

Methoden moderner Röntgenphysik: Streuung und Abbildung

Lecture 4	Vorlesung zum Haupt- oder Masterstudiengang Physik, SoSe 2019 G. Grübel, L. Müller, O. Seeck, L. Frenzel, F. Lehmkuhler, M. Martins, W. Wurth		
Location	Lecture hall AP, Physics, Jungiusstraße		
Date	Tuesdays	12:30 - 14:00	(starting 2.4.)
	Thursdays	8:30 - 10:00	(until 11.7.)



Methoden moderner Röntgenphysik: Streuung und Abbildung

Part I:

Basics of X-ray Physics

by Gerhard Grübel (GG)

- [2.4.] Organisation and Introduction
- [4.4.] X-ray Scattering Primer
- [9.4.] Sources of X-rays, Synchrotron Radiation
- [11.4.] Refraction and Reflection
- [16.4.] Kinematical Scattering Theory (I)
- [18.4.] Kinematical Scattering Theory (II), Applications
- [23.4.] Small Angle Scattering and Soft Matter
- [25.4.] Anomalous Scattering
- [30.4.] Introduction: Coherence I
- [2.5.] Coherence II; Applications of Coherent X-ray Beams



Methoden moderner Röntgenphysik: Streuung und Abbildung

Part I:

Basics of X-ray Physics

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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)

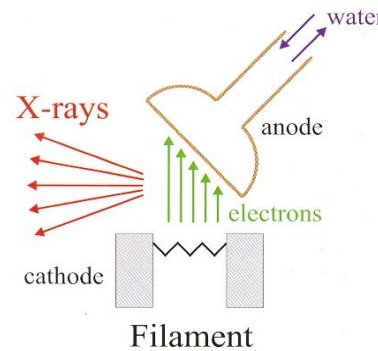
Diffraction from a Crystal, Reciprocal Lattice, Structure Factor, ...

Source of X-Rays

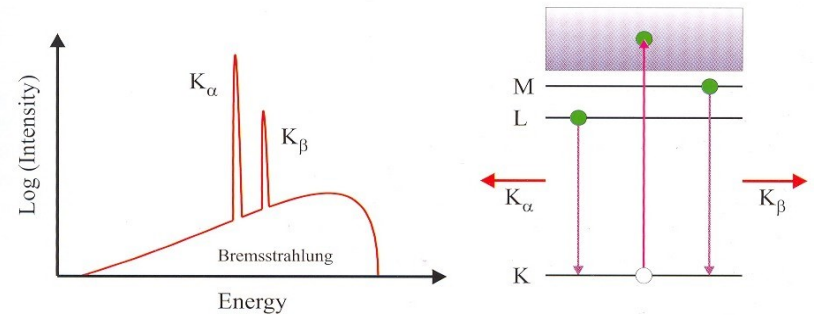
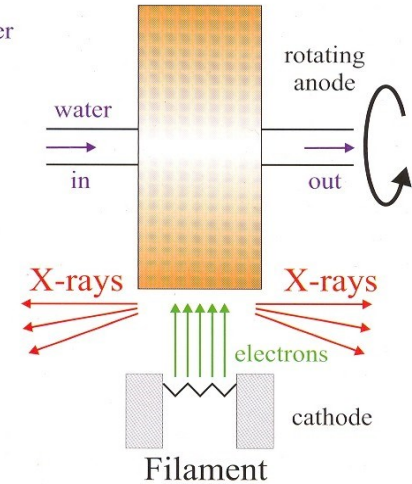
- 1895 Discovered by W.C. Röntgen
- 1912 First diffraction experiment (v. Laue)
- 1912 Coolidge tube (W.D. Coolidge, GE)
- 1946 Radiation from electrons in a synchrotron, GE, Physical Review, 71,829 (1947)



