Methoden moderner Röntgenphysik: Streuung und Abbildung

Lecture 1	Vorlesung zum Haupt- oder Masterstudiengang Physik, SoSe 2021
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Location	online

Date	Tuesdays	12:30 - 14:00	(starting 6.4.)
	Thursdays	8:30 - 10:00	(until 8.7.)

Methoden moderner Röntgenphysik: Online Info

Tuesday Zoom-Meeting
https://desy.zoom.us/j/92674682486
Meeting ID: 926 7468 2486
Passcode: 144456

Thursday Zoom-Meeting
https://desy.zoom.us/j/99738625981
Meeting ID: 997 3862 5981
Passcode: 841881

Tutorial Zoom-Meeting
https://desy.zoom.us/j/95288979489
Meeting ID: 952 8897 9489
Passcode: 832350

Literature

Basic concepts:

Elements of Modern X-Ray Physics
J. A. Nielsen and D. McMorrow, J. Wiley&Sons (2001)

X-Ray Diffraction
B.E. Warren, DOVER Publications Inc., New York

Principles of Optics
M. Born and E. Wolf, Cambridge University Press, 7^{th} ed.

Soft X-rays and Extreme Ultraviolet Radiation
D. Attwood, Cambridge University Press (2000)
http://www.coe.berkeley.edu/AST/sxreuv/

Physik der Teilchenbeschleuniger und Synchrotronstrahlungsquellen
K. Wille, Teubner Studienbücher 1996

Lecture Notes

https://photon-science.desy.de/research/students__teaching/lectures__seminars/ss_20/index_eng.html

https://photon-science.desy.de/research/research_teams/coherent_x_ray_scattering/teaching/index_eng.html

Methoden moderner Röntgenphysik: 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 & Sources of X-rays +Synchrotron Radiation
Elements of X-ray Scattering, 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: Streuung und Abbildung

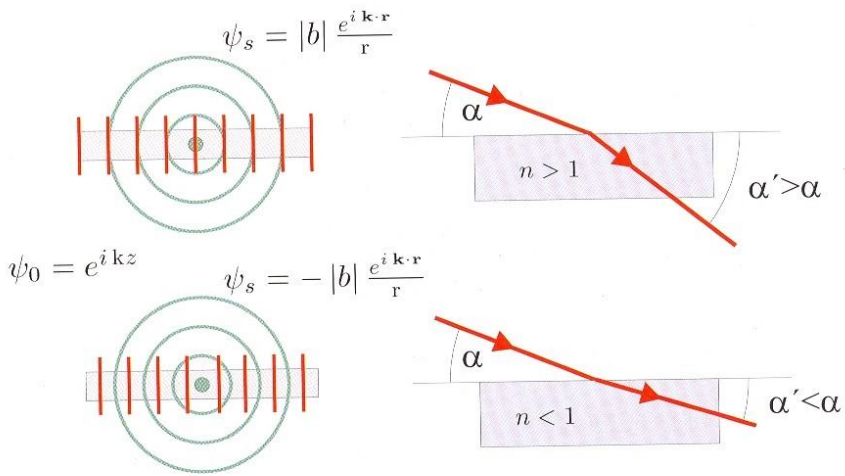
Small Angle Scattering, and Soft Matter
Introduction, Form Factor, Structure Factor, Applications, ...

Anomalous Diffraction
Introduction into Anomalous Scattering, ...

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

Coherent Scattering
Imaging and Correlation Spectroscopy, ...

