Methoden moderner Röntgenphysik I: Struktur und Dynamik kondensierter Materie

Vorlesung zum Haupt/Masterstudiengang Physik

WS 2008/9

G. Grübel, M. Martins, E. Weckert et al.

Location: SemRm 4, Physik, Jungiusstrasse

Thursdays 10.15 – 11.45

G.Grübel (GG), A.Meents (AM), C. Gutt (CG), S. Roth (SR)

Methoden moderner Röntgenphysik I: Struktur und Dynamik kondensierter Materie

Hard X-Rays - Sources of X-rays, refraction & reflexion

Lecture 2

23.10.	Introduction	(GG)
30.10.	Sources of X-rays, Refraction and Reflexion	(GG)
6.11.	Kinematical Scattering Theory	(GG)
13.11.	Small Angle and Anomalous Scattering	(GG)
20.11. - 11.12.	Modern Crystallography	(AM)
18.12. - 15. 1.	Coherence base techniques	(CG)
22. 1. - 5. 2.	Soft Matter Applications	(SR)

Coherence of light and matter I: from basic concepts to modern applications

Introduction into X-ray physics: 23.10.-13.11.

Introduction

Overview, Introduction to X-ray Scattering (Scattering from atoms, crystals,.., absorption, reflection,coherence,..)

Sources, Reflection and Refraction

Sources of X-rays, Refraction, reflection, Snell’s law, Fresnel equations

Kinematical Diffraction

Diffraction from an atom, molecule, crystal, reciprocal lattice, structure factor,..

SAXS, Anomalous Diffraction

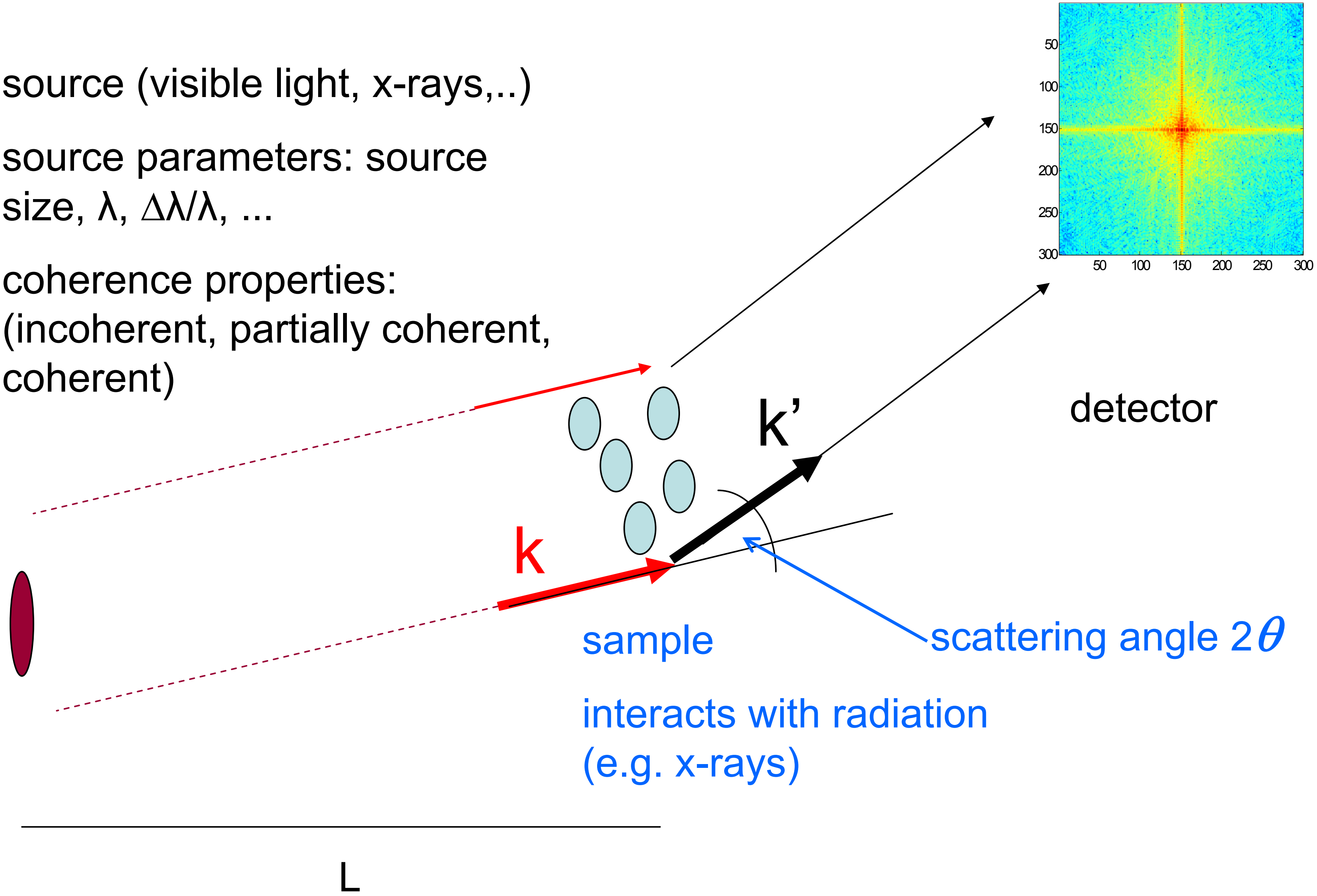
Introduction into small angle scattering and anomalous scattering

Experimental Set-Up for Scattering Experiments

source (visible light, x-rays,..)

source parameters: source size, λ, Δλ/λ, ...

coherence properties: (incoherent, partially coherent, coherent)



sample

scattering angle 2θ

interacts with radiation (e.g. x-rays)

