Methoden moderner Röntgenphysik: Streuung und Abbildung

Lecture 3	Vorlesung zum Haupt- oder Masterstudiengang Physik, SoSe 2018		
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Location	Lecture hall AP, Physics, Jungiusstraße		
Date	Tuesdays	13:00 - 14:30	(starting 3.4.)
	Thursdays	8:30 - 10:00	(until 12.7.)

Methoden moderner Röntgenphysik: Streuung und Abbildung

Part I:

Basics of X-ray Physics

by Gerhard Grübel (GG)

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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, …

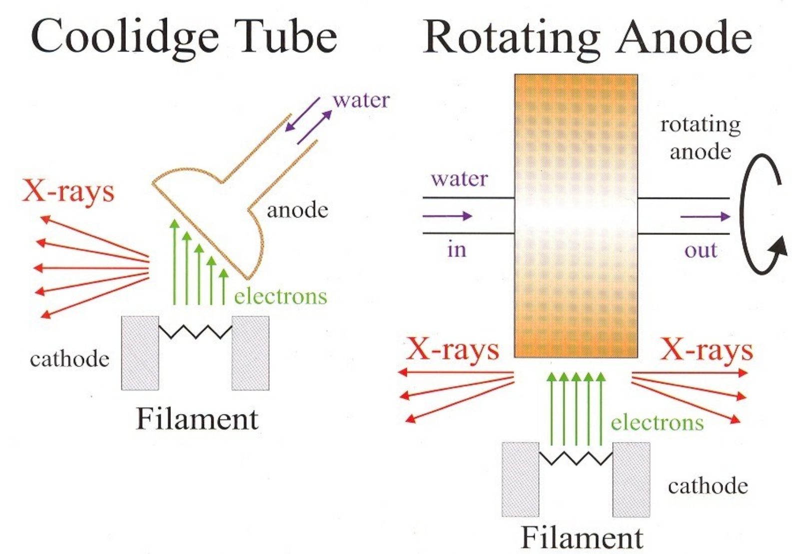
Source of X-Rays

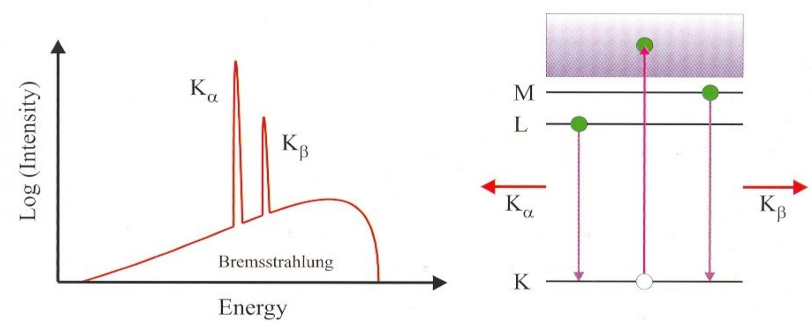
1895 Discovered by W.C. Röntgen

1912 First diffraction experiment (v. Laue)

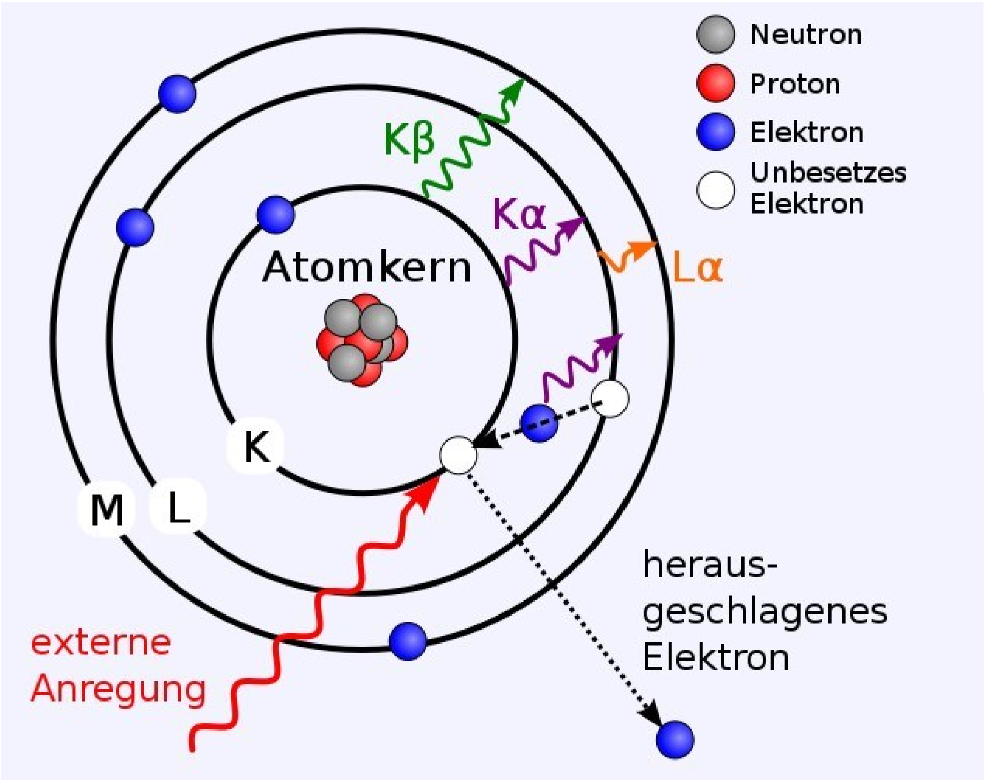
1912 Coolidge tube (W.D. Coolidge, GE)

