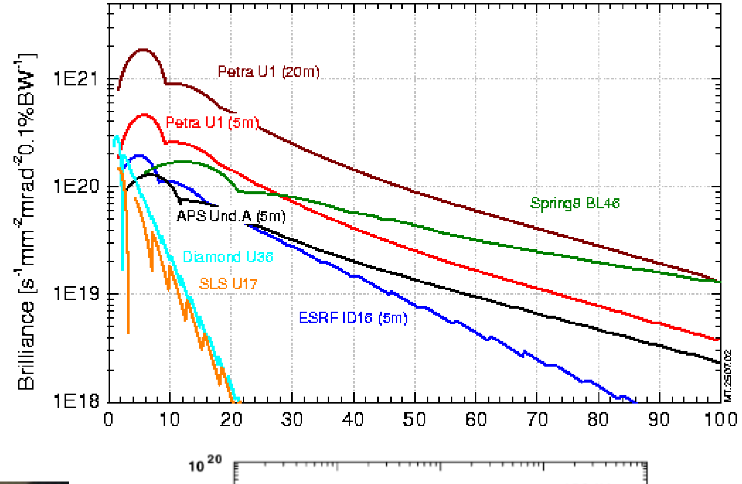

Neutron
Proton
Elektron
Unbesetzes Elektron
Kβ
Kα
Lα
Atomkern
K
L
M
externe Anregung
heraus-geschlagenes Elektron


Energie
n=4
n=3
n=2
n=1
K_α
K_β
K_γ

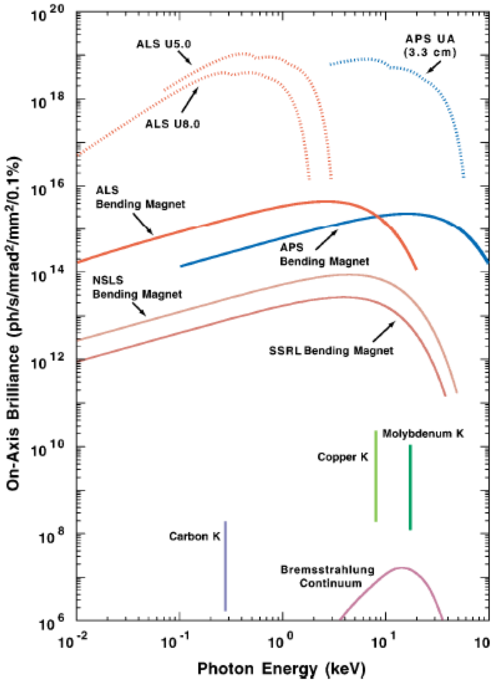
Synchrotron Radiation Storage Ring



The most recent third generation machine:



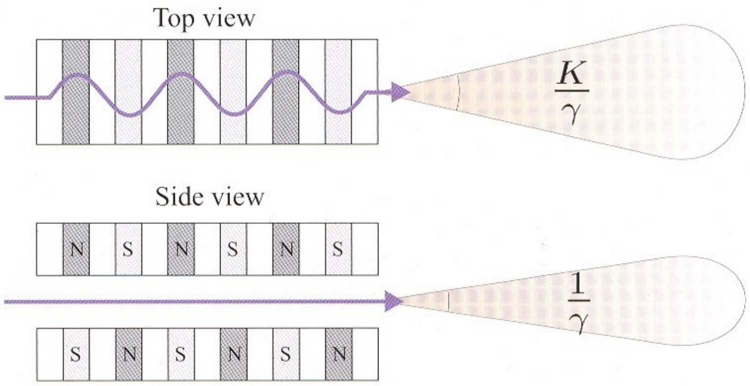
Petra III



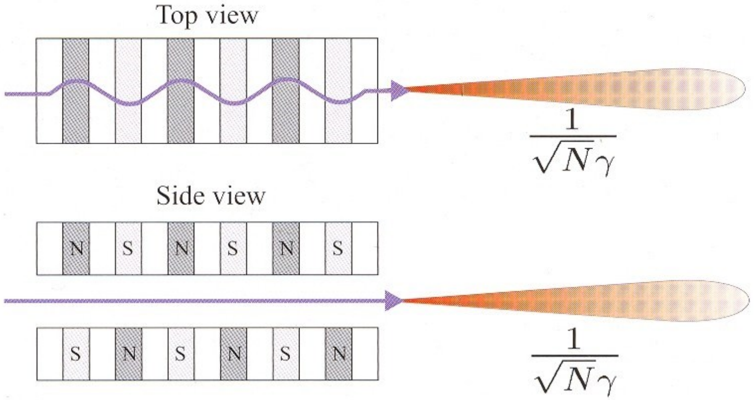
Petra III at DESY/Hamburg

Insertion Devices (Wigglers and Undulators)

(a) Wiggler



(b) Undulator



$$P[\mathrm{kW}] = 0.633 E^2_e\ [\mathrm{GeV}]\ B^2[\mathrm{T}]\ L[\mathrm{m}]\ I[\mathrm{A}]$$

$$K = eB / mc\,k_u = 0.934\,\lambda_u\,[\mathrm{cm}]\,B[\mathrm{T}]$$

with λ_u undulator period

<u>Wiggler</u>: K > 1

$$\mathrm{Flux} \sim E^2 \times N$$

N: number poles

<u>Undulator</u>: K ≤ 1

<u>undulator fundamental</u>:

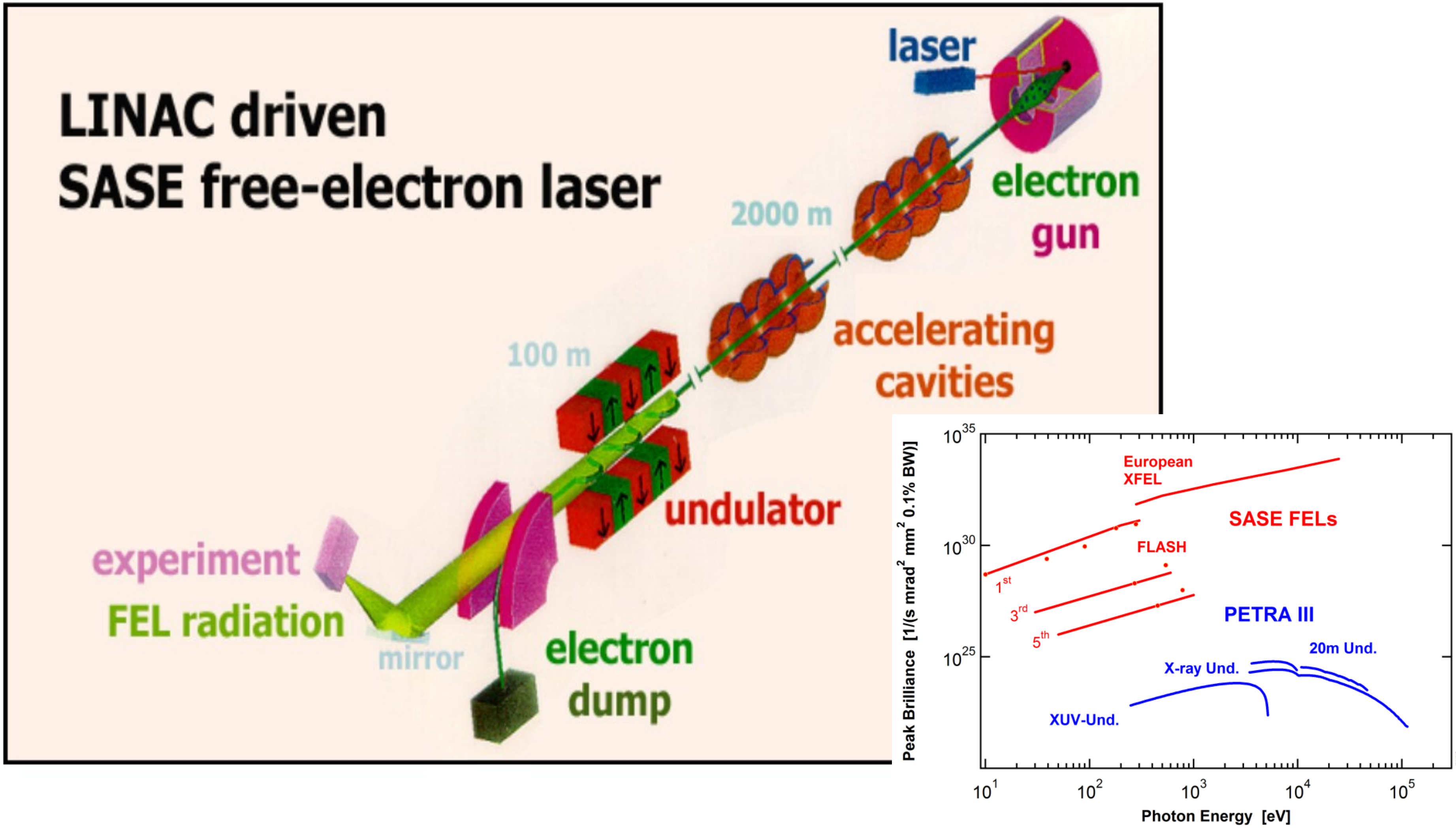
$$\lambda_0 = \frac{\lambda_u}{2\gamma^2}\left(1 + \frac{K^2}{2} \cancel{+ \gamma\theta)}\right.$$