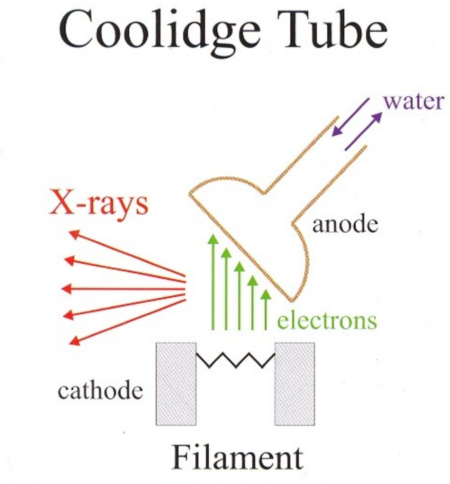
Sources of X-Rays

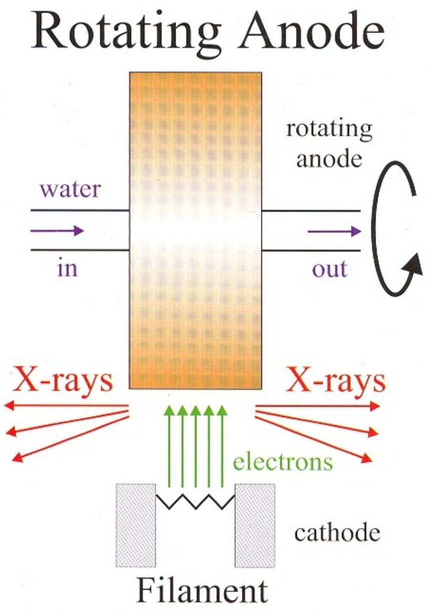
1895 discovered by W.C. Röntgen

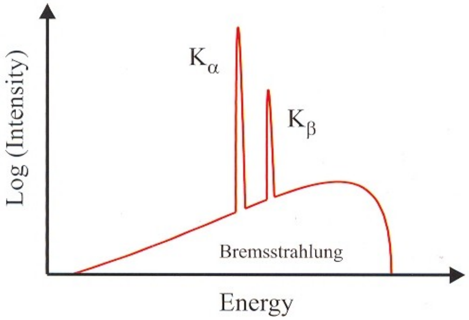
1912 First diffraction experiment (v. Laue)

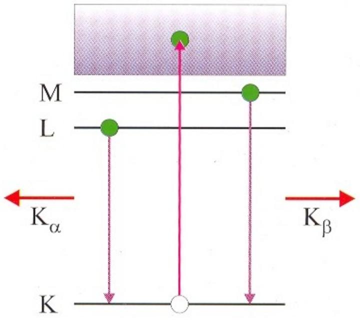
1912 Coolidge tube (W.D. Coolidge,GE)