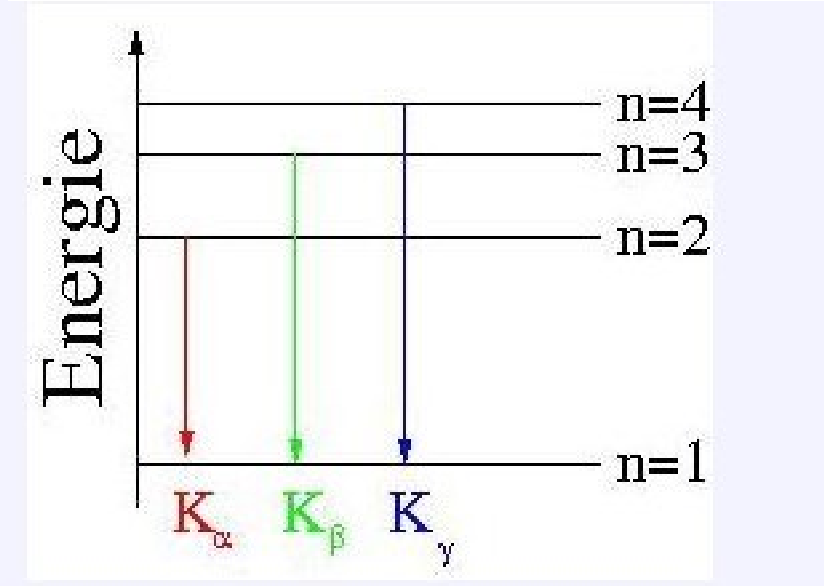
1946 Radiation from electrons in a synchrotron, GE, Physical Review, 71,829 (1947)



