Methoden moderner Röntgenphysik II: Streuung und Abbildung

Lecture 4

Vorlesung zum Haupt/Masterstudiengang Physik

SS 2013

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Location: Hörs AP, Physik, Jungiusstrasse

Tuesdays 12.45 – 14.15

Thursdays 8:30 – 10.00

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
Snell's law, Fresnel equations,

Kinematical Diffraction (I)
Diffraction from an atom, molecule, 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,..

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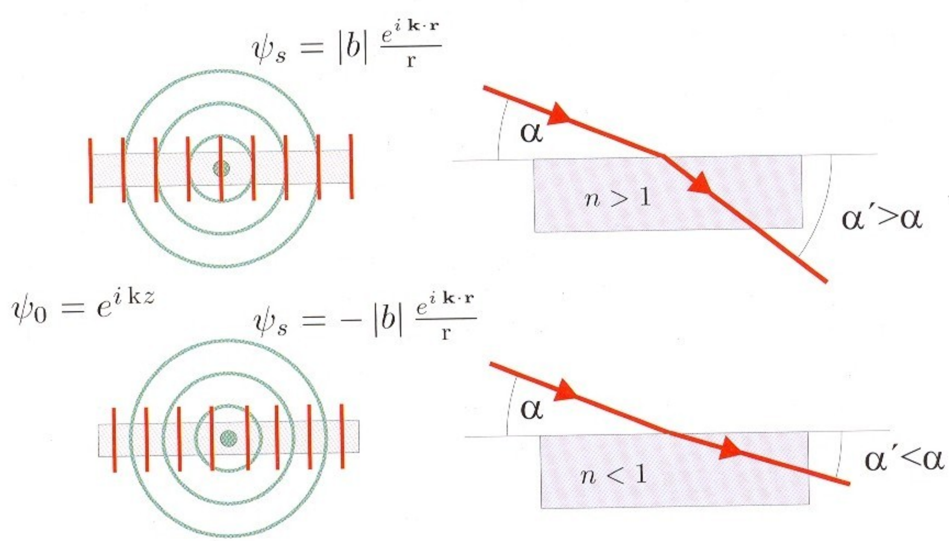
Refraction and Reflexion from Interfaces

Refraction and Reflexion from Interfaces



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

Governed by Snell's law:

cosα / cosα' = n (refractive index)

n = n(ω)   1.2 < n < 2 visible light

n < 1 X-rays (α' < α)

n = 1-δ $\delta \approx 10^{-5}$

Note: spherical wave exp(ik'r)

k' = nk =(n/c)ω = ω/v

with v=c/n phase velocity

(v>c for n<1; but group velocity dω/dk ≤ c)

total external reflexion:

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

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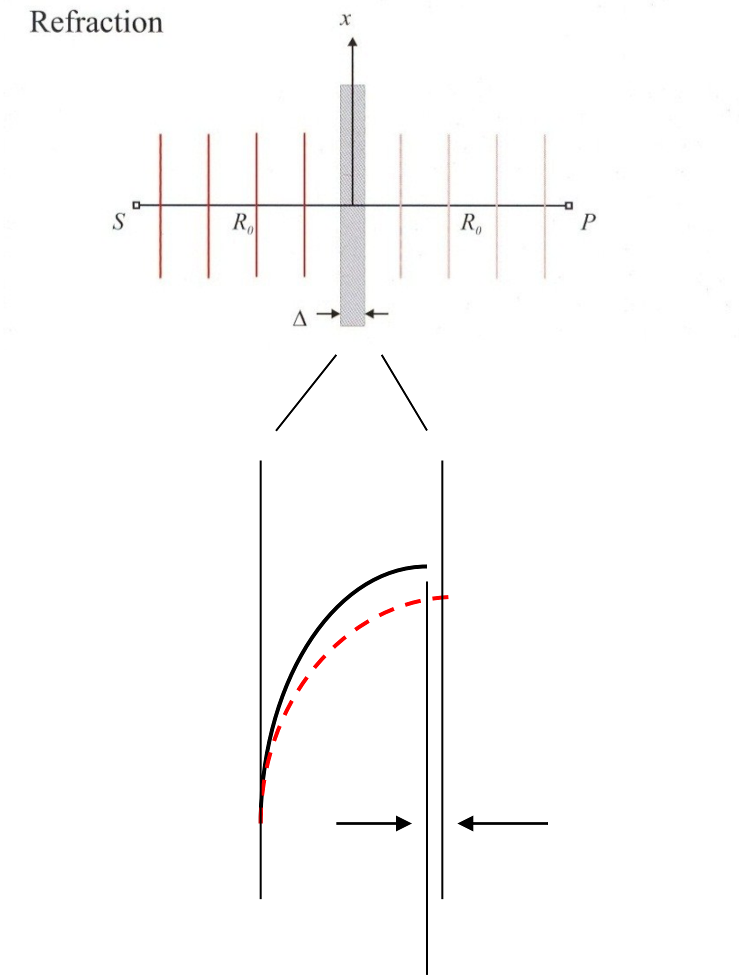
- # Refractive Index