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

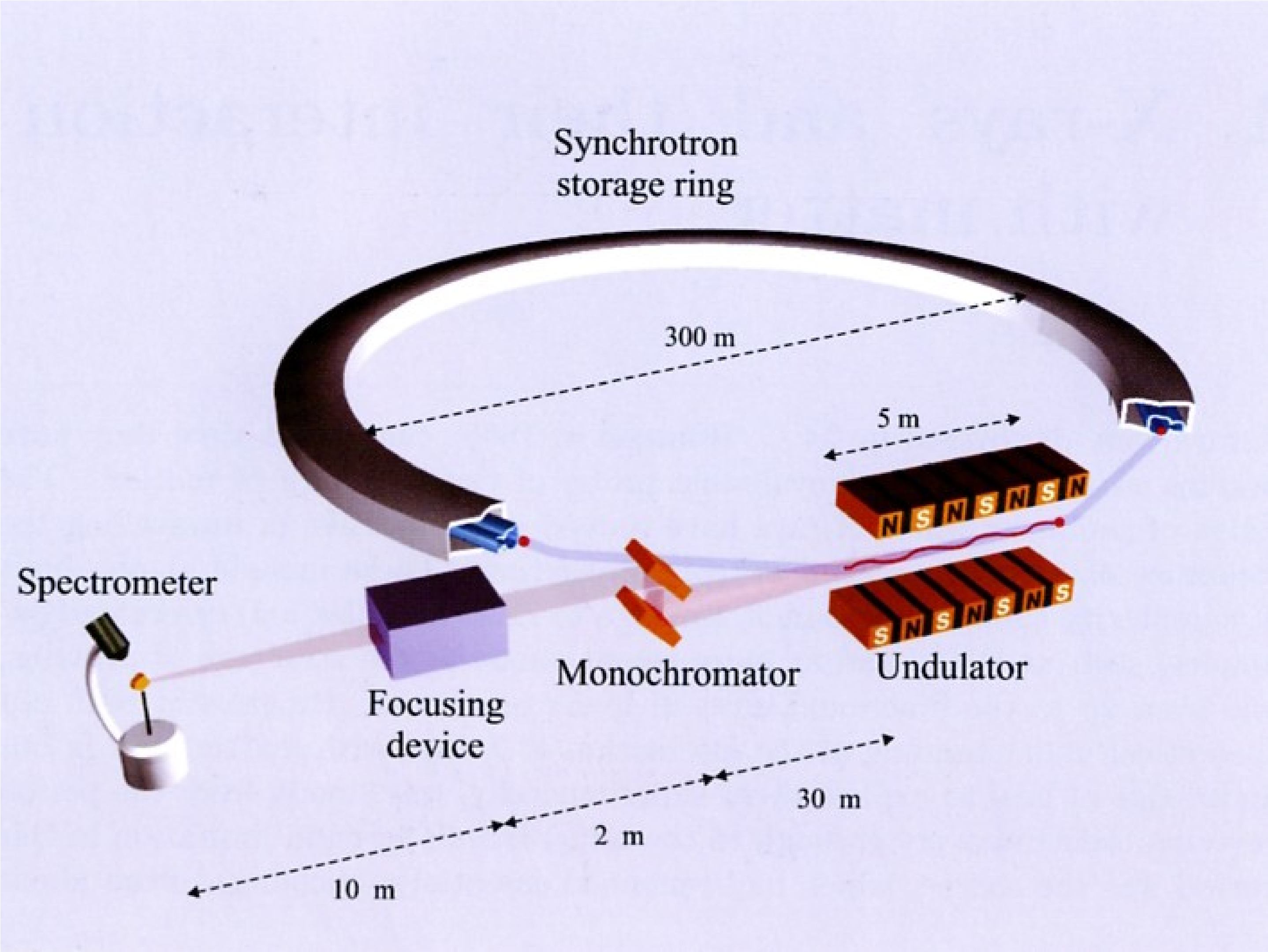

Coolidge Tube


Rotating Anode



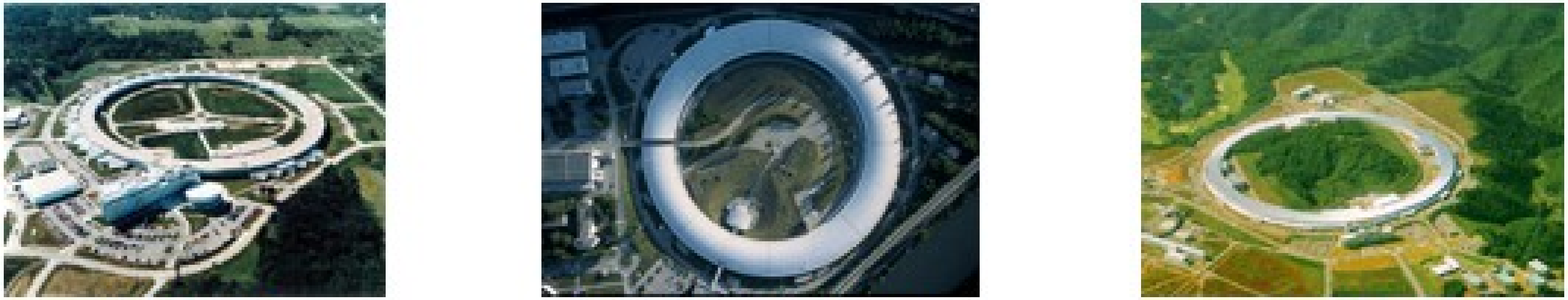


Synchrotron Radiation Storage Ring



Photos machines

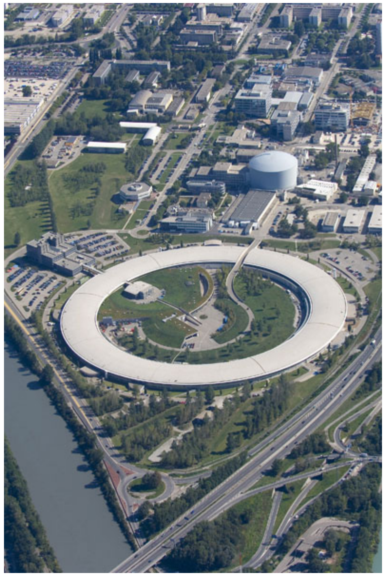
The three largest and most powerful synchrotrons in the world



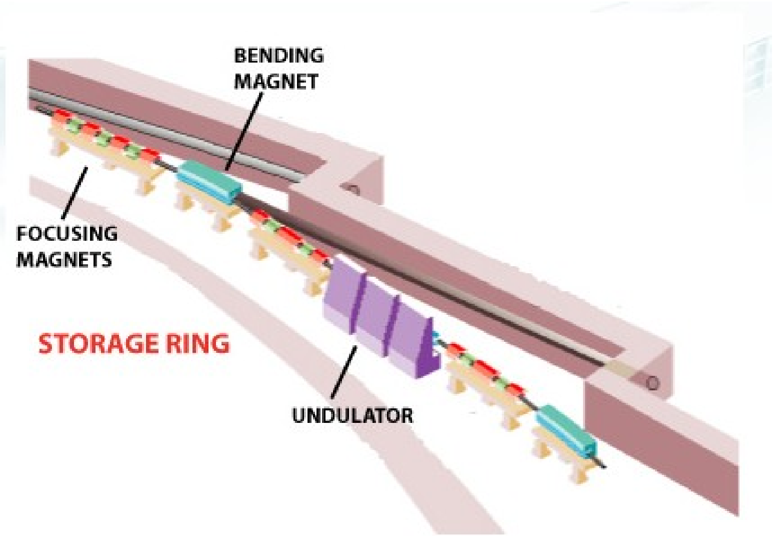
APS, USA

ESRF, Europe-France

Spring-8, Japan



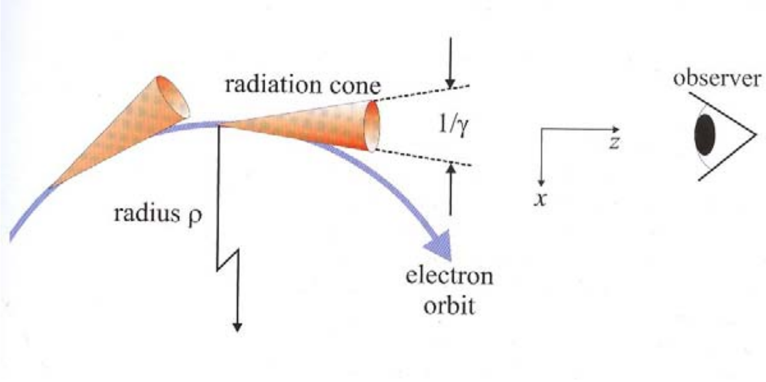
Synchrotron Radiation Primer



Energy E_e of an electron at speed v:

$$E_e = mc^2/\mathrm{sqrt}\{(1-(v/c)^2\} = \gamma\, mc^2$$

For 5GeV and mc^2=0.511 MeV get $\gamma \approx 10^4$



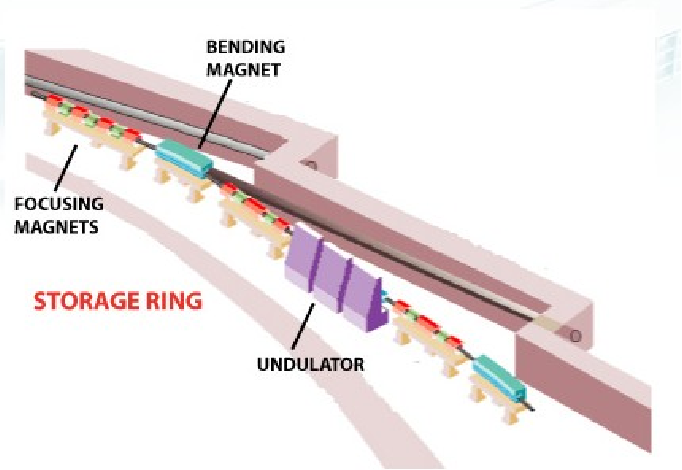
Centrifugal=Lorentz force yields for radius:

$\rho = \gamma mc /eB = 3.3\ E[\mathrm{GeV}]/B[\mathrm{T}] \approx 25$ m

$E_e \approx 6$ GeV, B=0.8 T

Opening angle is of order $1/\gamma \approx 0.1$ mrad

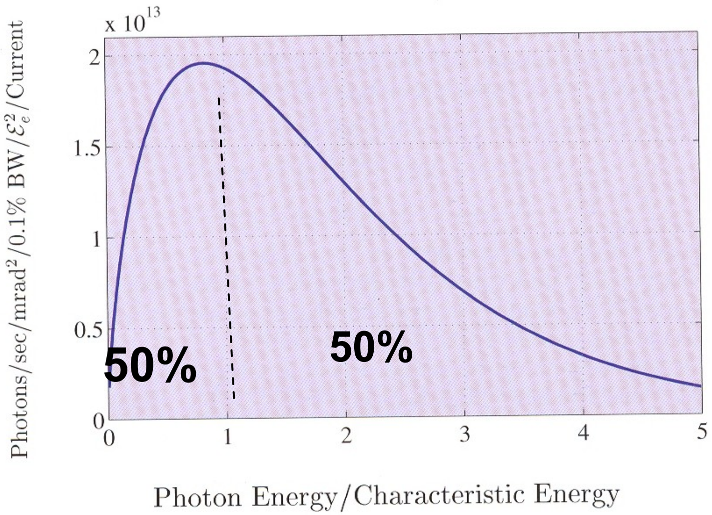
Bending magnets



<u>Characteristic energy $\hbar\omega_c$ for bend or wiggler:</u>

$\hbar\omega_c$ [keV] = 0.665 E_e^2[GeV] B(T) ≈20 keV

Flux ~ E^2



<u>Energy loss by synchrotron radiation per turn:</u>

ΔE [keV] = 88.5 E^4[GeV]/ρ[m]

For 1 GeV and ρ=3.33 m: ΔE =26.6 keV/turn

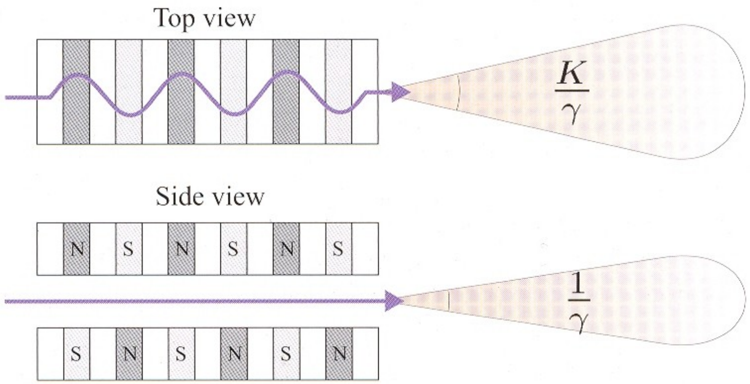
For I=500 mA ≡ 0.5 Cb/s =0.5x6.25x10^{18} e^-/s

➔P= 0.5x6.25x10^{18} e^-/sx26.6 keV

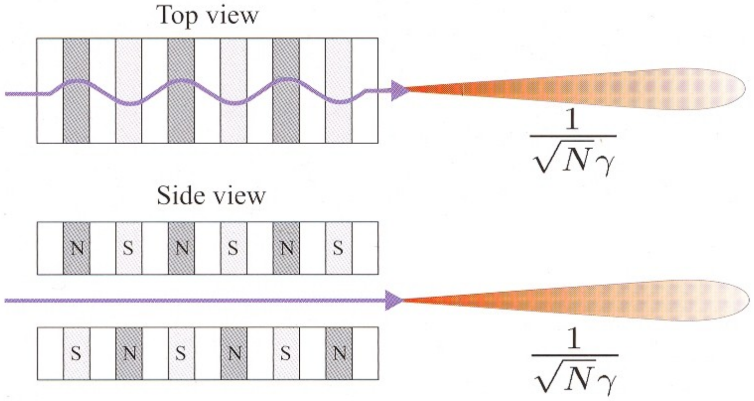
=8.3125x10^{22}x1.6x10^{-19} = 13.3 KJ/s =13.3 KW