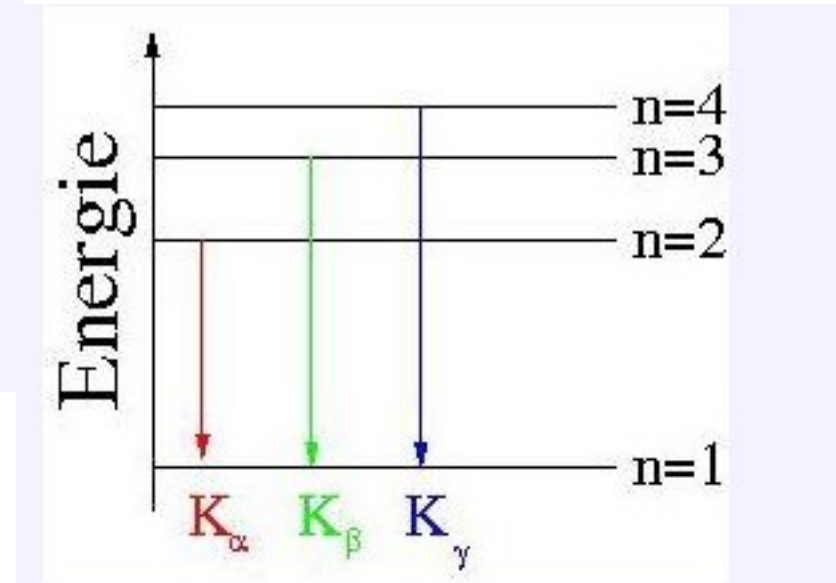
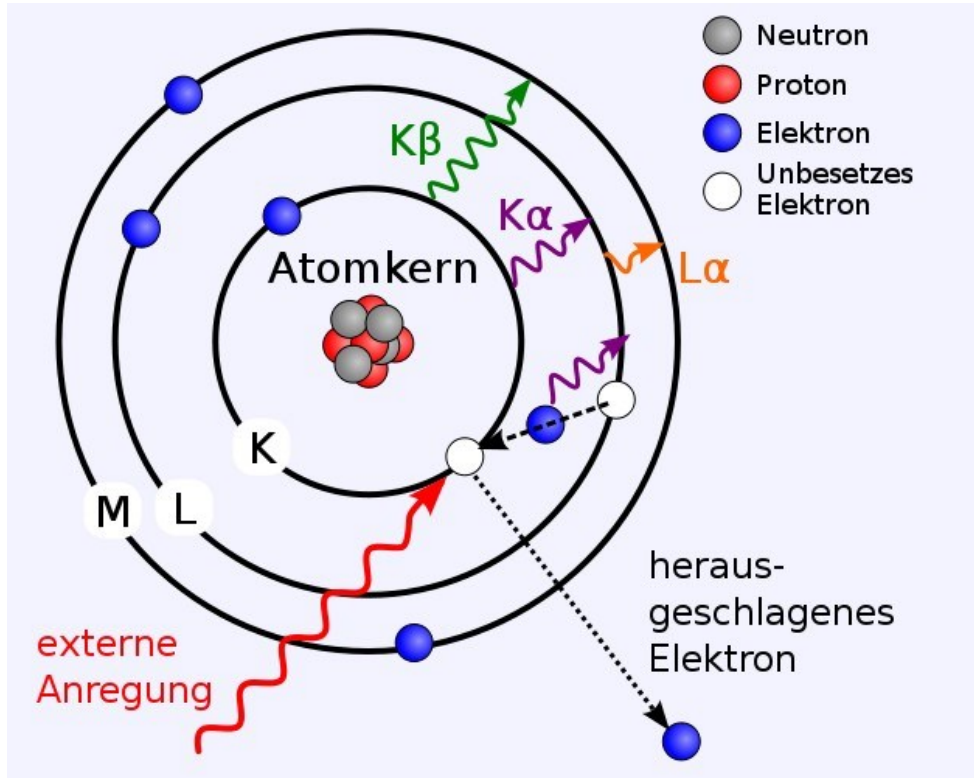
Coolidge Tube