on axis

$$\mathrm{Flux} \sim E^2 \times N^2$$

<u>bandwidth</u>: $\frac{\Delta\lambda}{\lambda} \sim \frac{1}{nN}$

Free Electron Lasers (FELs)



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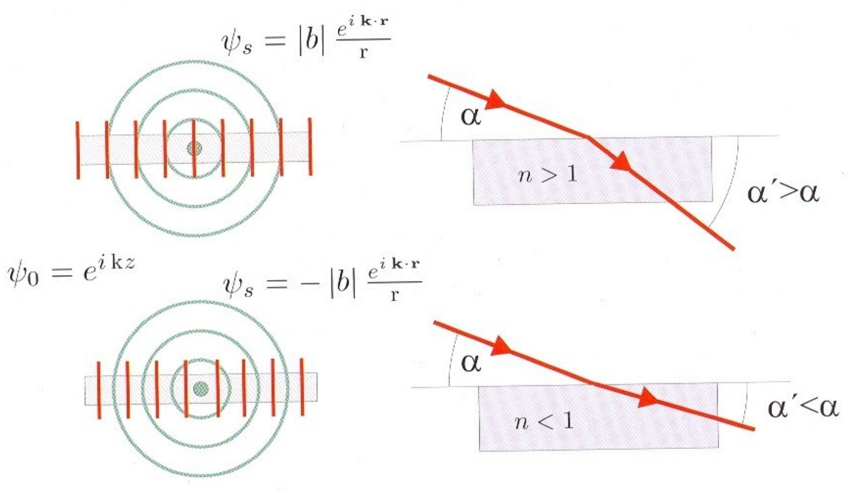


Rays of light propagating in air change direction when entering glass, water or another transparent material.

Governed by Snell's law:

$$\frac{\cos\alpha}{\cos\alpha'} = n \text{ (refractive index)}$$

$n = n(\omega)$ $\quad 1.2 < n < 2$ visible light

$n < 1$ X−rays $(\alpha' < \alpha)$

$n = 1 - \delta \quad \delta \approx 10^{-5}$

Total external reflection:

for $\alpha < \alpha_c$ (critical angle)

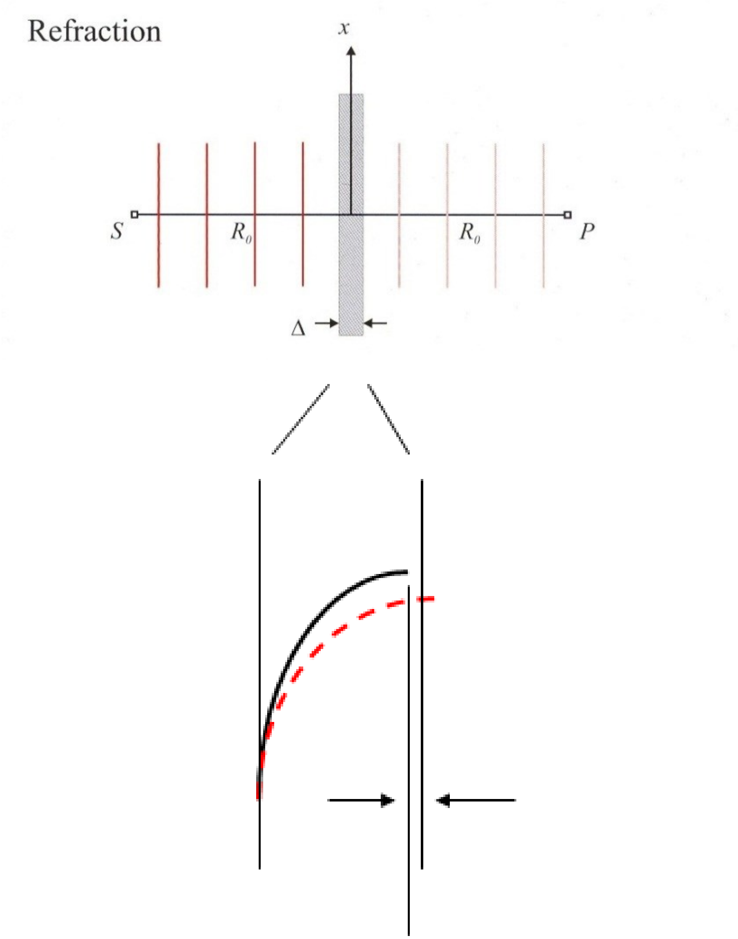
Note: spherical wave $e^{ik'r}$

$$k' = nk = \left(\frac{n}{c}\right)\omega = \frac{\omega}{v}$$

with $v = \frac{n}{c}$ phase velocity

$(v > c$ for $n < 1;$ but group velocity $\frac{d\omega}{dk} \leq c)$

Refractive Index



Phase difference

Refractive picture:

Consider plane wave impinging on a slab with thickness Δ and refractive index n. Evaluate amplitude at observation point P (compared to the situation without slab).