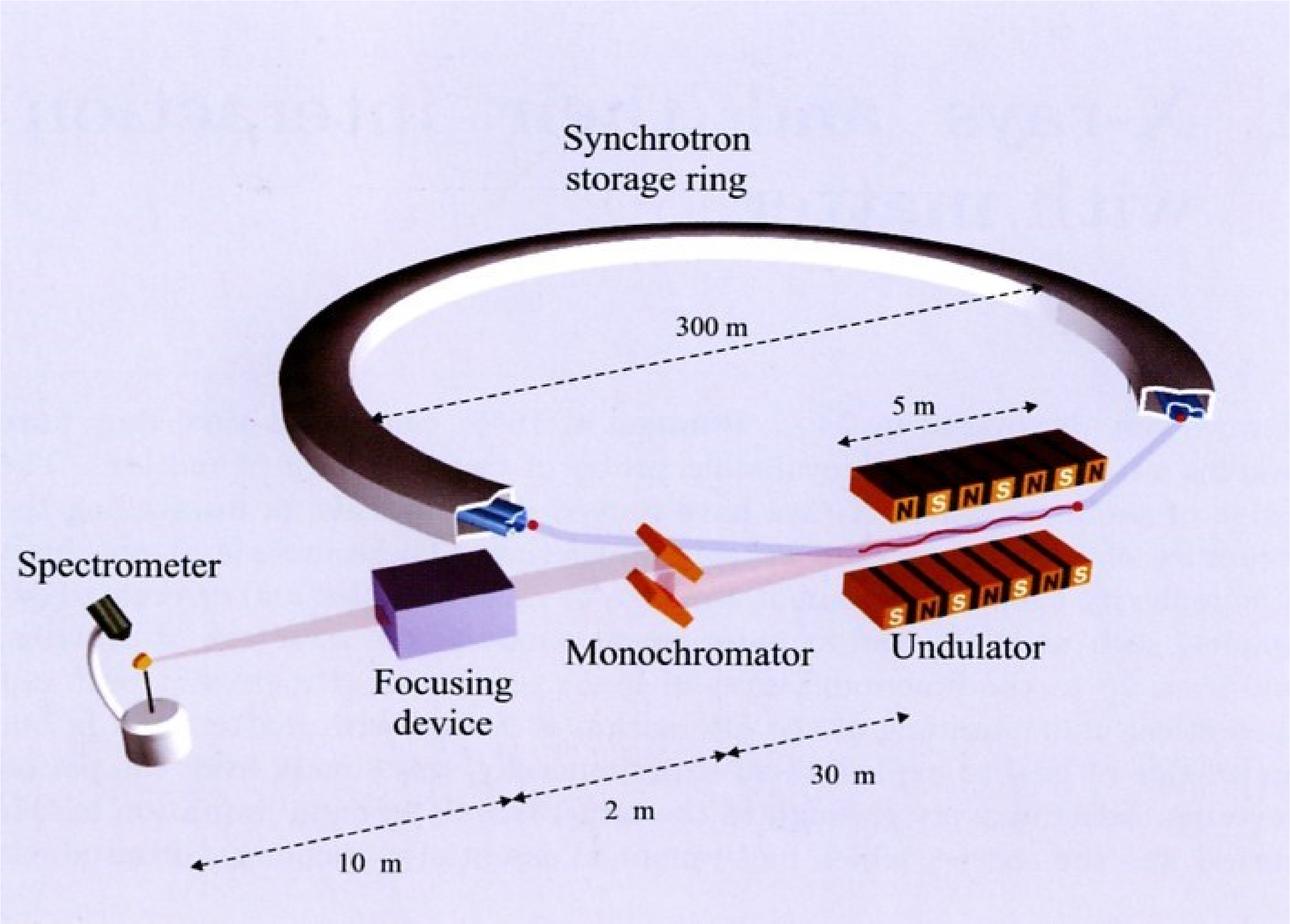


X-Ray Tube

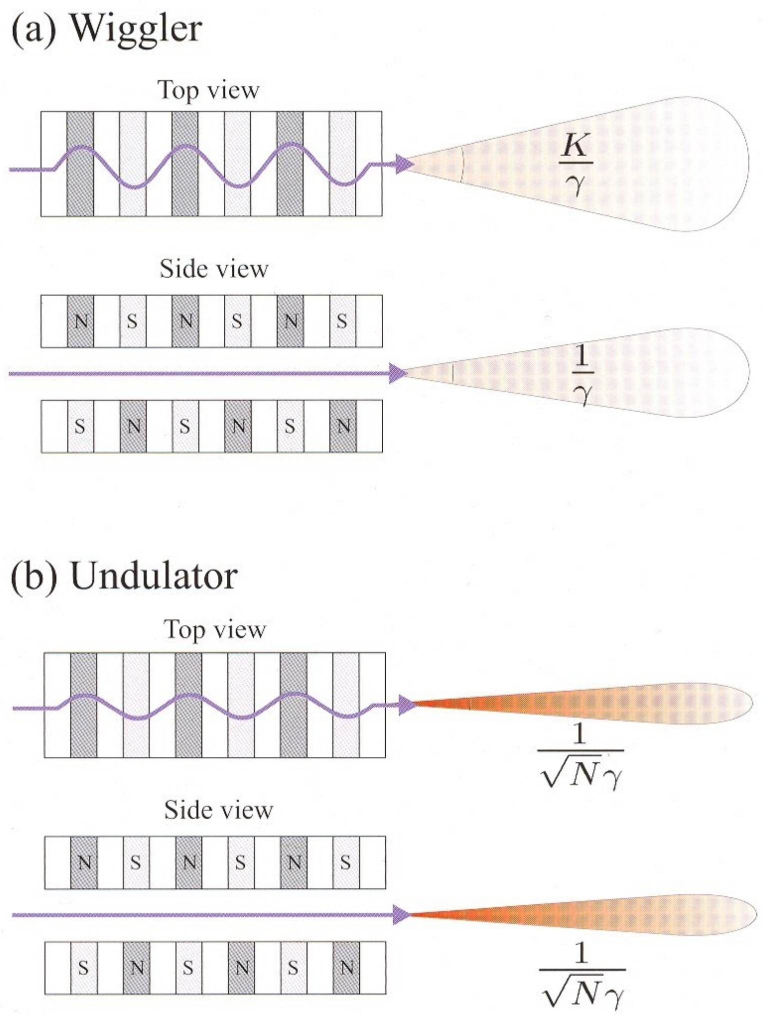

Neutron
Proton
Elektron
Unbesetzes Elektron
Kβ
Kα
Lα
Atomkern
K
M
L
externe Anregung
heraus-geschlagenes Elektron