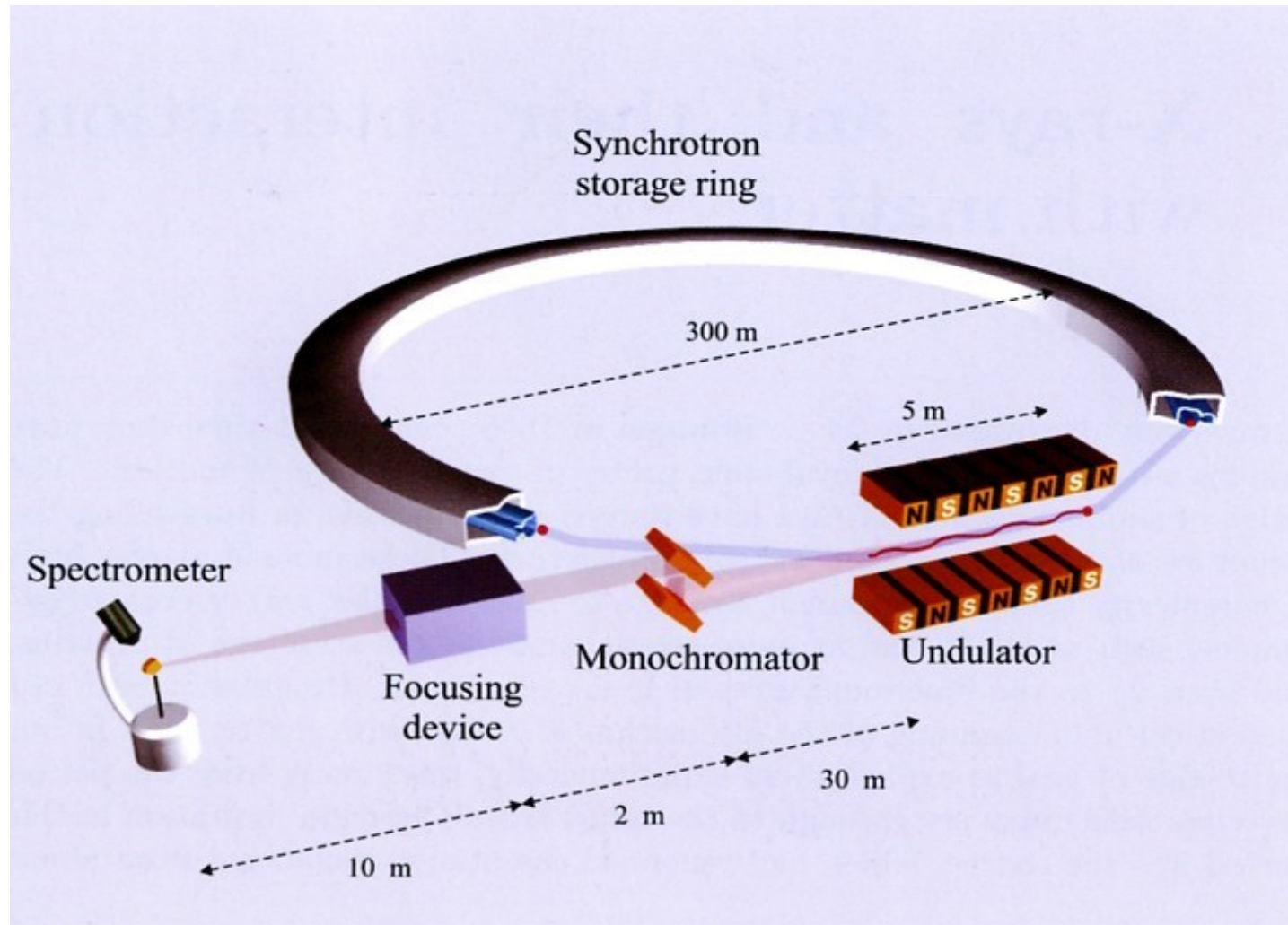
Rotating Anode



X-Ray Tube

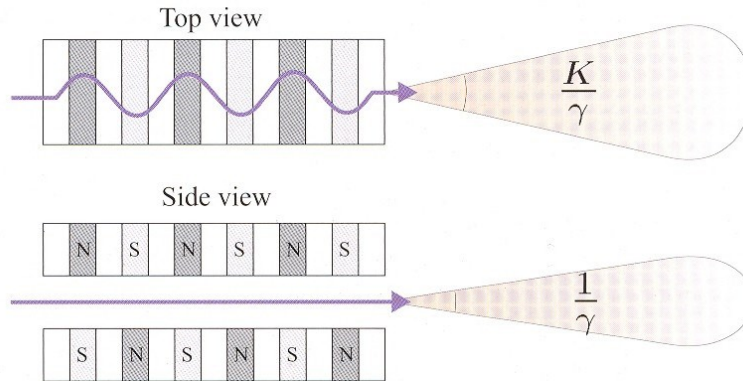


Synchrotron Radiation Storage Ring

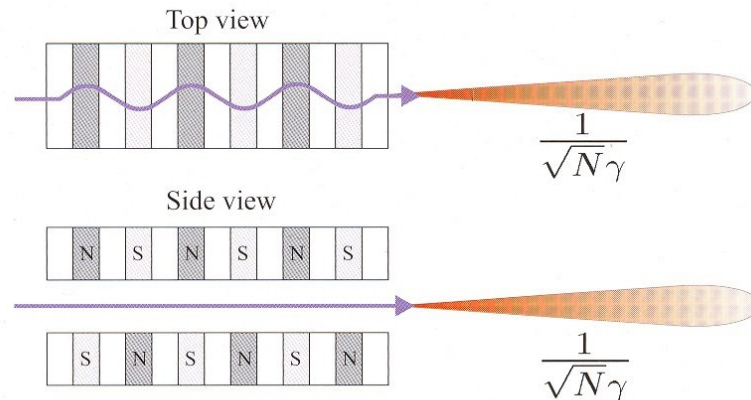


Insertion Devices (Wigglers and Undulators)

(a) Wiggler



(b) Undulator



Wiggler:

$$\begin{aligned}
 P[\text{kW}] &= 0.633 E_e^2 [\text{GeV}] B^2 [\text{T}] L [\text{m}] I [\text{A}] \\
 \text{Flux} &\sim E^2 \times N