no slab: $e^{ik\Delta}$

slab: $e^{ink\Delta}$

phase difference: $e^{i(nk-k)\Delta}$

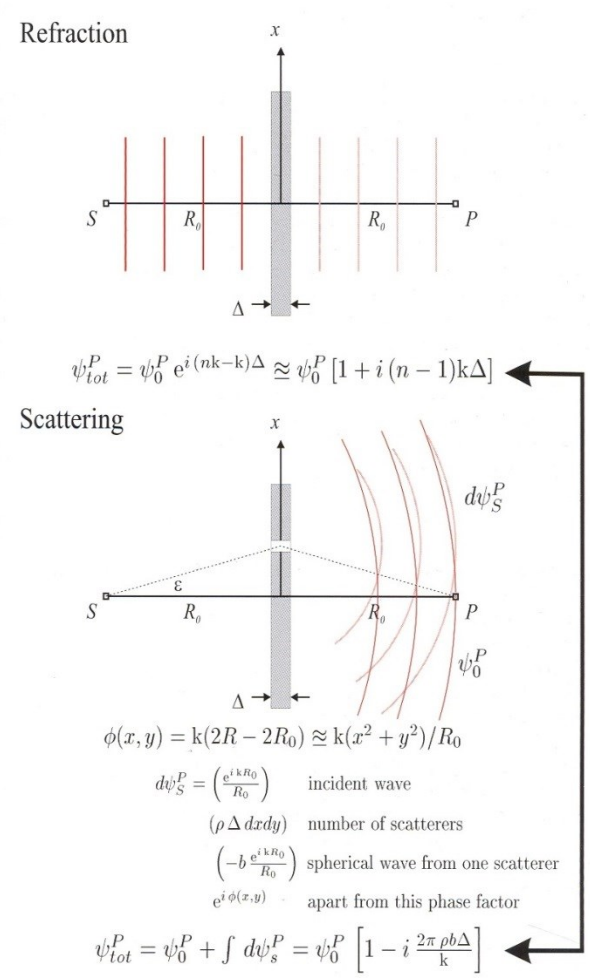
Amplitude: $$\frac{\psi^{P}_{tot}}{\psi^{P}_{0}} = \frac{e^{ink\Delta}}{e\ ik\Delta}$$

$$= e^{i(nk-k)\Delta}$$

$$e^{i\alpha} = \cos\alpha + i\sin\alpha \xrightarrow[\alpha\ \text{small}]{} 1 + i\alpha$$

$$\boxed{\psi^{P}_{tot} \approx \psi^{P}_{0}\,[1 + i\,k(n-1)\Delta]} \quad (\$)$$

Refractive Index



$$\psi_{tot}^P = \psi_0^P\,\mathrm{e}^{i\,(n\mathrm{k}-\mathrm{k})\Delta} \approxeq \psi_0^P\,[1 + i\,(n-1)\mathrm{k}\Delta]$$

$$\phi(x,y) = \mathrm{k}(2R - 2R_0) \approxeq \mathrm{k}(x^2+y^2)/R_0$$

$d\psi_S^P = \left(\frac{\mathrm{e}^{i\,\mathrm{k}R_0}}{R_0}\right)$ incident wave

$(\rho\,\Delta\,dxdy)$ number of scatterers

$\left(-b\,\frac{\mathrm{e}^{i\,\mathrm{k}R_0}}{R_0}\right)$ spherical wave from one scatterer

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

$$\psi_{tot}^P = \psi_0^P + \int d\psi_s^P = \psi_0^P\,\left[1 - i\,\frac{2\pi\,\rho b\Delta}{\mathrm{k}}\right]$$

Scattering picture:

$$R = \sqrt{R_0^2 + x^2} = \sqrt{R_0^2\left(1 + \frac{x^2}{R_0^2}\right)} \approx R_0\sqrt{1 + \frac{x^2}{R_0^2} + \frac{x^4}{4R_0^2}}$$

$$= R_0\sqrt{\left(1 + \frac{x^2}{2R_0^2}\right)^2} = R_0\left(1 + \frac{x^2}{2R_0^2}\right)$$

phase difference $(2k(R - R_0))$ between direct rays and rays following path R;

$$\frac{kx^2}{R_0}$$

Include *y* direction: $e^{i\Phi(x,y)} = e^{\frac{i(x^2+y^2)k}{R_0}}$

Amplitude at P: $d\psi_s^P \approx$

$$\underset{\text{incident wave}}{\frac{\mathbf{1}}{\mathbf{R_0}}\mathbf{e^{ikR_0}}} \quad \underset{\text{number of scatters in volume element } \rho dxdy}{(\boldsymbol{\rho\Delta dxdy})} \quad \underset{\text{scattered wave from 1 scatterer}}{\left(\mathbf{b}\,\frac{\mathbf{1}}{\mathbf{R_0}}\mathbf{e^{ikR_0}}\right)} \quad \underset{\text{phase factor}}{\mathbf{e^{i\Phi(x,y)}}}$$

Refractive Index

$$\psi_s^P = \int d\psi_s^P = -\rho b\Delta\left(\frac{\exp(i2kR_0)}{R_0^2}\right)\underbrace{\int \exp(i\Phi(x,y))dxdy}_{i\frac{\pi R_0}{k}} \qquad [1]$$

[Ref. 1]

Amplitude at P without slab:

$$\psi_0^P = \left(\frac{\exp(i2kR_0)}{2R_0}\right) \qquad [2]$$

$$\psi_{tot}^P = [1] + [2] = \psi_0^P\left[1 - \left(\frac{i2\pi\rho b\Delta}{k}\right)\right]$$

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

$$\boxed{n = 1 - \frac{2\pi\rho b}{k^2} = 1 - \delta}$$

If a homogenous electron density ρ is replaced by a plate composed of atoms:

$$\rho = \rho_a f^0(0)$$

atomic density X atomic scattering factor

$$\boxed{\delta = \frac{2\pi\rho_a f^0(0) r_0}{k}}$$

Total external reflection $(\alpha' = 0)$ **for** $\alpha = \alpha_c$ **:**

$$\cos\alpha = n\cos\alpha'$$

$$\cos\alpha_c = 1 - \frac{\alpha_c^2}{2}$$

$$\boxed{\alpha_c = \sqrt{2\delta} = \sqrt{\frac{4\pi\rho r_0}{k^2}}}$$

$k = \frac{2\pi}{\lambda} = 6Å^{-1}$, $b = r_0 = 2.82 \times 10^{-5}Å$, $\rho = \frac{1e^-}{Å^3}$: $\delta \approx 10^{-5}$

[Ref. 1: Als-Nielsen and McMorrow, p. 66]

Critical Angle for Si

$$\alpha_c = \sqrt{2\delta} = \sqrt{\frac{4\pi\rho r_0}{k^2}}$$

Silicon: $\rho = \frac{0.699e^-}{Å^3}$, $\lambda = 1Å$

$$\alpha_c = \sqrt{(4\pi \times 0.699 \times 2.82e^{-5}) \times \frac{1}{(2\pi)^2}}$$
$$= 0.0025 \text{ rad}$$