Energie
n=4
n=3
n=2
n=1
Kα
Kβ
Kγ

Synchrotron Radiation Storage Ring



Insertion Devices (Wigglers and Undulators)



Wiggler:

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

$Flux \sim E^2 \times N$

N: number poles

Undulator:

$k = eB / mc\ k_u = 0.934\ \lambda_u\ [cm]\ Bo[T]$

with λ_u undulator period

undulator fundamental:

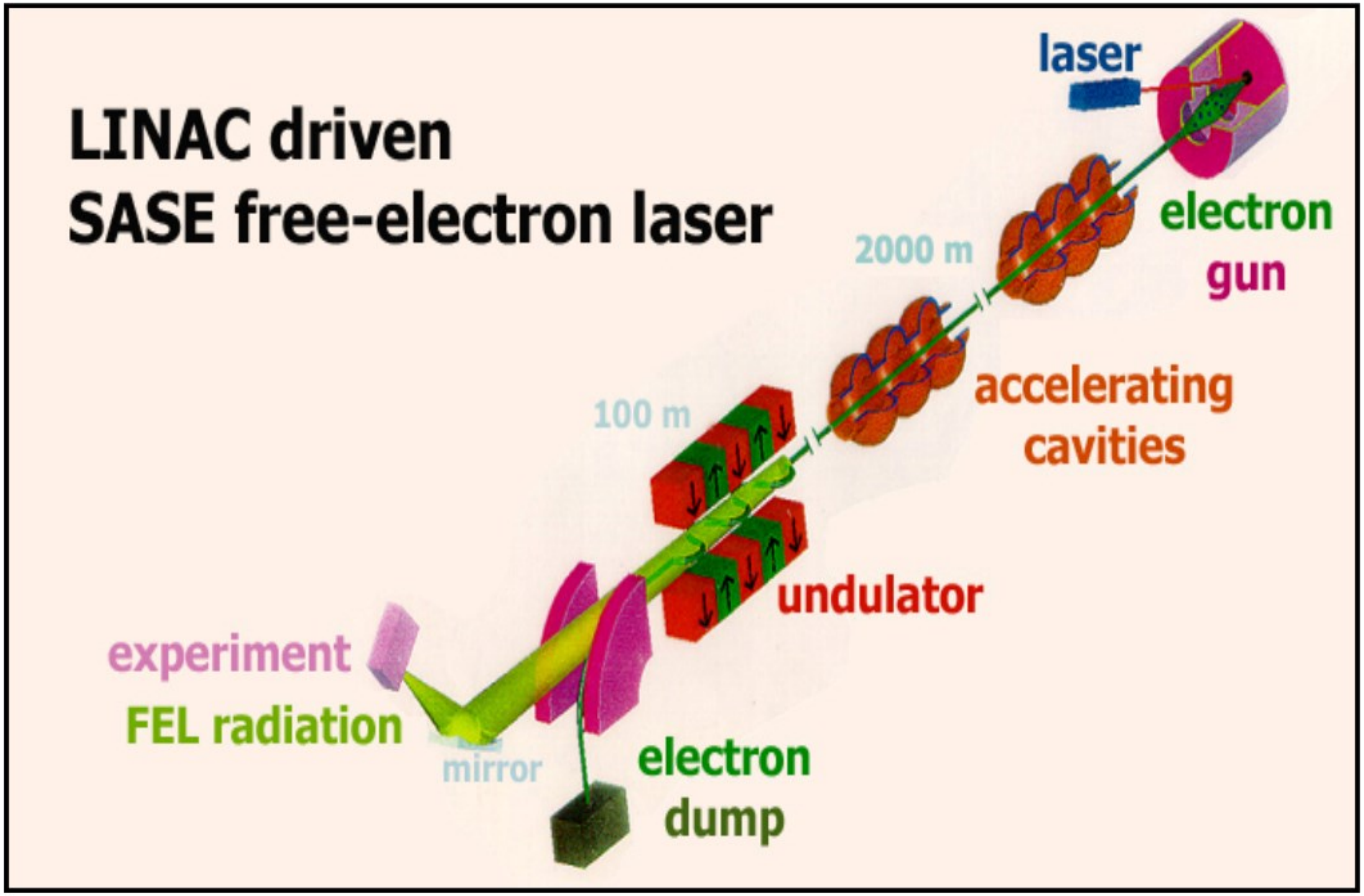
$$\lambda_0 = \frac{\lambda_u}{2_{\gamma^2}}(1 + \frac{k^2}{2} + \gamma\theta)$$