 \end{aligned}$$

$$P[\text{kW}] = 0.633 E_e^2 [\text{GeV}] B^2 [\text{T}] L [\text{m}] I [\text{A}]$$

N: number poles

Undulator:

$$k = eB / mc \quad k_u = 0.934 \lambda_u [\text{cm}] B_0 [\text{T}]$$

with λ_u undulator period

undulator fundamental:

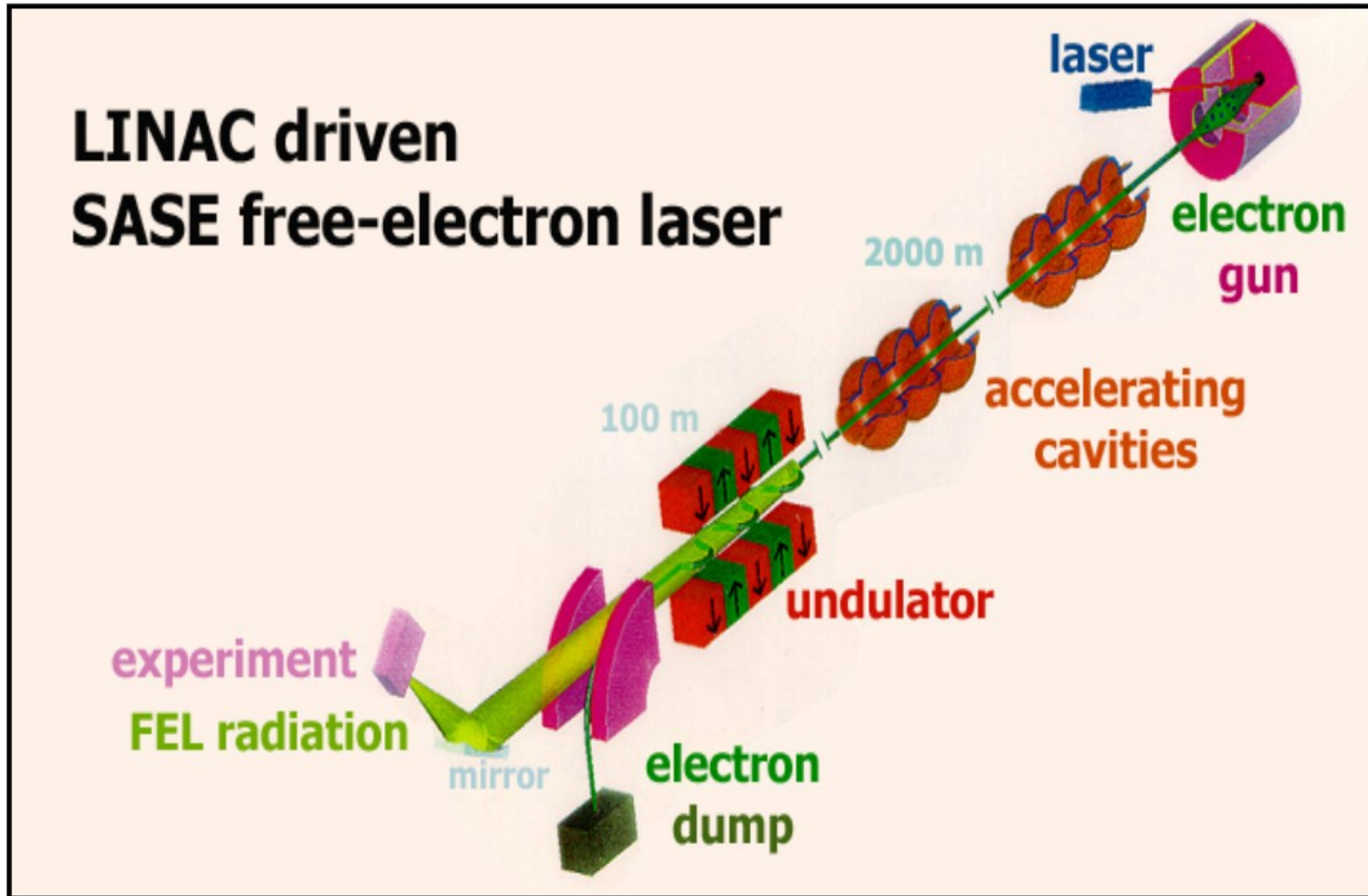
$$\lambda_0 = \frac{\lambda_u}{2\gamma^2} \left(1 + \frac{k^2}{2} + \gamma\theta \right)$$