$$Q_c = \left(\frac{4\pi}{\lambda}\right) \sin\alpha_c = 0.032Å^{-1}$$

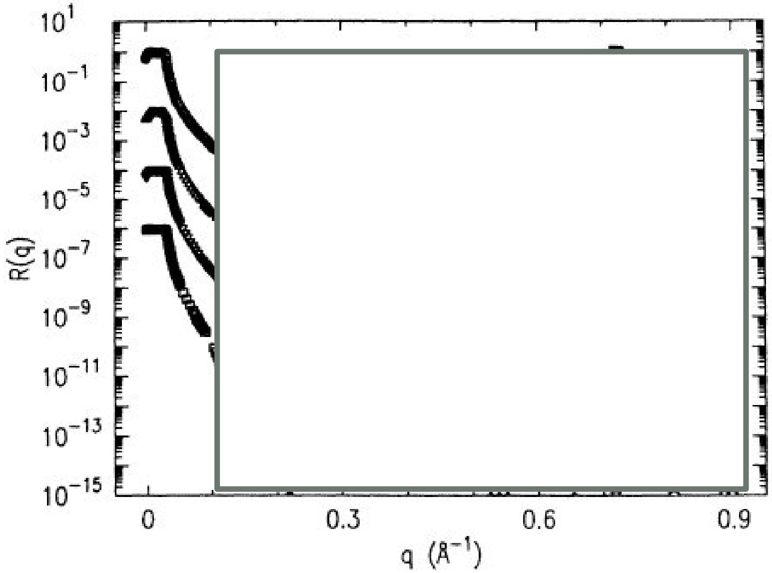
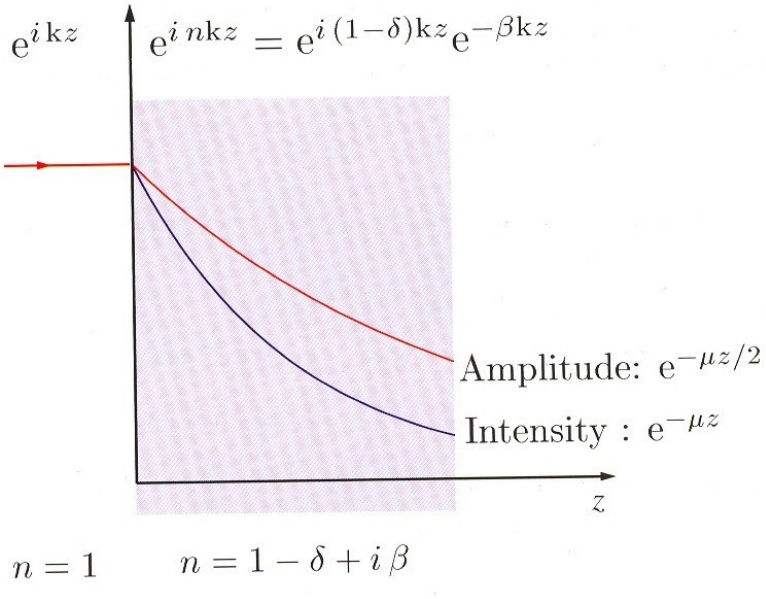


FIG. 1. Normalized reflectivity data from several samples. Successive data sets are displaced by 100 times and error bars omitted for clarity. (——) Theoretical reflectivity from an ideal step interface with bulk silicon density. (○) Uncoated silicon sample in helium; the "pairing" of points occurs for two scans taken 60 min apart and is probably due to the build up of contaminants on the surface. (△) 10-carbon chain alkylsiloxane. (▽) 12-carbon chain alkylsiloxane. (□) 18-carbon chain alkylsiloxane. The inset shows a schematic diagram of the scattering vectors for the specular reflectivity condition, where $2(\phi) = 2\theta$.

Refraction Including Absorption



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

Wave propagating in a medium:

$$e^{i\,nkz} = e^{i(1-\,\delta)kz}e^{-\beta kz}$$

Attenuation of amplitude: $e^{-\frac{\mu z}{2}}$

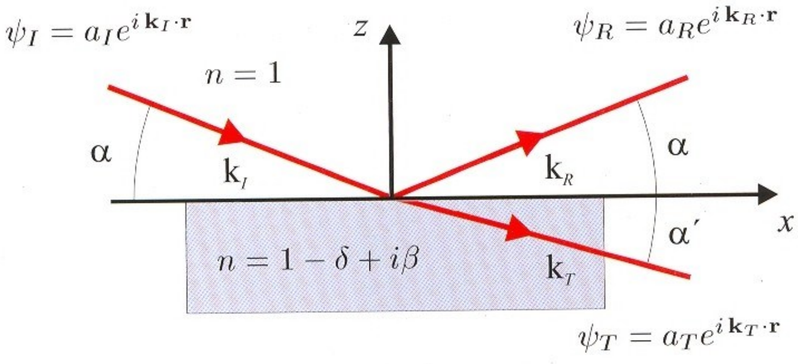
(when intensity drops according to $e^{-\mu z}$)

$$\boxed{\beta = \frac{\mu}{2k}}$$

Snell’s Law and the Fresnel Equations

Snell's Law and the Fresnel Equations

$$k = |\mathbf{k}_I| = |\mathbf{k}_R|$$



Assume that the wave and its derivative is continuous at the interface:

$$a_I + a_R = a_T \qquad \text{(A)}$$

$$a_I\mathbf{k}_I + a_R\mathbf{k}_R = a_T\mathbf{k}_T \qquad \text{(B)}$$

$$||:\ a_I k\cos\alpha + a_R k\cos\alpha = a_T(nk)\cos\alpha' \qquad \text{(B')}$$

$$|:\ -(a_I - a_R)k\sin\alpha = -a_T(nk)\sin\alpha' \qquad \text{(B'')}$$

$$\boxed{\cos\alpha = n\cos\alpha'} \qquad \text{(B'+A)}$$

<u>α, α′small</u>: $(\cos z = 1 - \frac{z^2}{2})$

$$\alpha^2 = \alpha'^2 + 2\delta - 2i\beta$$

$$= \alpha'^2 + \alpha_c^2 - 2i\beta \qquad \text{(C)}$$

$$\frac{a_I - a_R}{a_I + a_R} = n\frac{\sin\alpha'}{\sin\alpha} \approx \frac{\alpha'}{\alpha} \qquad \text{(B''+A)}$$

<u>Fresnel equations</u>:

$$\boxed{r = \frac{a_R}{a_I} = \frac{\alpha-\alpha'}{\alpha+\alpha'} \quad ; \quad t = \frac{a_T}{a_I} = \frac{2\alpha}{\alpha+\alpha'}}$$

r: reflectivity **t: transmittivity**

Snell's Law and the Fresnel Equations (2)

Note: α' is a complex number

$$\alpha' = \mathrm{Re}(\alpha') + \mathrm{i}\,\mathrm{Im}(\alpha')$$

Consider z-component of transmitted wave:

$$= a_T e^{ik \sin \alpha' z} \approx a_T e^{ik\alpha' z}$$

$$= a_T e^{ik\mathrm{Re}(\alpha')z}\ e^{-k\,\mathrm{Im}(\alpha')z}$$

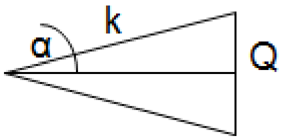
exponential damping

intensity fall-off: $e^{-2k\,\mathrm{Im}(\alpha')z}$

1/e penetration depth Λ: $z\,2k\,\mathrm{Im}(\alpha') = 1\ (z = \Lambda)$

$$\boxed{\Lambda = \frac{1}{2k\,\mathrm{Im}(\alpha')}}$$

Use wavevector notation:



$$\sin\alpha = \frac{\left(\frac{Q}{2}\right)}{k}$$

$$Q \equiv 2\,k \sin\alpha \approx 2\,k\,\alpha$$

$$Q_c \equiv 2\,k \sin\alpha_c \approx 2\,k\,\alpha_c$$

use dimensionless units:

$$q \equiv \frac{Q}{Q_c} \approx \left(\frac{2k}{Q_c}\right)\alpha\ ; \qquad q' \equiv \frac{Q'}{Q_c} \approx \left(\frac{2k}{Q_c}\right)\alpha'$$

$$\boxed{q^2 = q'^2 + 1 - 2\,\mathrm{i}\,b_\mu} \qquad \text{(D)}$$

$$b_\mu = \left(\frac{2k}{Q_c}\right)^2 \beta = \left(\frac{4k^2}{Q_c^2}\right)\frac{\mu}{2k} = \frac{2k}{Q_c^2}\mu$$