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: exp(ikΔ)
slab: exp(inkΔ)

phase difference: exp(i(nk-k)Δ)

amplitude:

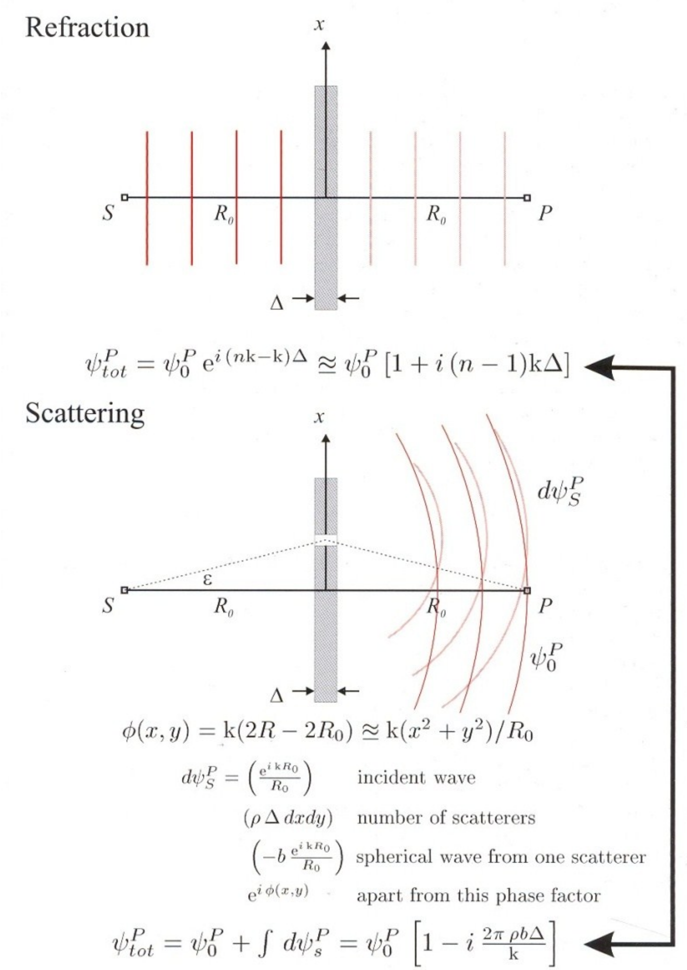
$$\psi_{tot}^P / \Psi_0^P = \exp(ink\Delta) / \exp(ik\Delta)$$

$$= \exp(i(nk-k)\Delta)$$

$$\exp(i\alpha) = \cos\alpha + i\sin\alpha \xrightarrow[\alpha \text{ small}]{} 1+i\alpha$$

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

Refractive Index



Scattering picture:

$R = \mathrm{sqrt}(Ro^2+x^2) = \mathrm{sqrt}[Ro^2(1+x^2/Ro^2)]$

$\approx Ro\ \mathrm{sqrt}[1+x^2/Ro^2 + x^4/4Ro^4]$

$= Ro\ \mathrm{sqrt}\{[1+x^2/2Ro^2]^2\} = Ro[1 + \mathbf{x^2/2Ro^2}]$

phase difference (2kR) btw. direct rays and rays following path R;

$2k\mathbf{x^2}/2Ro = k\mathbf{x^2}/Ro$

include y direction:

$\exp(i\,\Phi(x,y)) = \exp(i(\mathbf{x^2}+\mathbf{y^2})k/Ro$

amplitude at P:

$d\psi_S^P \approx$

$\exp(ikRo)/Ro)\ (\rho\Delta dxdy)\ (b\exp(ikRo)/Ro)\ \exp(i\Phi(x,y))$

phase factor

incident wave

number of scatters in volume element ρdxdy

scattered wave from 1 scatterer

Refractive Index

$$\Psi_S^P = \int d\Psi_S^P = -\rho b\Delta\{\exp(i2kRo)\}/Ro^2 \bullet \frac{\int \exp(i\Phi(x,y)dxdy}{} \quad [1]$$