on axis

$Flux \sim E^2 \times N^2$

bandwidth: $\frac{\Delta\lambda}{\lambda} \sim \frac{1}{nN}$

Free Electron Lasers (FELs)



Methoden moderner Röntgenphysik II: Streuung und Abbildung

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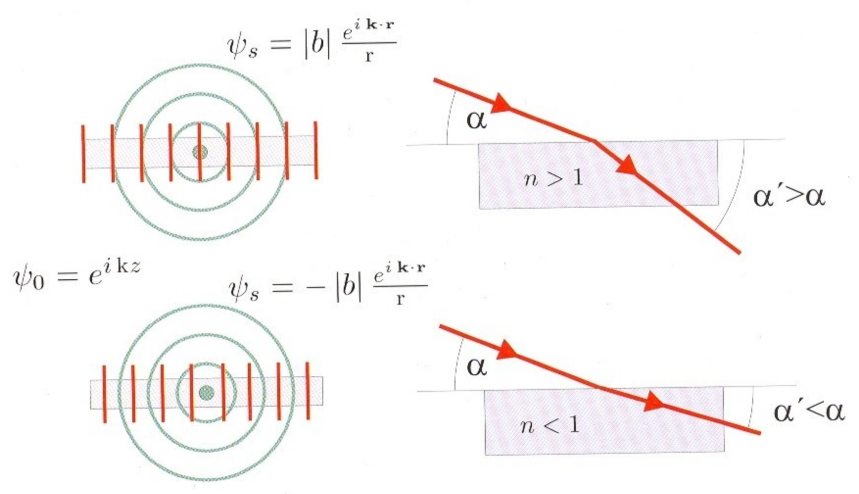


Rays of light propagating in air change direction when entering glass, water or another transparent material.

Governed by Snell's law:

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

$$\mathrm{n} = \mathrm{n}(\omega) \qquad 1.2 < \mathrm{n} < 2 \text{ visible light}$$

$$\mathrm{n} < 1 \text{ X-rays } (\alpha' < \alpha)$$

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

Total external reflection:

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

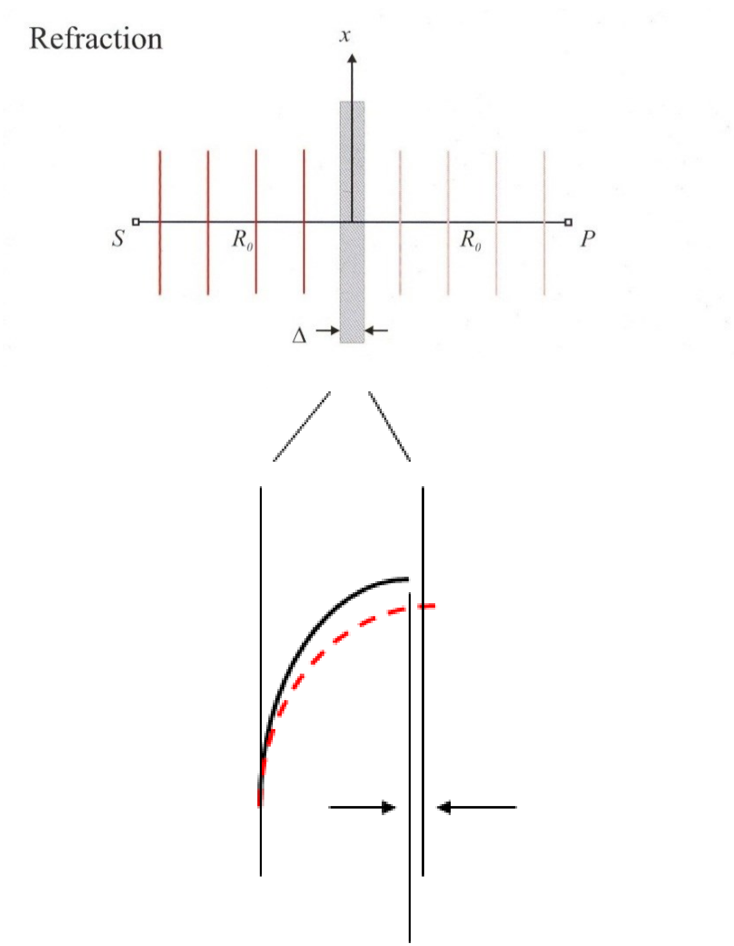
Note: spherical wave $e^{ik'r}$

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

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:

$$\frac{\psi^P_{tot}}{\psi^P_0} = \frac{e^{ink\Delta}}{e\ ik\Delta}$$

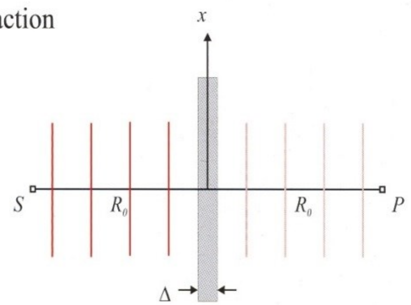
$$= e^{i(nk-k)\Delta}$$

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

$$\psi^P_{tot} \approx \psi^P_0\,[1 + i\,k(n-1)\Delta] \qquad (\$)$$

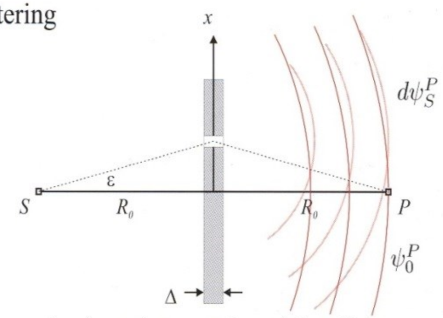
Refractive Index

Refraction



$\psi^P_{tot} = \psi^P_0\, e^{i(nk-k)\Delta} \approx \psi^P_0\,[1 + i\,(n-1)k\Delta]$

Scattering



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

$d\psi^P_S = \left(\frac{e^{ikR_0}}{R_0}\right)$	incident wave
$(\rho\,\Delta\,dxdy)$	number of scatterers
$\left(-b\,\frac{e^{ikR_0}}{R_0}\right)$	spherical wave from one scatterer
$e^{i\phi(x,y)}$	apart from this phase factor

$\psi^P_{tot} = \psi^P_0 + \int d\psi^P_s = \psi^P_0\left[1 - i\,\frac{2\pi\rho b\Delta}{k}\right]$

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 $(2kR)$ between direct rays and rays following path R;

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

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

Amplitude at P: $d\psi^P_s \approx$

$$e^{\frac{ikR_0}{R_0}} \quad (\rho\Delta dxdy) \quad \left(b\, e^{\frac{ikR_0}{R_0}}\right) \quad e^{i\Phi(x,y)}$$

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

Refractive Index

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

$$i\frac{\pi R_0}{k}$$ [Ref. 1]

Amplitude at P without slab:

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

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

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

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

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

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

number density x atomic scattering factor

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

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

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

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

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

$k = \frac{2\pi}{\lambda} = 4\text{Å} - 1$, $b = r_0 = 2.82 \times 10^{-5}\text{Å}$, $\rho = \frac{1e^-}{\text{Å}^3}$: $\delta \approx 10^{-5}$ *[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: $\rho = \frac{0.699e^-}{\text{Å}^3}$, $\lambda = 1\text{Å}$