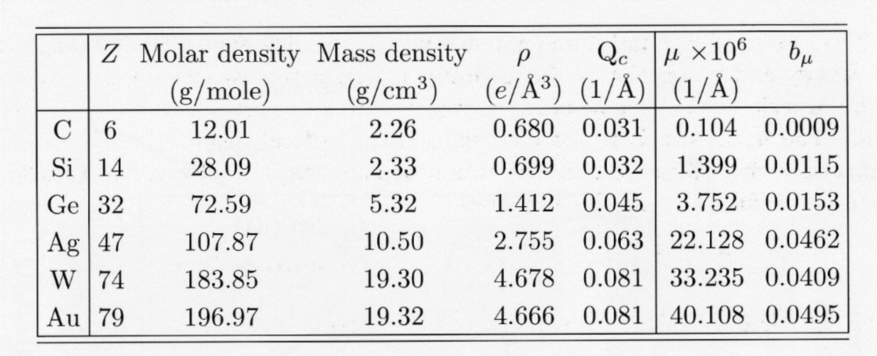
$$Q_c = 2k\alpha_c = 2k\sqrt{2\delta}$$

Snell's Law and the Fresnel Equations (3)

Use table to extract μ, ρ, f' yielding Q_c

and calculate b_μ $(b_\mu \ll 1)$:

$$b_\mu = \frac{2k\mu}{Q_c^2}$$



	Z	Molar density (g/mole)	Mass density (g/cm^3)	ρ (e/Å^3)	Q_c (1/Å)	$\mu \times 10^6$ (1/Å)	b_μ
C	6	12.01	2.26	0.680	0.031	0.104	0.0009
Si	14	28.09	2.33	0.699	0.032	1.399	0.0115
Ge	32	72.59	5.32	1.412	0.045	3.752	0.0153
Ag	47	107.87	10.50	2.755	0.063	22.128	0.0462
W	74	183.85	19.30	4.678	0.081	33.235	0.0409
Au	79	196.97	19.32	4.666	0.081	40.108	0.0495

Use (D): $q^2 = q'^2 + 1 - 2\,i\,b_\mu$

Get:

$$\boxed{r(q) = \frac{q - q'}{q + q'}}$$

$$t(q) = \frac{2q}{q + q'}$$

$$\Lambda(q) = \frac{1}{Q_c \mathrm{Im}(q')}$$

Snell's Law and the Fresnel Equations (4)

Fresnel equations:

$\mathbf{q \gg 1}$: $R(Q) \sim \frac{1}{q^4}$,

$\Lambda \approx \mu^{-1}$,

$T \approx 1$,

no phase shift

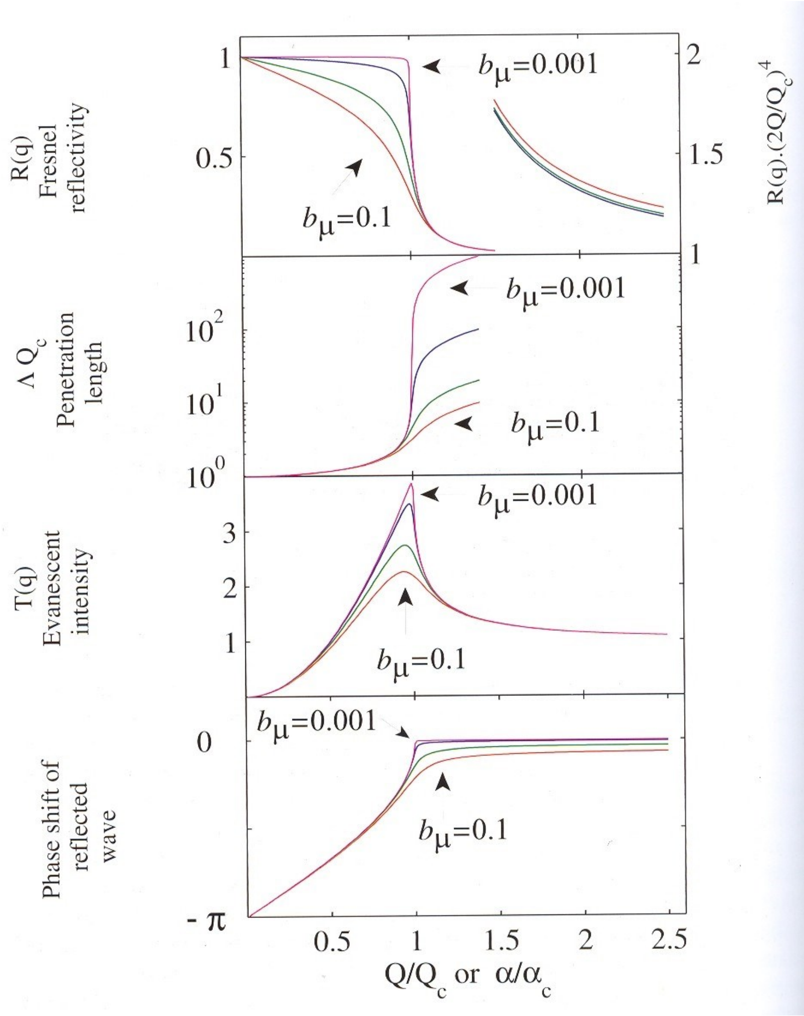
$\mathbf{q \ll 1}$: $R \approx 1$,

$\Lambda \approx \frac{1}{q_c}$ small ,

T very small ,

$-\pi$ phase shift

$\mathbf{q = 1}$: $T(q = 1) \approx 4a_I$



Examples

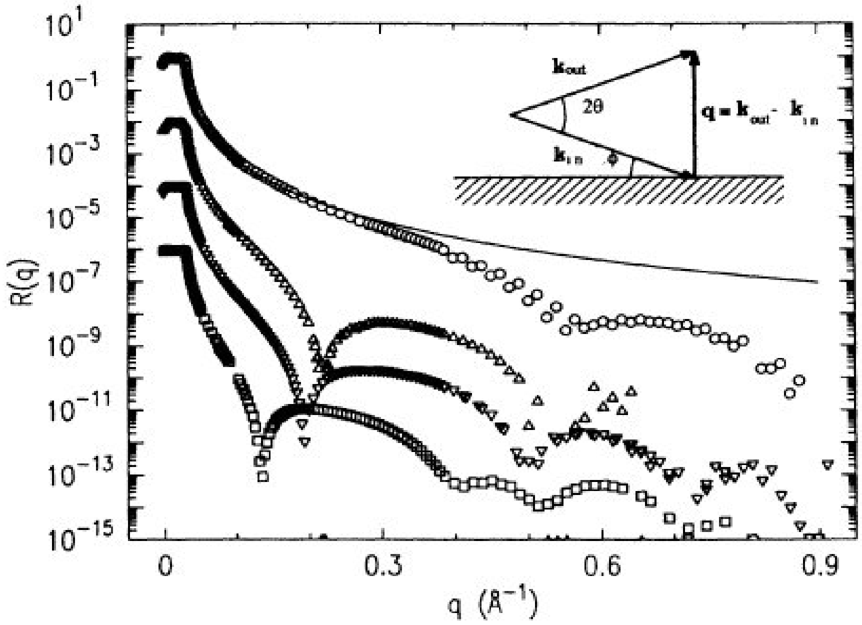
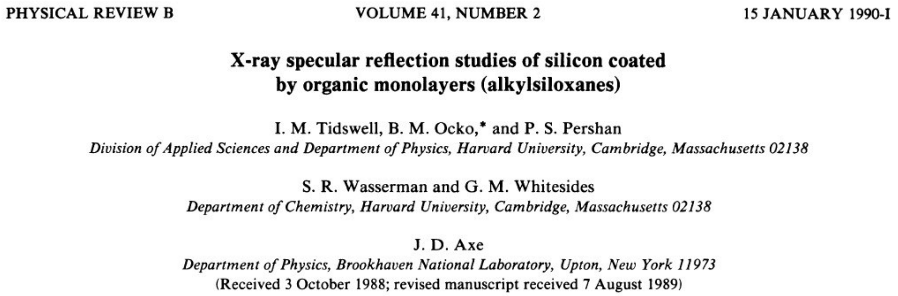


FIG. 1. Normalized reflectivity data from several samples. Successive data sets are displaced by 100 times and error bars omitted for clarity. (——) Theoretical reflectivity from an ideal step interface with bulk silicon density. (○) Uncoated silicon sample in helium; the "pairing" of points occurs for two scans taken 60 min apart and is probably due to the build up of contaminants on the surface. (△) 10-carbon chain alkylsiloxane. (▽) 12-carbon chain alkylsiloxane. (□) 18-carbon chain alkylsiloxane. The inset shows a schematic diagram of the scattering vectors for the specular reflectivity condition, where $2(\phi) = 2\theta$.