Insertion Devices (wigglers and undulators)

(a) Wiggler



(b) Undulator



<u>Wiggler:</u>

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

Flux ~ $E^2 \times N$

N: number poles

<u>Undulator:</u>

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

with λ_u undulator period

<u>undulator fundamental:</u>

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

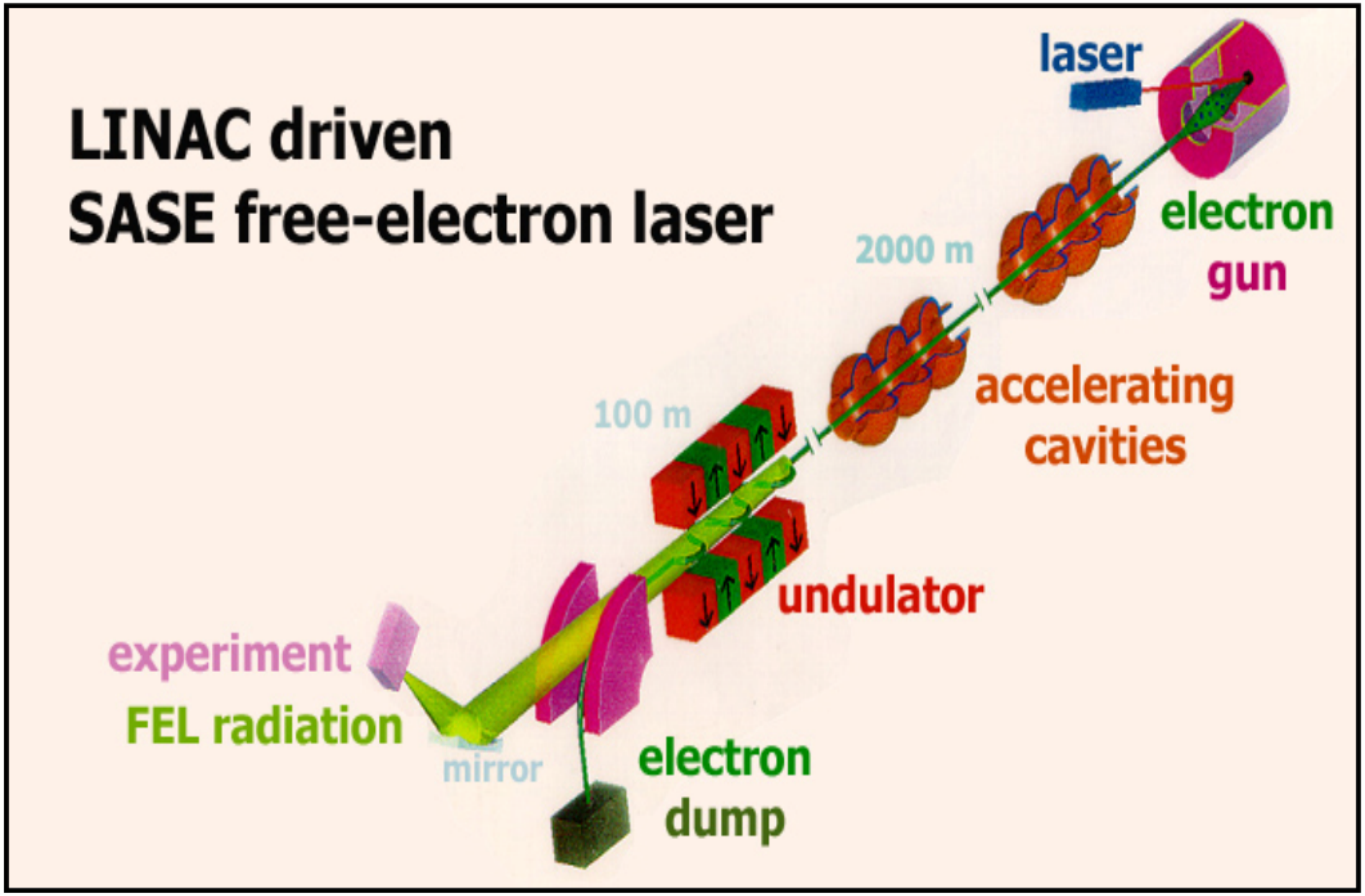
on axis

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

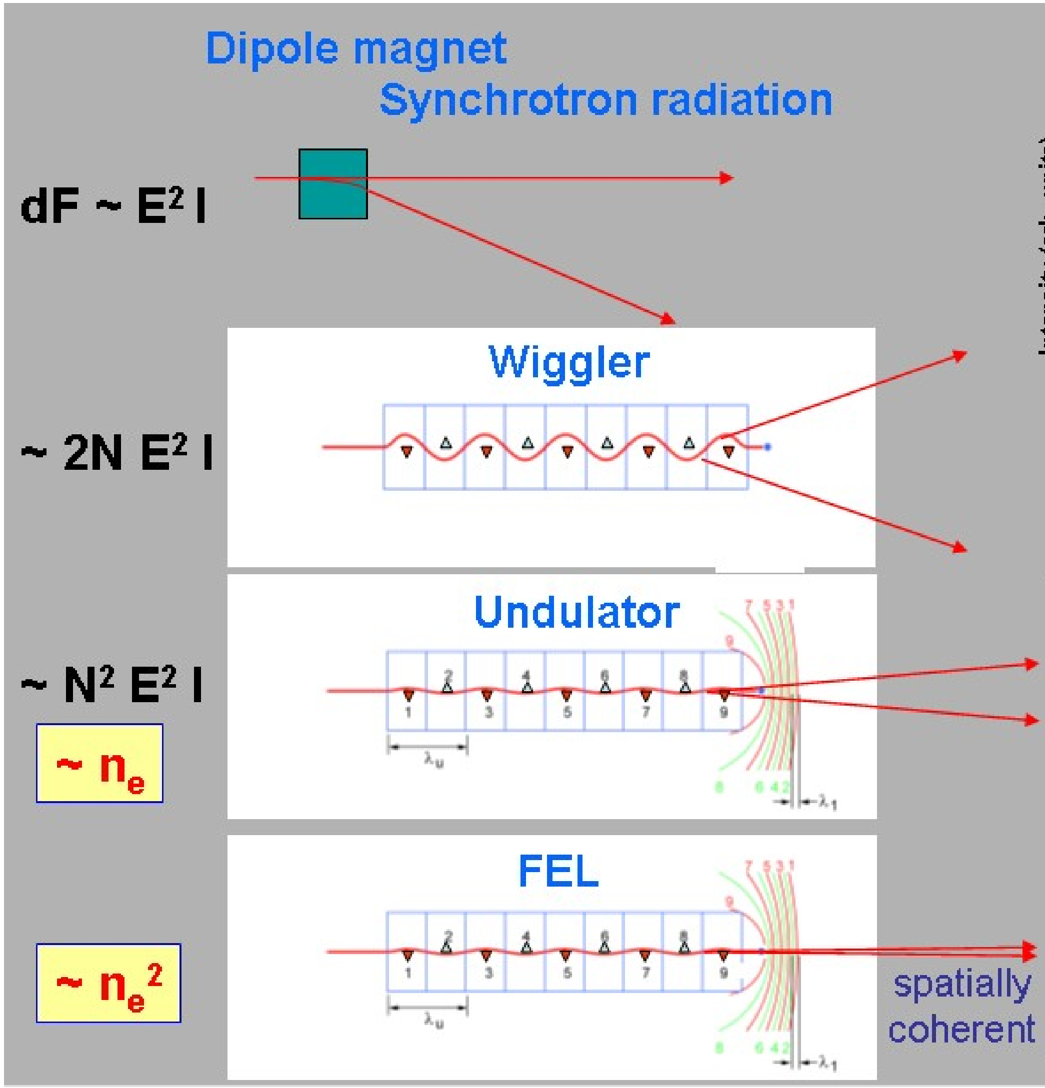
<u>bandwidth:</u>

$\Delta\lambda/\lambda \sim 1/nN$

Free Electron Lasers (FELs)