$i\pi Ro/k$ *[Ref.1]*

Amplitude at P without slab:

$$\Psi_o^P = \{\exp(ik2Ro)\}/2Ro \quad [2]$$

$$\Psi_{tot}^P = [1]+[2] = \Psi_o^P\,[1 - i2\pi\rho b\Delta/k\,] \equiv$$

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

➔ $n = 1 - 2\pi\rho b/k^2 = 1 - \delta$

$k=2\pi/\lambda=4Å\text{-}1$, $b=ro=2.82\times10^{-5}Å$, $\rho=1e^-/Å^3$: $\delta \approx 10^{-5}$

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

$$\rho = \rho_a f^{\,0}(0)$$

Number density x atomic scattering factor

$$\delta = 2\pi\rho_a f^0(0) r_0/k^2$$

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

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

$$\cos\alpha_c = 1 - \delta = 1 - \alpha_c^2/2$$

$$\alpha_c = \mathrm{sqrt}(2\delta) = \mathrm{sqrt}\,(4\pi\rho r_0/k^2)$$

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

critical angle for Si

$\alpha_c = \mathrm{sqrt}(2\delta) = \mathrm{sqrt}\,(4\pi\rho r_0/k^2)$

<u>Silicon:</u> $\rho = 0.699$ e-/Å^3, $\lambda = 1$Å

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

$= 0.0025$ rad

$Q_c = (4\pi/\lambda)\,\sin\alpha_c = 0.032$ Å^{-1}

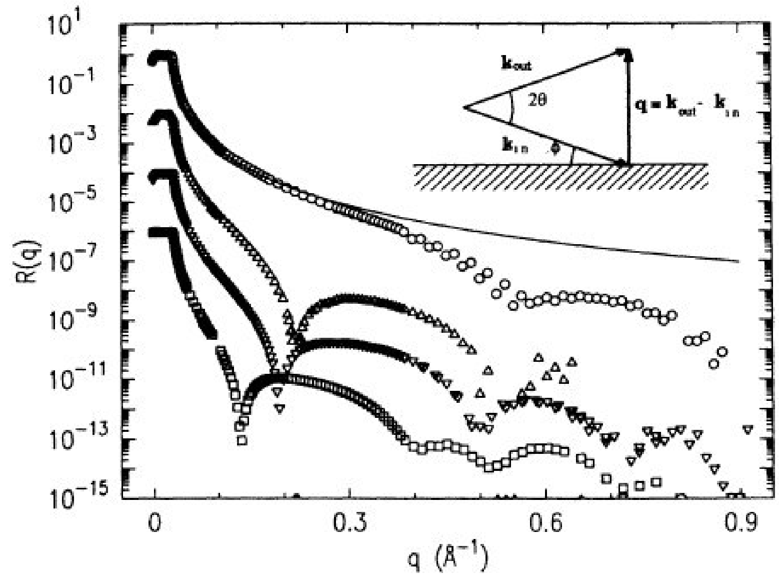
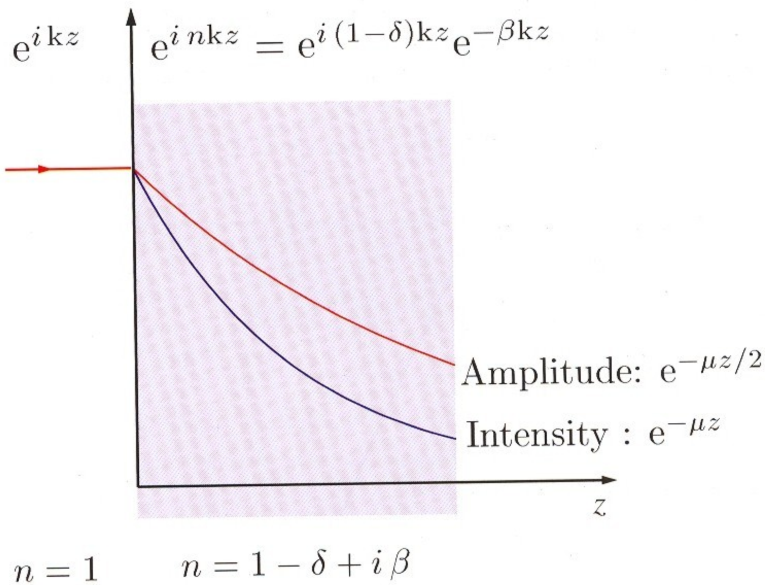