PHYSICAL REVIEW B VOLUME 41, NUMBER 2 15 JANUARY 1990-I

X-ray specular reflection studies of silicon coated by organic monolayers (alkylsiloxanes)

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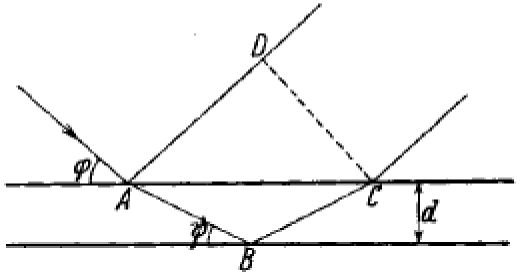
(Received 3 October 1988; revised manuscript received 7 August 1989)

Examples- Thin Films



Darstellung des Strahlenganges bei den Röntgeninterferenzen an dünnen Schichten

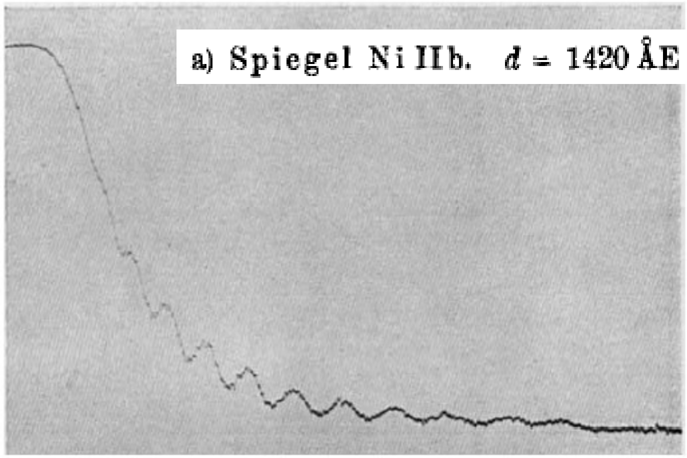
Fig. 1

ANNALEN DER PHYSIK

5. FOLGE, 1931, BAND 10, HEFT 7

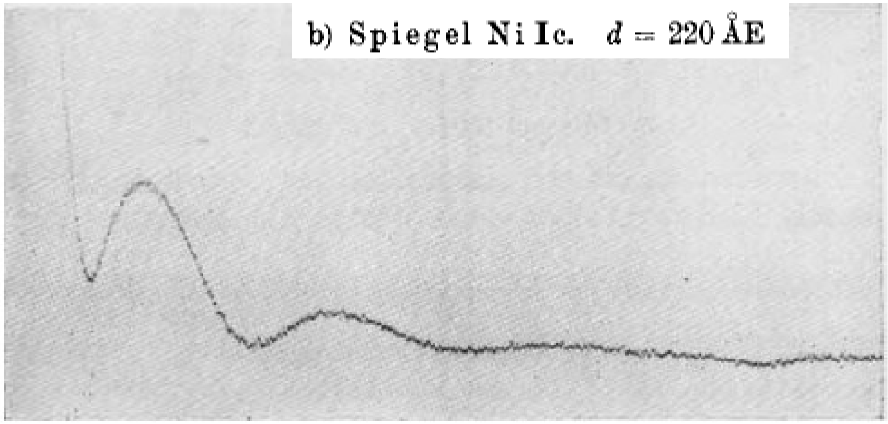
Interferenz von Röntgenstrahlen an dünnen Schichten

Von Heinz Kiessig



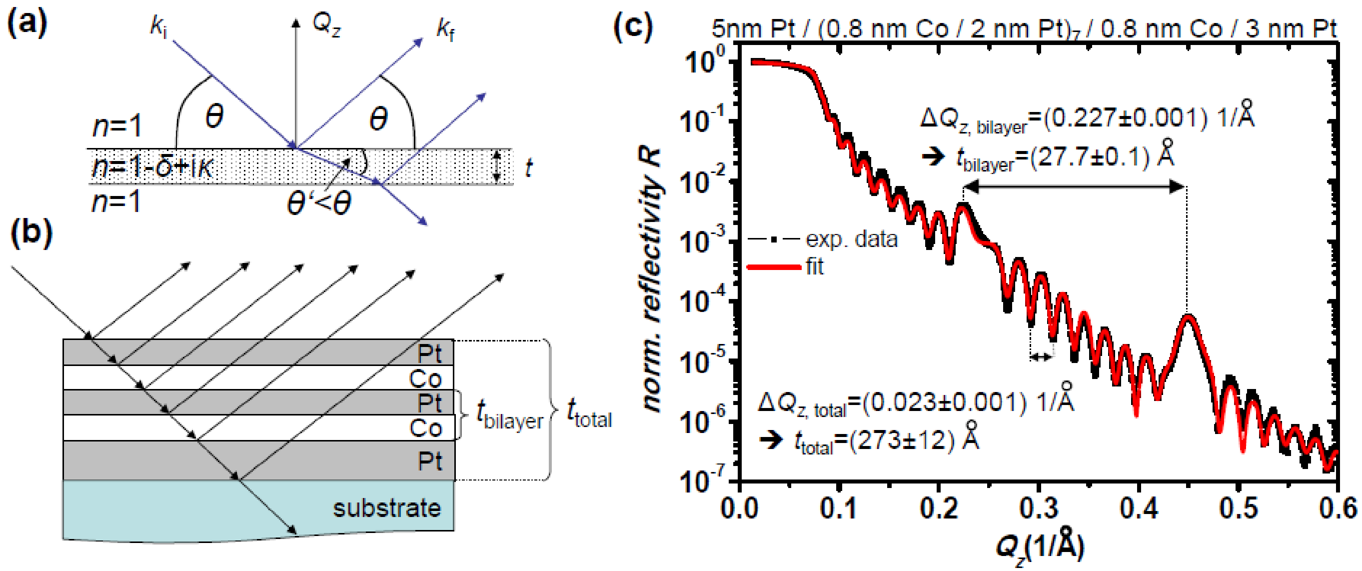
Photometerkurve von der Aufnahme in Fig. 1

Fig. 3



$$\Delta Q_{z,\text{ total}} = \frac{2\pi}{t_{\text{total}}}$$

Examples- Multilayers



$$\Delta Q_{z,\text{ total}} = \frac{2\pi}{t_{\text{total}}}$$

$$\Delta Q_{z,\text{ bilayer}} = \frac{2\pi}{t_{\text{bilayer}}}$$

Figure 5.27: (a) Refraction and reflection of an x-ray beam hitting a thin layer with thickness t. The interference of the partial waves refracted from the two interfaces generates oscillations (Kiessig fringes) in the reflectivity profile $R(\theta)$. (b) In a periodically layered structure the interferences of the reflected partial waves additionally yield beating waves in $R(\theta)$. (c) Reflectivity R in dependence of the scattering vector Q_z for a multilayer with $n = 8$ and a Pt interlayer thickness of $t_{\text{Pt}} = 2$ nm. From the oscillation and beating wave period the total thickness of the stacking and the bilayer thickness was verified utilizing Eq. 5.64 and Eq. 5.65, respectively. The red solid line is a fit utilizing the software PARRAT32 [715], which is used in particular to determine the thickness of the roughness/interdiffusion regions.