Synchrotron and FEL sources



Dipole magnet

Synchrotron radiation

dF ~ E^2 I

Wiggler

~ 2N E^2 I

Undulator

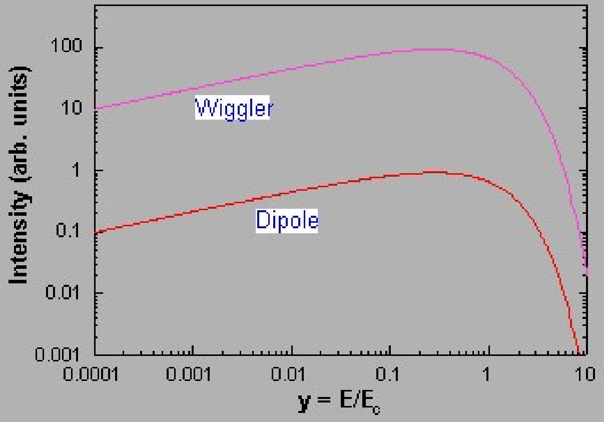
~ N^2 E^2 I

~ n_e

FEL

~ n_e^2

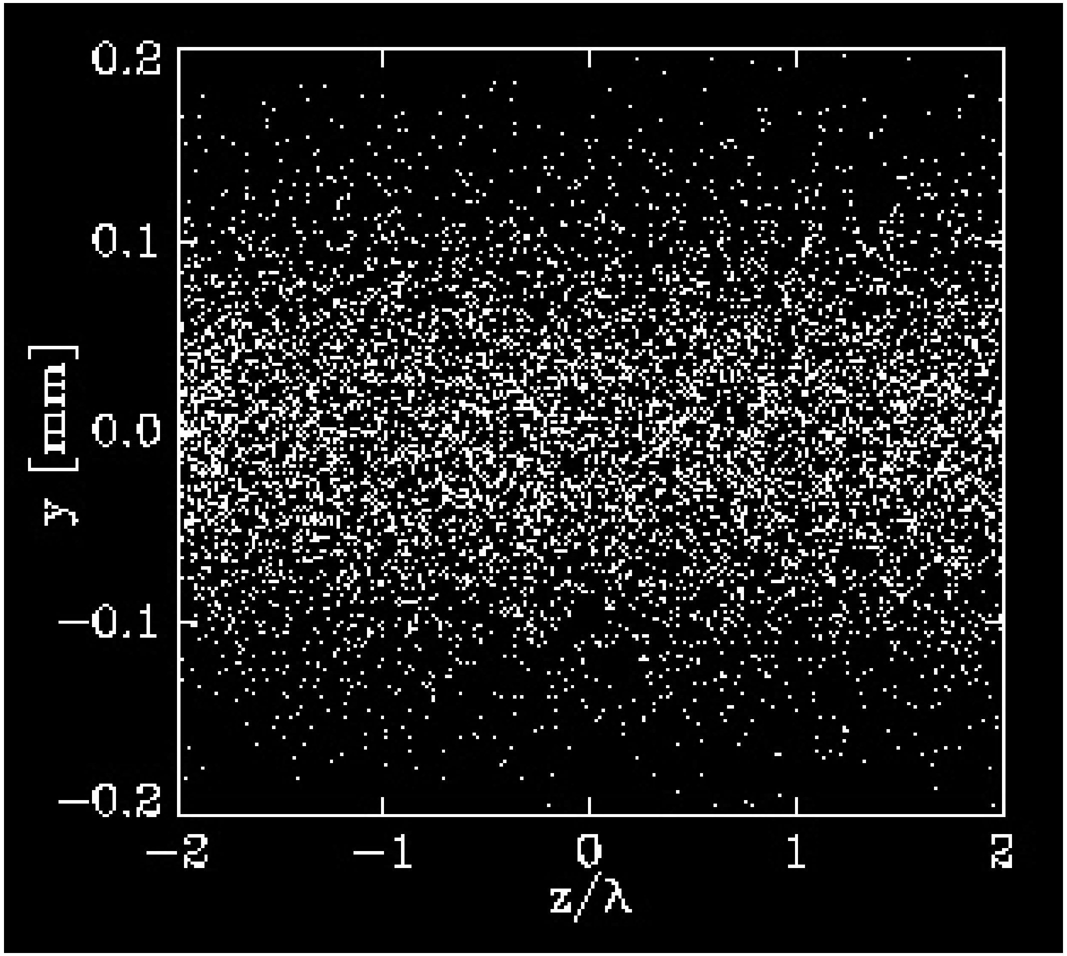
spatially coherent



The radiation emitted by a single electron in subsequent oscillations in an undulator is in phase. Radiation from different electrons is NOT (positional disorder in bunch).