~~on axis~~

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

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

Free Electron Lasers (FELs)



Methoden moderner Röntgenphysik II: Streuung und Abbildung

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**



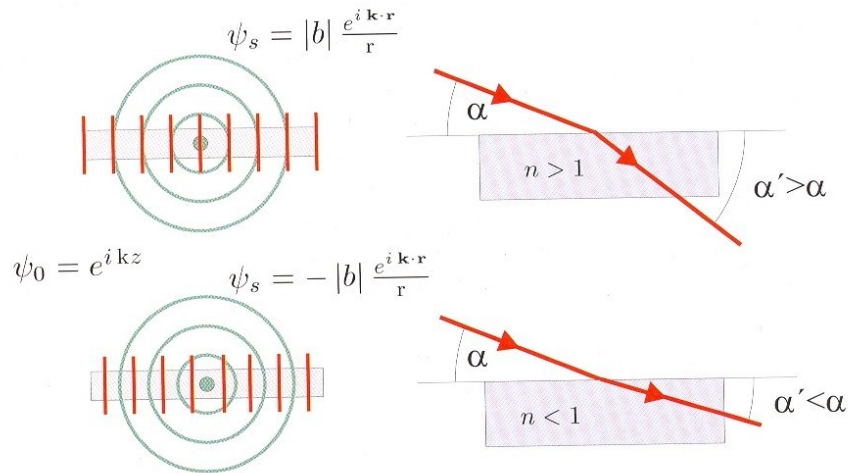
Kinematical Diffraction (I)

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Kinematical Diffraction (II)

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Reflection and Refraction from Interfaces



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

Governed by Snell's law:

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

$$\begin{aligned}
 n = n(\omega) \quad & 1.2 < n < 2 \text{ visible light} \\
 & n < 1 \text{ X-rays } (\alpha' < \alpha) \\
 & n = 1 - \delta \quad \delta \approx 10^{-5}
 \end{aligned}$$

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

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



Refractive Index

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).

$$\left. \begin{array}{l} \text{no slab: } e^{ik\Delta} \\ \text{slab: } e^{ink\Delta} \end{array} \right\} \text{phase difference: } e^{i(nk-k)\Delta}$$

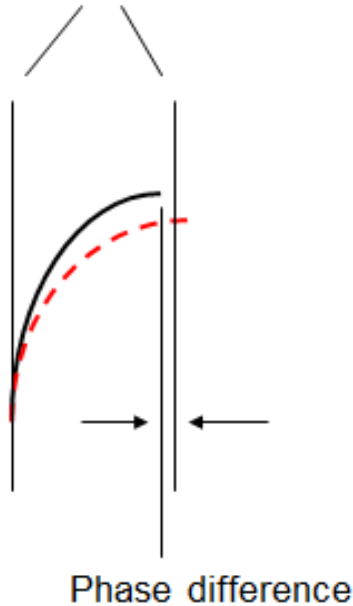
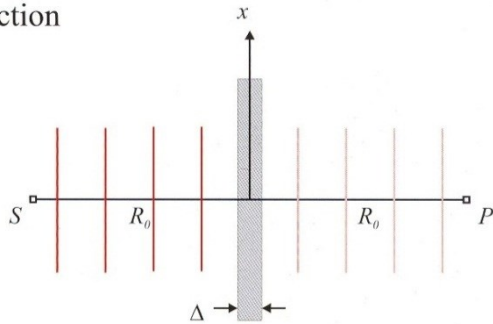
Amplitude:

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

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

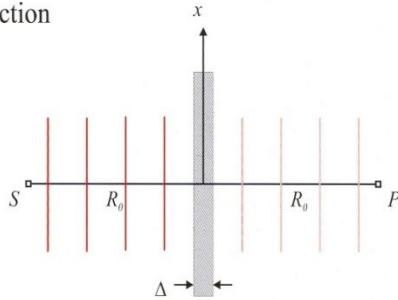
$$\psi_{\text{tot}}^P \approx \psi_0^P [1 + i k(n-1)\Delta] \quad (\$)$$

Refraction



Refractive Index

Refraction



Scattering picture:

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

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

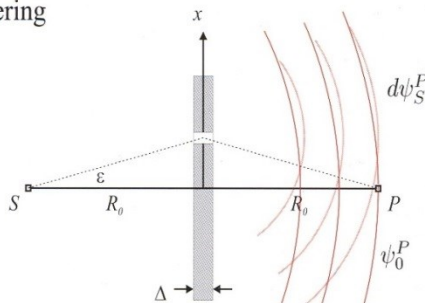
phase difference ($2kR$) between direct rays and rays following path R ;

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

Include y direction:

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

Scattering



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

$$d\psi_S^P = \left(\frac{e^{ikR_0}}{R_0}\right) \text{ incident wave}$$

$(\rho \Delta dx dy)$ number of scatterers

$(-b \frac{e^{ikR_0}}{R_0})$ spherical wave from one scatterer

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

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

Amplitude at P:

$$d\psi_S^P \approx$$

$$e^{\frac{ikR_0}{R_0}}$$

$$(\rho \Delta dx dy)$$

$$\left(b e^{\frac{ikR_0}{R_0}}\right)$$

$$e^{i\Phi(x,y)}$$

incident wave

number of scatterers in volume element $\rho dx dy$

scattered wave from 1 scatterer

phase factor

Refractive Index

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

[Ref. 1]

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

Amplitude at P without slab:

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

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

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

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

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

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

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

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

➔

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

$$k = \frac{2\pi}{\lambda} = 4\text{\AA}^{-1}, \quad b = r_0 = 2.82 \times 10^{-5}\text{\AA}, \quad \rho = \frac{1e^-}{\text{\AA}^3} : \delta \approx 10^{-5} \quad [\text{Ref. 1: Als-Nielsen and McMorow, p. 66}]$$



Critical Angle for Si

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

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

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

$$= 0.0025 \text{ rad}$$

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

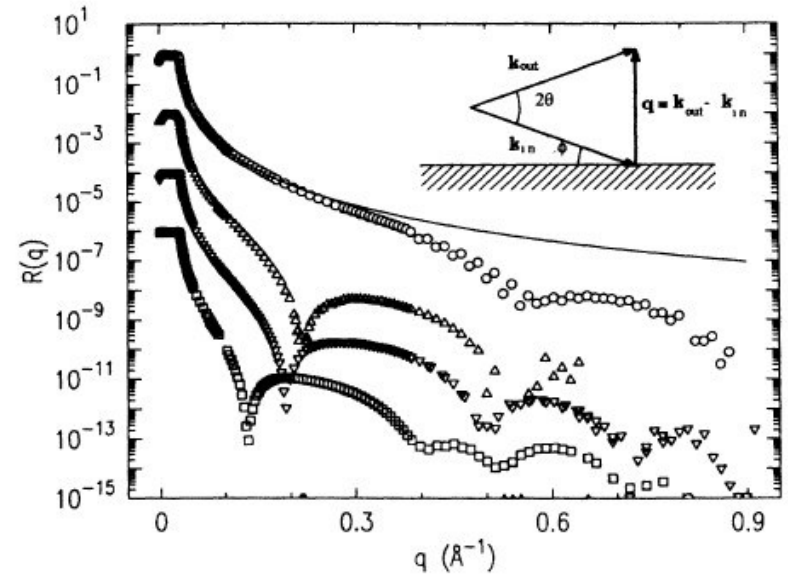
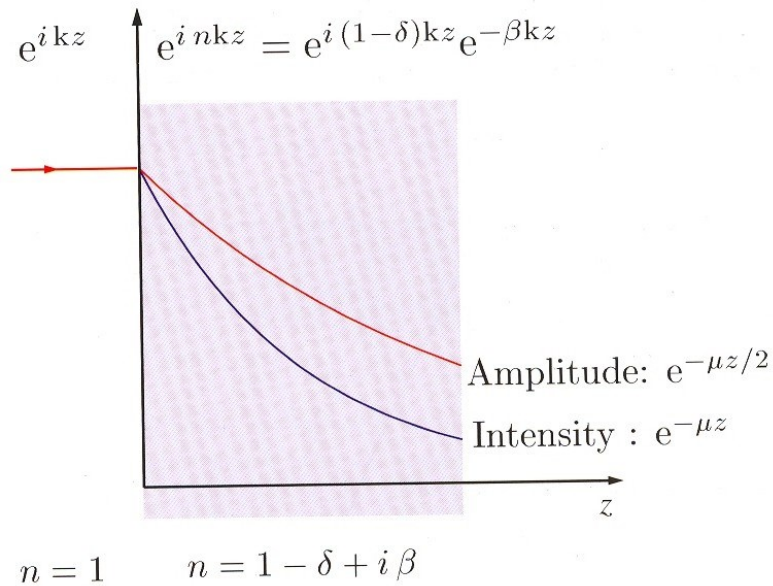