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

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

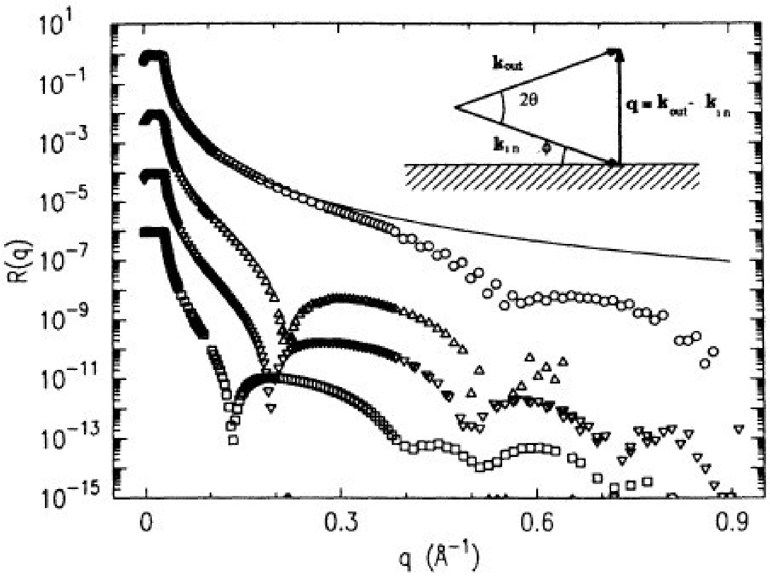
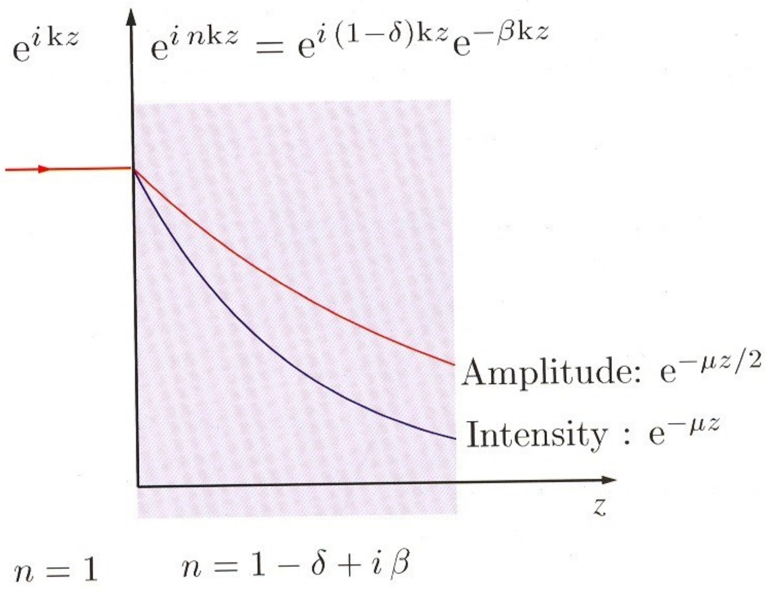


FIG. 1. Normalized reflectivity data from several samples. Successive data sets are displaced by 100 times and error bars omitted for clarity. (——) Theoretical reflectivity from an ideal step interface with bulk silicon density. (○) Uncoated silicon sample in helium; the "pairing" of points occurs for 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: $e^{-\frac{\mu z}{2}}$

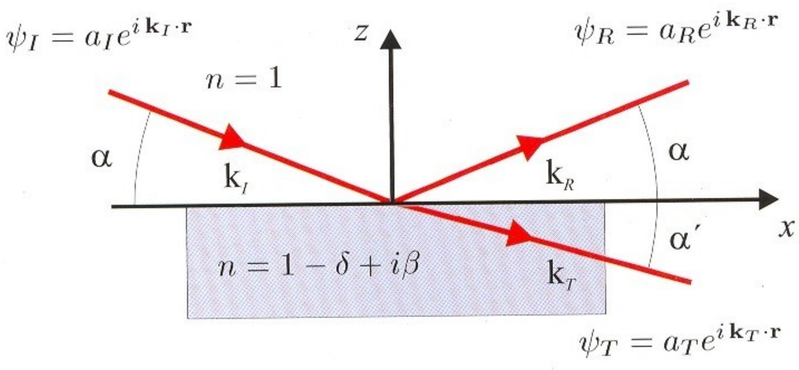
(when intensity drops according to $e^{-\mu z}$)

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

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:

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

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

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

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

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

α, α' small: $(\cos z = 1 - \frac{z^2}{2})$

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

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

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

Fresnel equations:

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

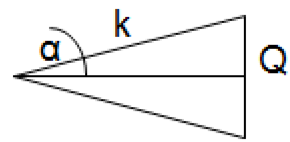
r: reflectivity **t: transmittivity**

Snell's Law and the Fresnel Equations (2)

Note: α' is a complex number

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

Use wavevector notation:



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

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: $z\,2k\,\mathrm{Im}(\alpha') = 1 \; (z = \Lambda)$

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

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

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

use dimensionless units:

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

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

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

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

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

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

<u>Get:</u>

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

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

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

Snell's Law and the Fresnel Equations (4)