Methoden moderner Röntgenphysik II: Streuung und Abbildung – Next Lecture

Introduction
Overview, Introduction to X-ray Scattering

X-ray Scattering Primer
Elements of X-ray Scattering

Sources of X-rays, Synchrotron Radiation
Laboratory Sources, Accelerator Bases Sources

Reflection and Refraction from Interfaces
Snell’s Law, Fresnel Equations

Kinematical Diffraction (I)
Diffraction from an Atom, a Molecule, from Liquids, Glasses, … ⇦

Kinematical Diffraction (II)
Diffraction from a Crystal, Reciprocal Lattice, Structure Factor, …

Methoden moderner Röntgenphysik II: Streuung und Abbildung

Small Angle Scattering, and Soft Matter
Introduction, Form Factor, Structure Factor, Applications, ...

Anomalous Diffraction
Introduction into Anomalous Scattering, ...

Introduction into Coherence
Concept, First Order Coherence, ...

Coherent Scattering
Spatial Coherence, Second Order Coherence, ...

Applications of Coherent Scattering
Imaging and Correlation Spectroscopy, ...

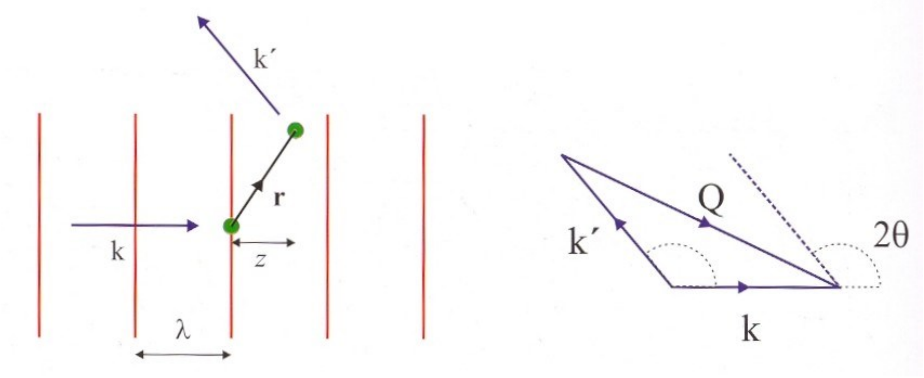
Kinematical Diffraction

Kinematical Diffraction

One of the main applications of X-rays is the determination of structure(s) using diffraction.

Assume the scattering to be weak; multiple scattering effects are to be neglected: weak scattering limit ≡ kinematical approximation.

Consider a 2 electron system:



$$z = r\cos\alpha;\ k\,z = k\,r\cos\alpha = \mathbf{k} \bullet \mathbf{r}$$

$$y = r\cos\beta;\ k'y = k'r\cos\beta = \mathbf{k'} \bullet \mathbf{r}$$

Path- or phase difference:

$$\Delta\Phi = z - y = \mathbf{k} \bullet \mathbf{r} - \mathbf{k'} \bullet \mathbf{r} = \mathbf{Q} \bullet \mathbf{r}$$

with

$$Q = \left(\frac{4\pi}{\lambda}\right)\sin\theta$$

Scattering amplitude for 2 electrons:

$$A(\mathbf{Q}) = -r_{\mathbf{0}}\,[1 + e^{i\mathbf{Qr}}]$$

$$I(\mathbf{Q}) = A(\mathbf{Q})A(\mathbf{Q})^*$$

$$= 2{r_{\mathbf{0}}}^{\mathbf{2}}\,[1 + \cos(Qr)]$$

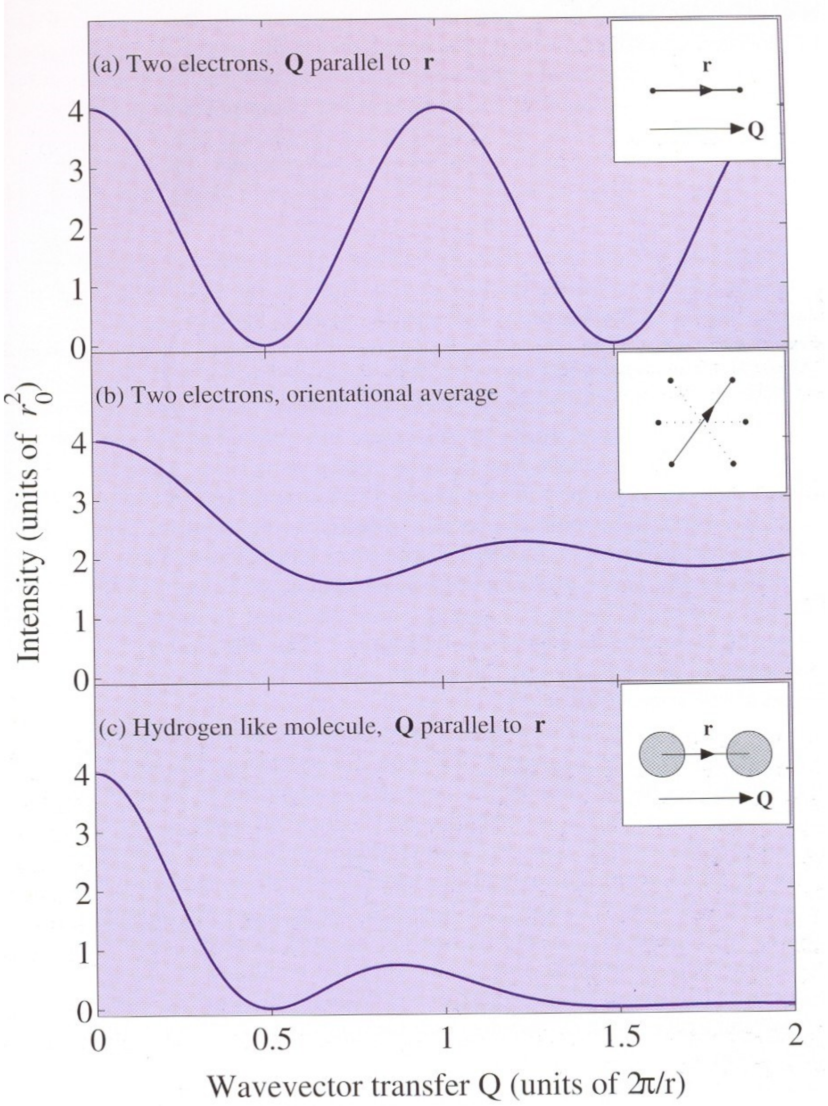
see Fig. 4.2

For many electrons:

$$A(\mathbf{Q}) = -r_0 \sum r_{j'}\, e^{i\mathbf{Q}\mathbf{r}_{j'}}$$

Geben Sie hier eine Formel ein.