"Phasing" is achieved via positional order in the bunch (micro-bunching) with a period equal to the x-ray wavelength.

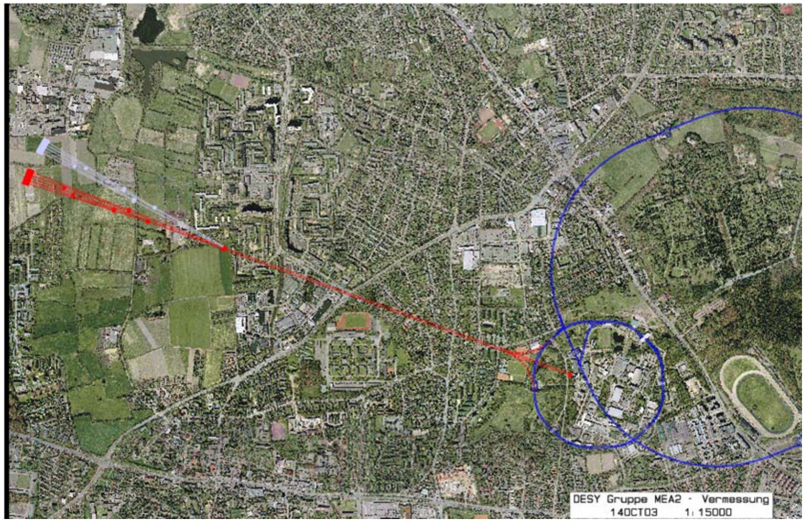
Electron bunching

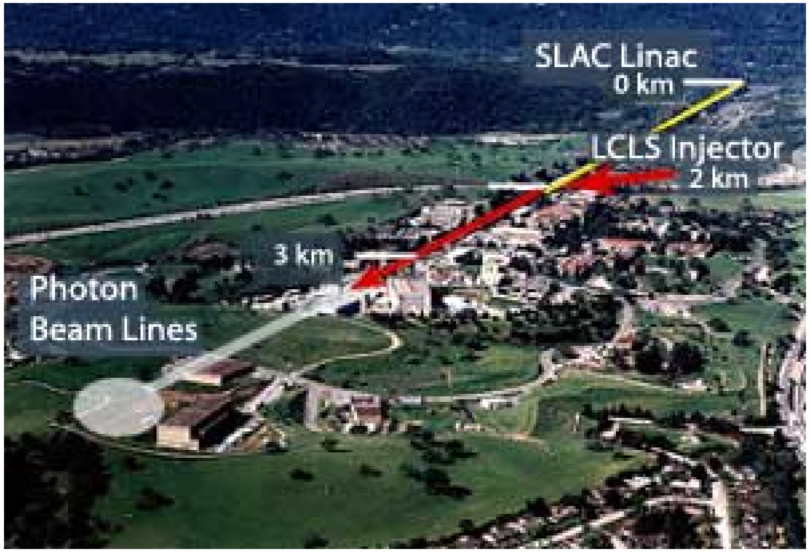


GENESIS – simulation for TTF parameters

Courtesy Sven Reiche (UCLA)

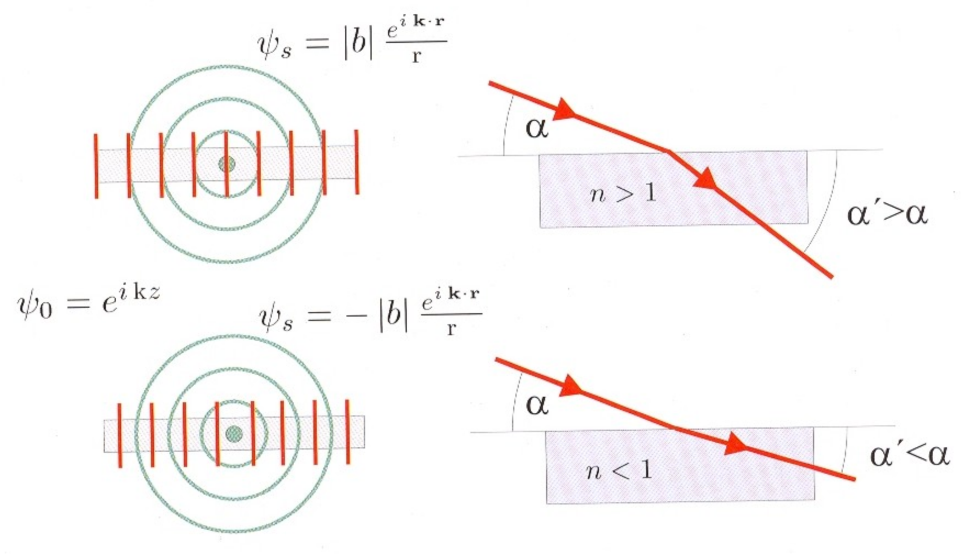
VUV and X-Ray FELs





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.