FIG. 1. Normalized reflectivity data from several samples. Successive data sets are displaced by 100 times and error bars omitted for clarity. (——) Theoretical reflectivity from an ideal step interface with bulk silicon density. (○) Uncoated silicon sample in helium; the "pairing" of points occurs for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

wave propagating in a medium:

exp(inkz) = exp(i(1-δ)kz exp(-ßkz)

attenuation of amplitude: exp (-μz/2)

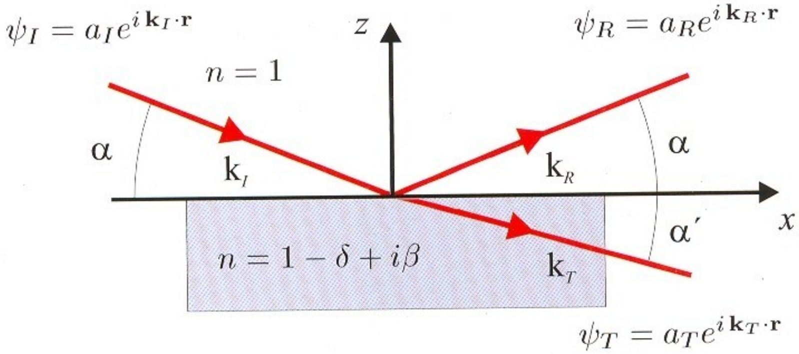
(when intensity drops according to exp(-μz))

ß = μ/2k

Snell's law and the Fresnel equations

Snell's law and the Fresnel equations

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



$|\mathbf{k}_T| = nk$

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

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

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

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

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

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

<u>α, α' small:</u> $(\cos z = 1 - z^2/2)$

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

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

<u>Fresnel equations:</u>

$$r = a_R / a_I = (\alpha - \alpha') / (\alpha + \alpha')$$

$$t = a_T / a_I = 2\alpha / (\alpha + \alpha')$$

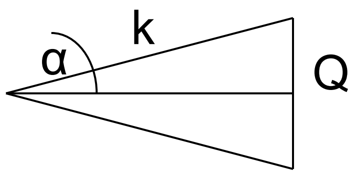
r: reflectivity t: transmittivity

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:



$\sin\alpha = (Q/2)/k$

Consider z-component of transmitted wave:

$= a_T \exp(ik\sin\alpha' z) \approx a_T \exp(ik\alpha' z)$

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

exponential damping

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

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

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

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

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

use dimensionless units:

$q \equiv Q/Qc \approx (2k/Q_c)\alpha$

$q' \equiv Q'/Qc \approx (2k/Q_c)\alpha'$

$$q^2 = q'^2 + 1 - 2ib_u \qquad \text{(D)}$$

$b_u = (2k/Q_c)\beta = (4k^2/Q_c^2)\mu/2k = 2k\mu/Q_c^2$

$Q_c = 2k\alpha_c = 2k\,\mathrm{sqrt}(2\delta)$

Snell's law and the Fresnel equations (3)

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

and calculate b_u ($b_u \ll 1$):

	Z	Molar density (g/mole)	Mass density (g/cm^3)	ρ ($e/\text{Å}^3$)	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

$$b_u = 2k\mu / Q_c^2$$

use (D): $q^2 = q'^2 + 1 - 2\,i b_u$

get:

$$r(q) = (q - q') / (q + q')$$

$$t(q) = 2q / (q + q')$$

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

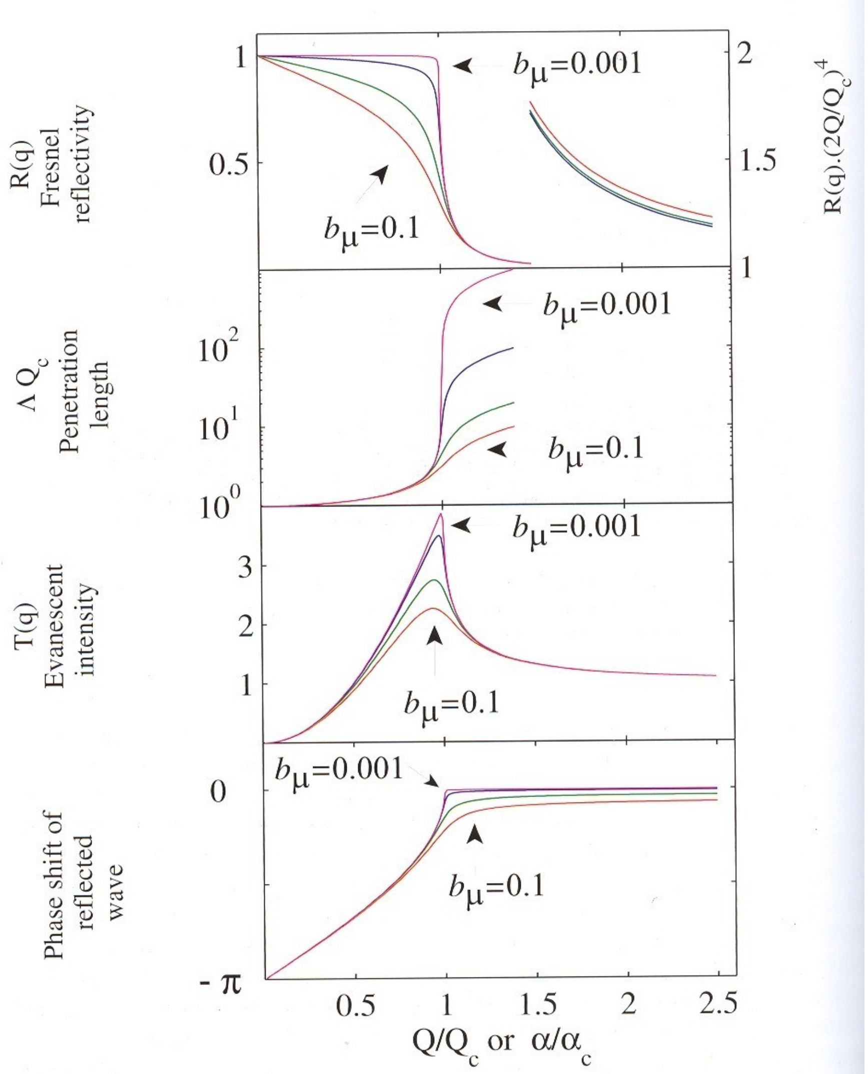
Snell's law and the Fresnel equations (4)

Fresnel equations:

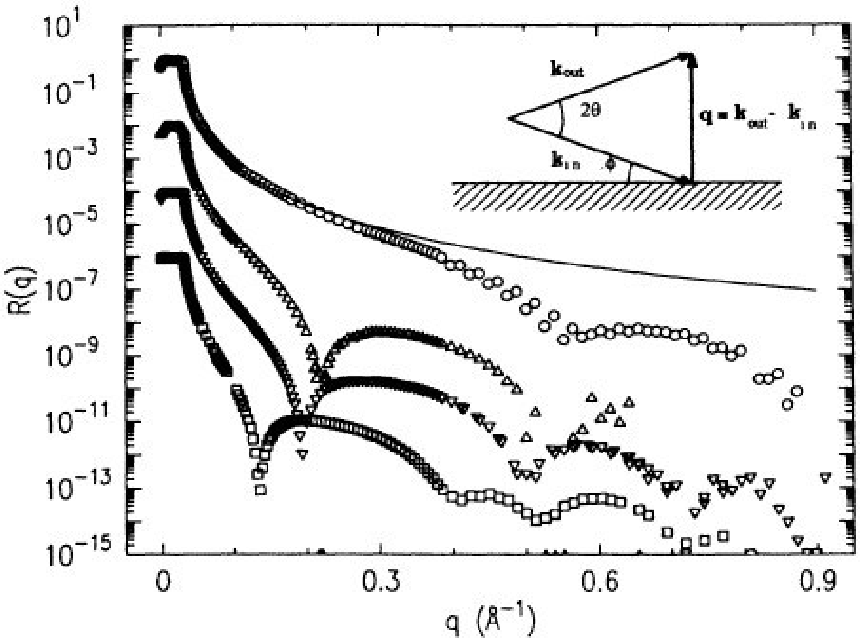
q>>1: $R(Q) \sim 1/q^4$,
$\Lambda \approx \mu^{-1}$,
$T \approx 1$,
no phase shift

q<<1: $R \approx 1$,
$\Lambda \approx 1/q_c$ small,
T very small,
$-\pi$ phase shift

q=1: $T(q=1) \approx 4\, a_l$



▪ Examples



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

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