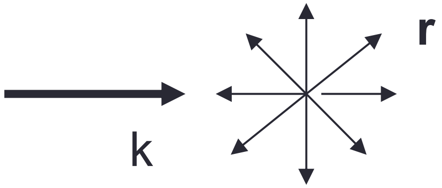
Kinematical Diffraction



Two electron system:

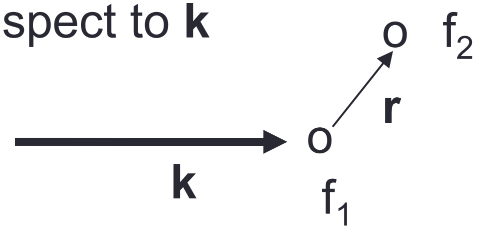
$$I(Q) = 2r_0^2[1 + \cos(Qr)]$$
$$Q \parallel r$$

orientational average



"smeared", no more "point-like" particles

For many systems, e.g. molecules the orientation of **r** will be random with respect to **k**



Orientational averaging: assume one electron at r=0, a second at r

$$A(Q) = f1 + f_2 e^{iQr}$$

$$I(Q) = f_1^2 + f_2^2 + f_1 f_2 e^{iQr} + f_1 f_2 e^{-iQr}$$

Orientational averaging: $<e^{iQr}> = <e^{-iQr}>$

$$< I(Q) > = f_1^2 + f_2^2 + 2 f_1 f_2 < e^{iQr} >$$

$$< e^{iQr} > = \frac{\int e^{iQr\cos\theta} \sin\theta \, d\theta}{\int \sin\theta \, d\theta d\phi}$$

4π

$$\int \exp(iQr\cos\theta) \sin\theta \, d\theta d\Phi$$
$$= 2\pi \int e^{iQr\cos\theta} \sin\theta \, d\theta$$
$$= 2\pi \left(-\frac{1}{iQr}\right) \int_{iQr}^{-iQr} e^x \, dx$$
$$= 4\pi \frac{\sin(Qr)}{Qr}$$

$$< I(Q) > = f_1^2 + f_2^2 + 4\pi f_1 f_2 \frac{\sin(Qr)}{Qr}$$

see figure 4.2 b

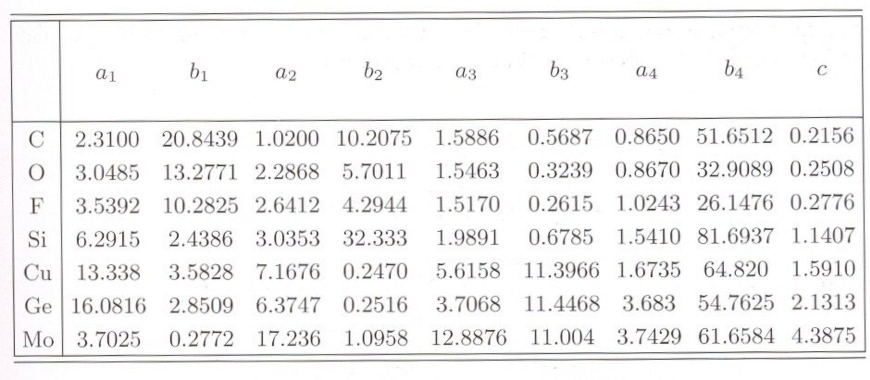
if the position of the electrons distributed or smeared: see Figure 4.2c

Scattering From an Atom

Scattering amplitude of an atom ≡ atomic form factor $f_0(\mathbf{Q})$ [in units of r_0]

ρ(**r**): electronic number density ≡ charge density

$$f_0(\mathbf{Q}) = \int \rho(\mathbf{r}) e^{i\mathbf{Q}\mathbf{r}} d\mathbf{r} = \begin{cases} Z \text{ for } \mathbf{Q} \to 0 \\ 0 \text{ for } \mathbf{Q} \to \infty \end{cases}$$



	a_1	b_1	a_2	b_2	a_3	b_3	a_4	b_4	c
C	2.3100	20.8439	1.0200	10.2075	1.5886	0.5687	0.8650	51.6512	0.2156
O	3.0485	13.2771	2.2868	5.7011	1.5463	0.3239	0.8670	32.9089	0.2508
F	3.5392	10.2825	2.6412	4.2944	1.5170	0.2615	1.0243	26.1476	0.2776
Si	6.2915	2.4386	3.0353	32.333	1.9891	0.6785	1.5410	81.6937	1.1407
Cu	13.338	3.5828	7.1676	0.2470	5.6158	11.3966	1.6735	64.820	1.5910
Ge	16.0816	2.8509	6.3747	0.2516	3.7068	11.4468	3.683	54.7625	2.1313
Mo	3.7025	0.2772	17.236	1.0958	12.8876	11.004	3.7429	61.6584	4.3875

Table 4.1: J. Als-Nielsen & D. McMorrow

Note: atomic form factor is FT of electronic charge distribution

$f_0\left(\frac{Q}{4\pi}\right)$ tabulated:

$$f_0\left(\frac{Q}{4\pi}\right) = \sum_{j=1}^{4} a_j e^{-b_j\left(\frac{Q}{4\pi}\right)^2} + c$$

Note:

$$f = f_0(Q) + f' + f''$$

corrections f' and f'' arise from the fact that the electrons are bound in the atom

Scattering from a Molecule

$$F^{\mathrm{mol}}(Q) = \sum_{rj} f_j(Q) e^{i\mathbf{Q}\mathbf{r}_j}$$

—— CF$_4$

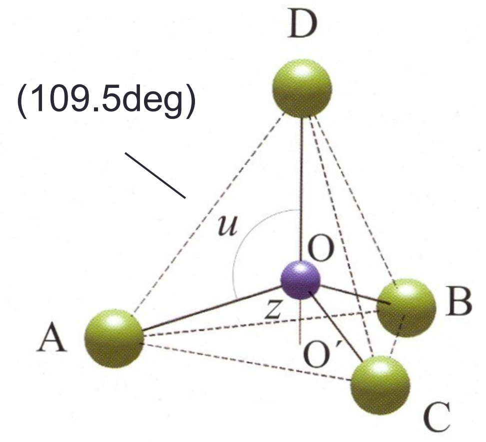
-. - . - CF$_4$ Q not || C-F

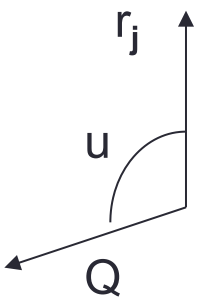
- - - - - molybdenum (also 42 electrons)

Example: CF$_4$:

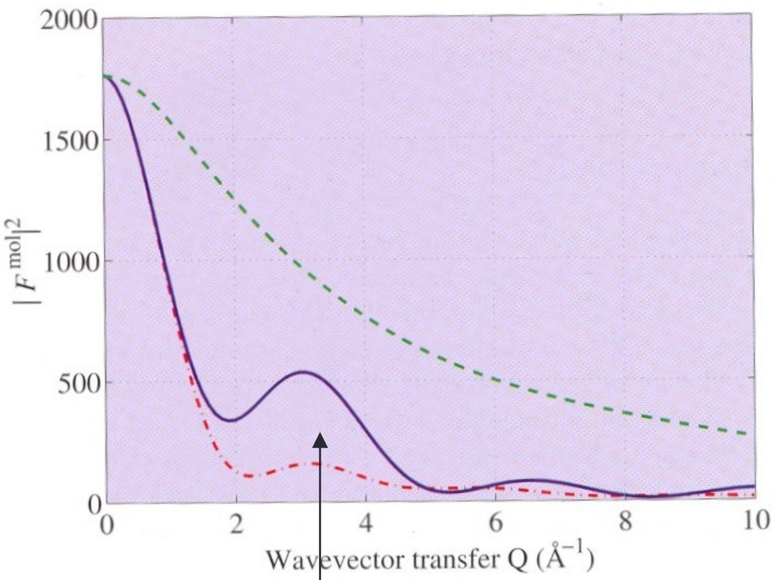
assume $OA = OB = OC = OD = 1;\ z = OO' = \cos(u) = \frac{1}{3}$

(109.5deg)





$$\mathbf{Q}\mathbf{r}_j = Qr_j \cos(u) = \left(\frac{1}{3}\right)Qr_j$$



(F-F bond)