Fresnel equations:

q ≫ 1: $R(Q) \sim \frac{1}{q^4}$,

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

$T \approx 1$,

no phase shift

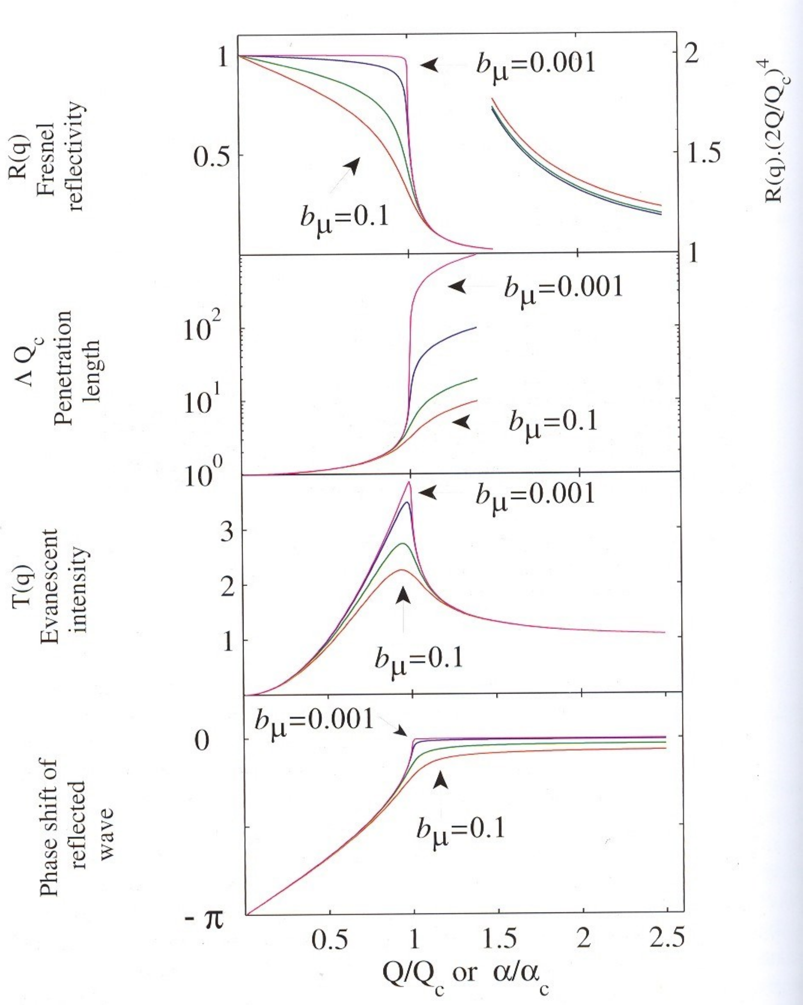
q ≪ 1: $R \approx 1$,

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

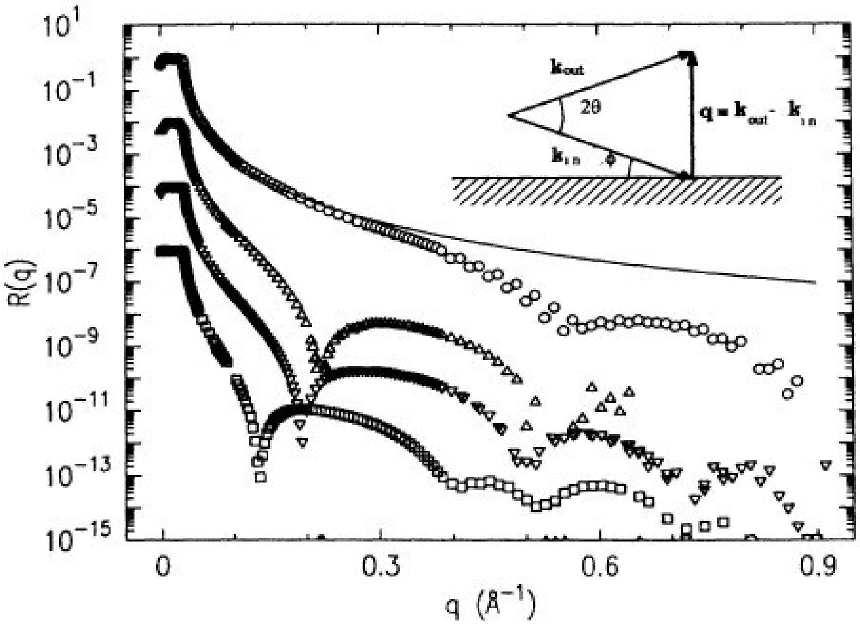
T very small ,

$-\pi$ phase shift

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



Examples



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

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