FIG. 1. Normalized reflectivity data from several samples. Successive data sets are displaced by 100 times and error bars omitted for clarity. (—) Theoretical reflectivity from an ideal step interface with bulk silicon density. (○) Uncoated silicon sample in helium; the “pairing” of points occurs for 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:

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

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

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

$$\parallel: a_I k \cos \alpha + a_R k \cos \alpha = a_T (nk) \cos \alpha' \quad (B')$$

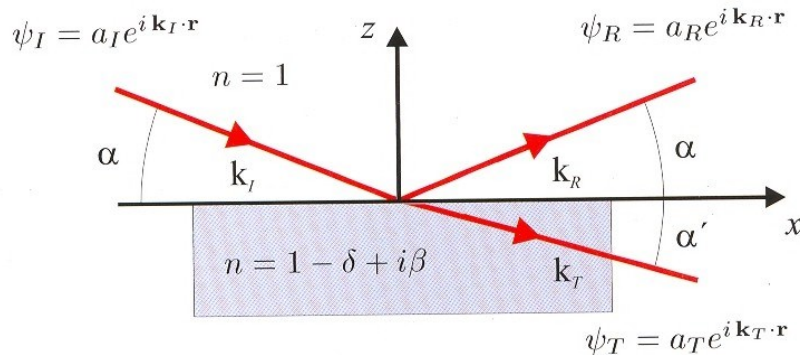
$$\perp: -(a_I - a_R) k \sin \alpha = -a_T (nk) \sin \alpha' \quad (B'')$$

$$\cos \alpha = n \cos \alpha' \quad (B'+A)$$

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

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

$$= \alpha'^2 + \alpha_c^2 - 2i\beta \quad (C)$$



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

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

$$a_I + a_R = a_T \quad (A)$$

Fresnel equations:

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

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

r: reflectivity

t: transmittivity



Snell's Law and the Fresnel Equations (2)

Note: α' is a complex number

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

Consider z-component of transmitted wave:

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

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

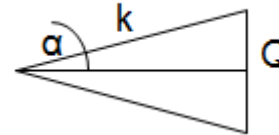
exponential damping

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

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

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

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:

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

$$q^2 = q'^2 + 1 - 2 i b_\mu \tag{D}$$

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

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



Snell's Law and the Fresnel Equations (3)

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

and calculate b_μ ($b_\mu \ll 1$):

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

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

Get:

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

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

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

	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

Snell's Law and the Fresnel Equations (4)

Fresnel equations:

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

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

$T \approx 1$,

no phase shift

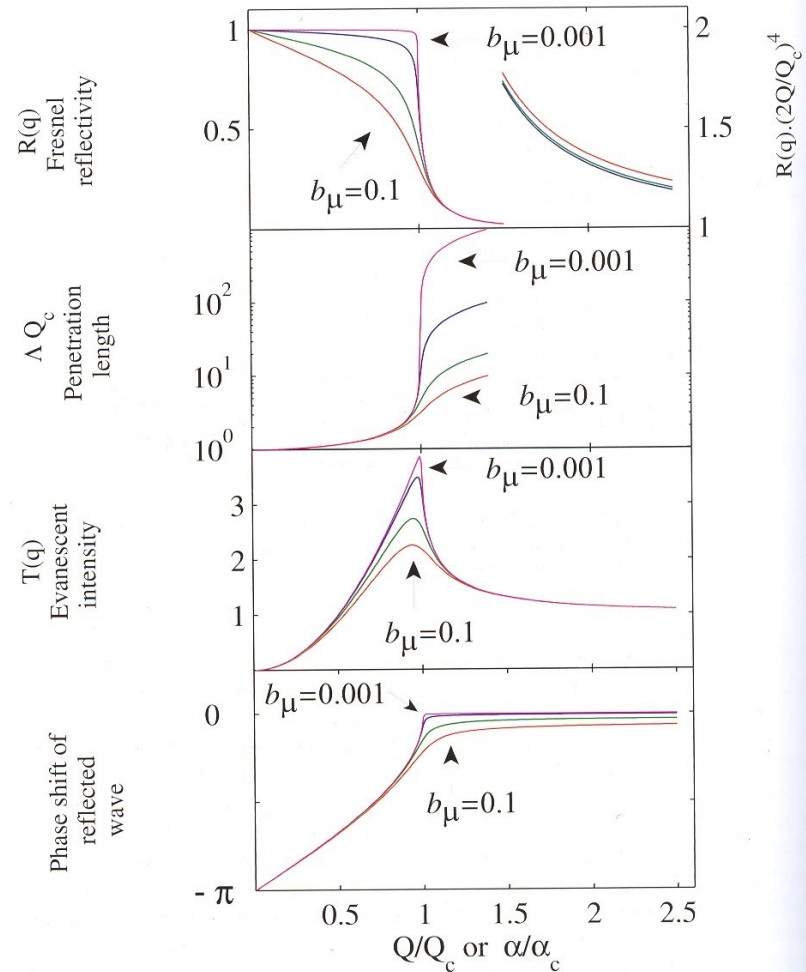
$q \ll 1$: $R \approx 1$,

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

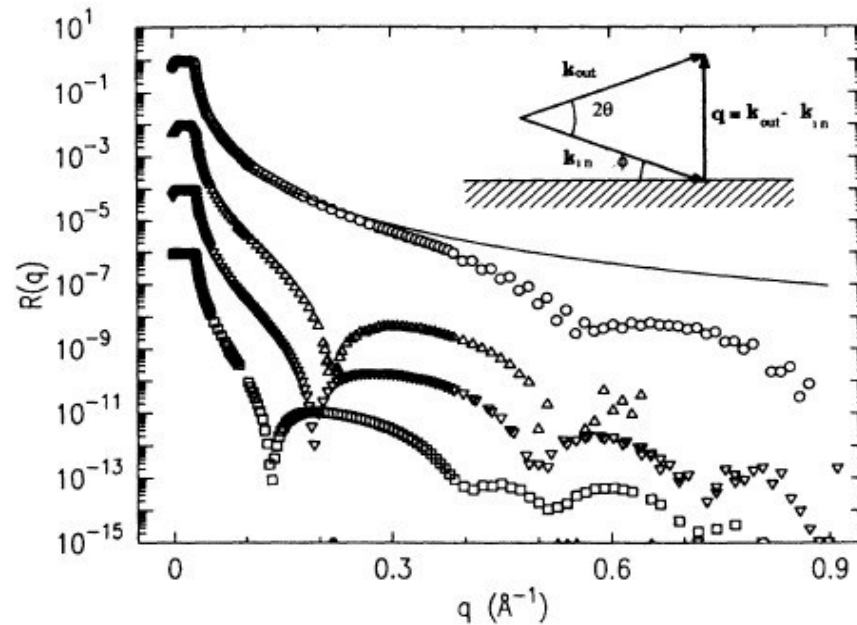
T very small,

$-\pi$ phase shift

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



Examples



PHYSICAL REVIEW B

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15 JANUARY 1990-1

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

I. M. Tidswell, B. M. Ocko,* and P. S. Pershan

Division of Applied Sciences and Department of Physics, Harvard University, Cambridge, Massachusetts 02138

S. R. Wasserman and G. M. Whitesides

Department of Chemistry, Harvard University, Cambridge, Massachusetts 02138

J. D. Axe

Department of Physics, Brookhaven National Laboratory, Upton, New York 11973

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

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