Reflection and Refraction from Interfaces



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

<u>Governed by Snell's law:</u>

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

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

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

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

<u>Total external reflection:</u>

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

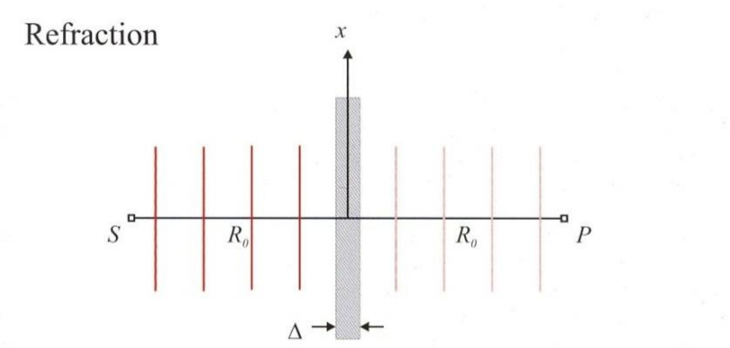
<u>Note</u>: spherical wave $e^{ik'r}$

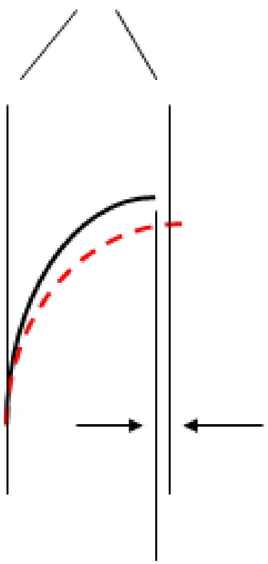
$$k' = nk = \left(\frac{n}{c}\right)\omega = \frac{\omega}{v}$$

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

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

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).

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

slab: $e^{ink\Delta}$

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

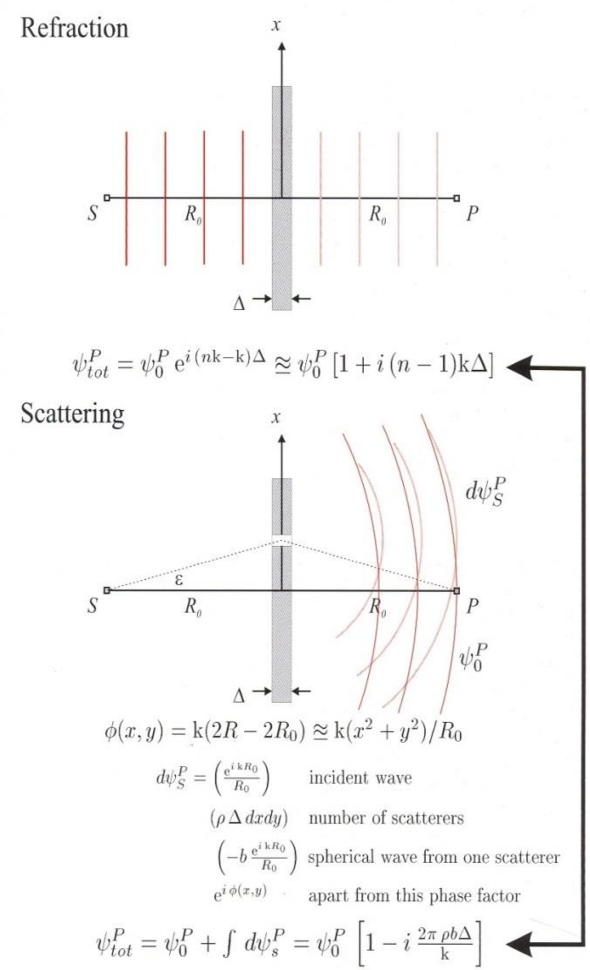
Amplitude: $\frac{\psi_{tot}^{P}}{\psi_{0}^{P}} = \frac{e^{ink\Delta}}{e^{ik\Delta}}$

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

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

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

Refractive Index



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:

$$d\psi_S^P \approx$$

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

incident wave

number of scatters in volume element $\rho dxdy$

scattered wave from 1 scatterer

phase factor

Refractive Index

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

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

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

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

Amplitude at P without slab:

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

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

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

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

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

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

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

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

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

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

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

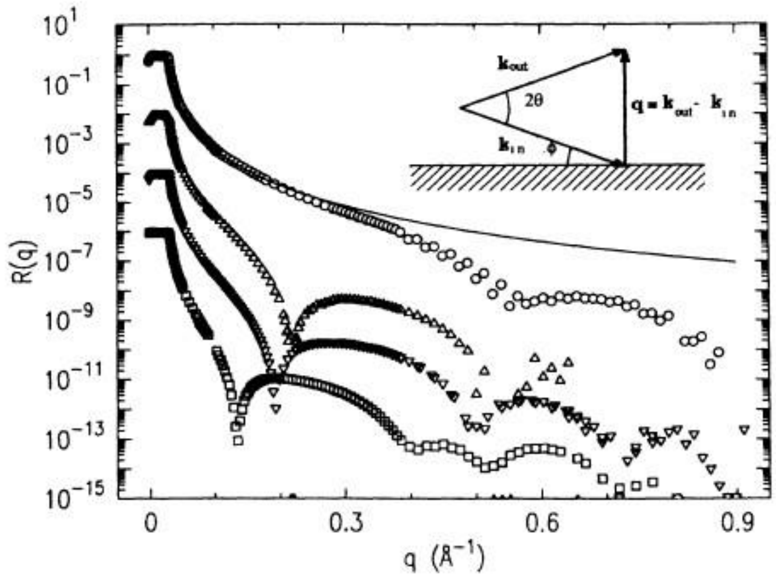
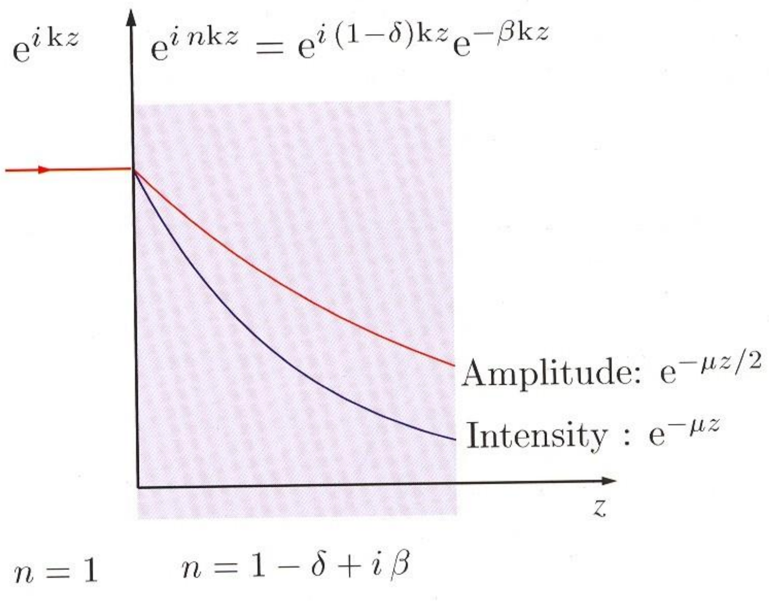


FIG. 1. Normalized reflectivity data from several samples. Successive data sets are displaced by 100 times and error bars omitted for clarity. (——) Theoretical reflectivity from an ideal step interface with bulk silicon density. (○) Uncoated silicon sample in helium; the "pairing" of points occurs for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

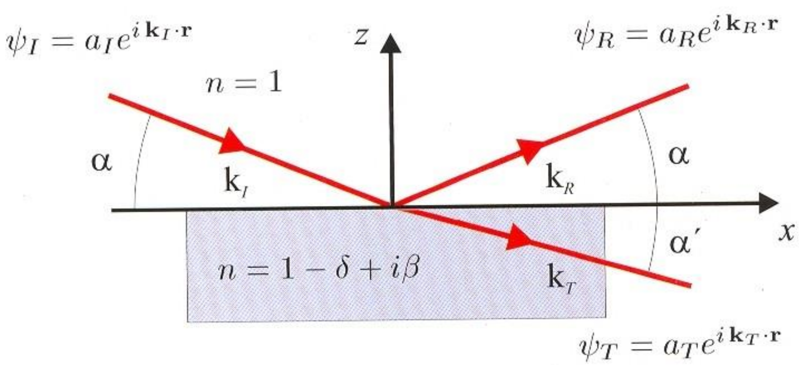
(when intensity drops according to $e^{-\mu z}$)

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

Snell's Law and the Fresnel Equations

Snell's Law and the Fresnel Equations

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



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

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

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

$\underline{\alpha, \alpha' \text{small}}$: $\left(\cos z = 1 - \frac{z^2}{2}\right)$

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

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

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

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

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

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

Fresnel equations:

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

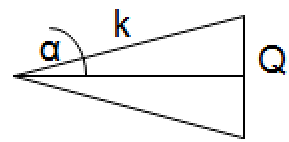
r: reflectivity **t: transmittivity**

Snell’s Law and the Fresnel Equations (2)

Note: α' is a complex number

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

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

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

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

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

use dimensionless units:

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

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

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

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

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:

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

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

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

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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

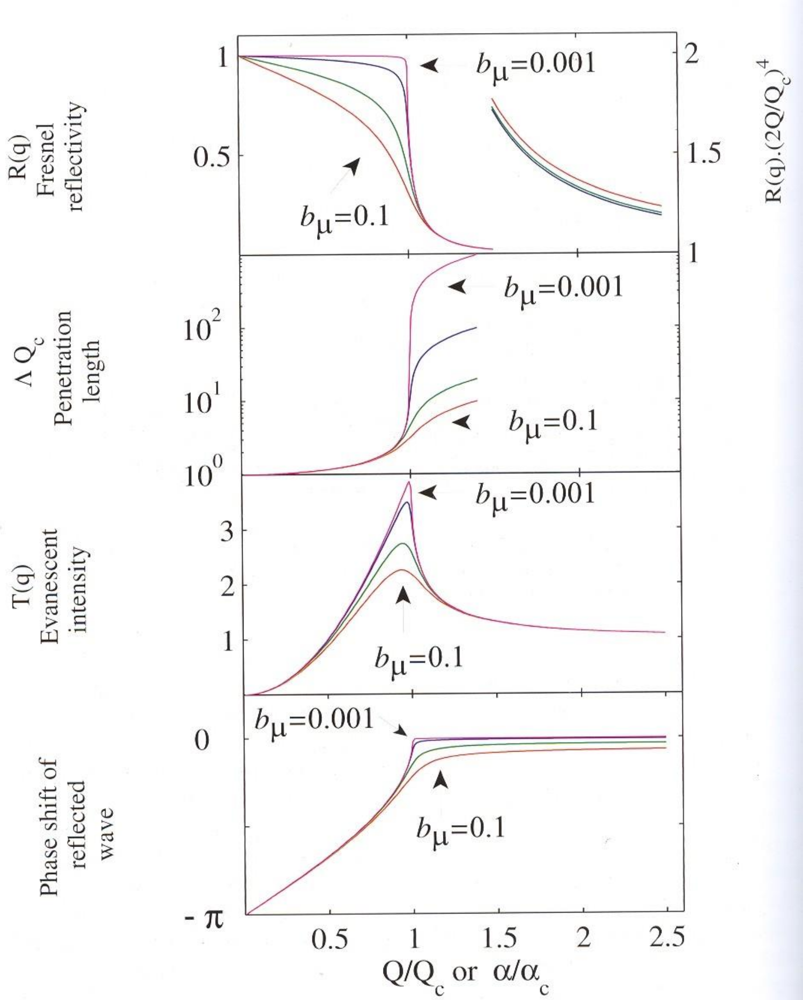
q ≪ 1: $R \approx 1$,

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

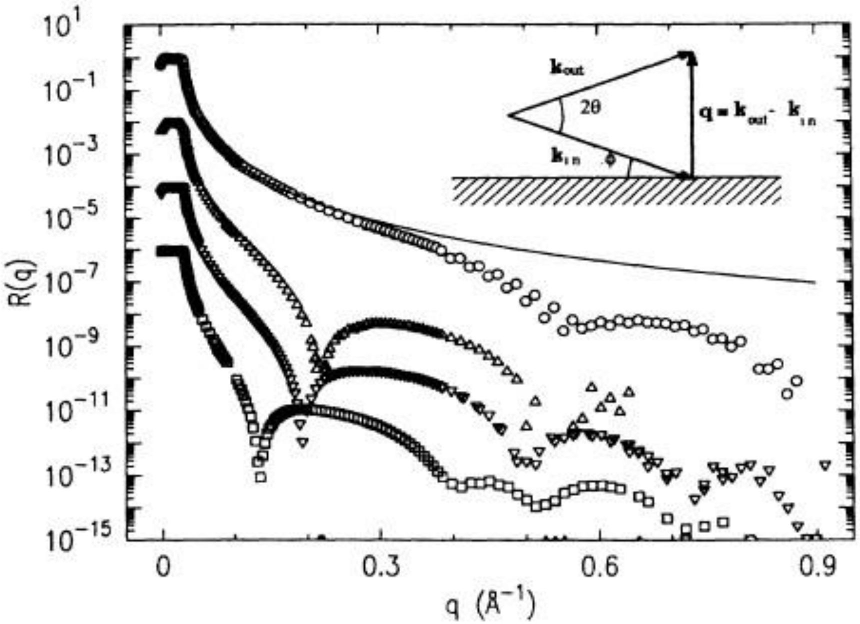
T very small ,

$-\pi$ 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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