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

$\cos\alpha / \cos\alpha' = n$ (refractive index)

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

$n < 1$ X-rays ($\alpha' < \alpha$)

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

<u>total external reflexion:</u>

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

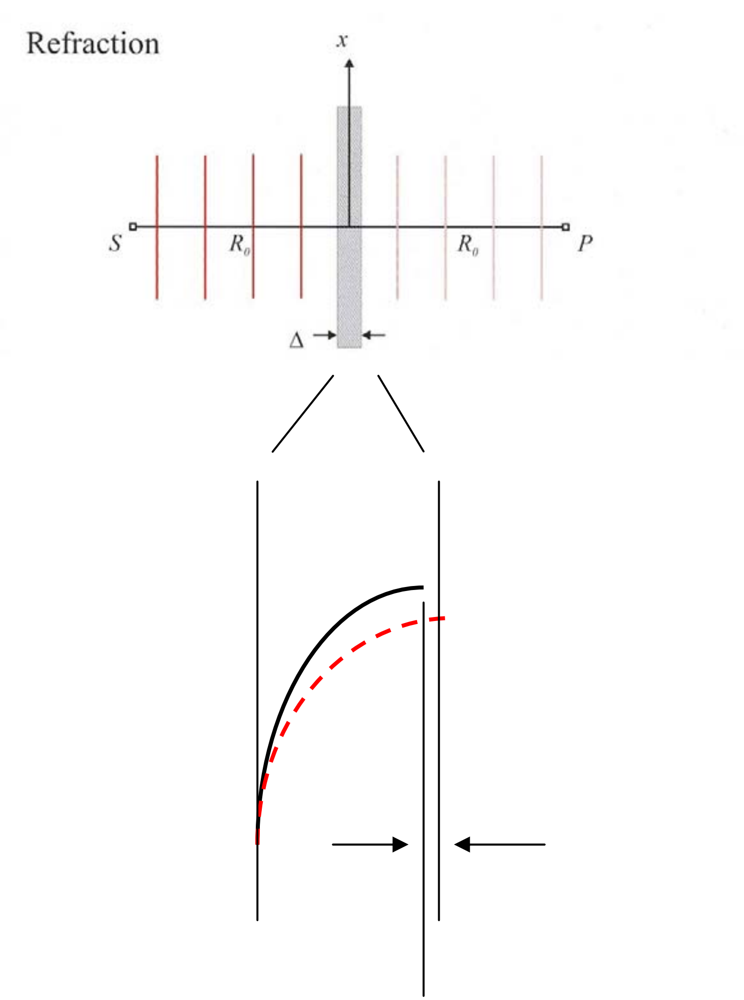
<u>Note:</u> spherical wave exp(ik'r)

$k' = nk = (n/c)\omega = \omega/v$

with $v=c/n$ phase velocity

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

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: $\exp(ik\Delta)$

slab: $\exp(ink\Delta)$

phase difference: $\exp(i(nk-k)\Delta)$

amplitude:

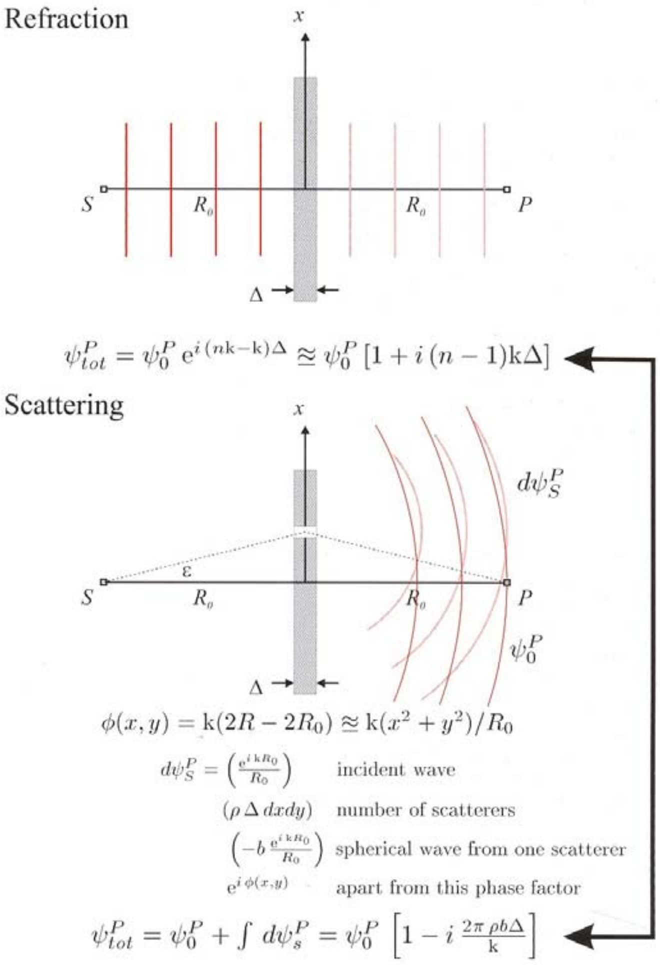
$$\psi_{tot}^{P} / \Psi_{0}^{P} = \exp(ink\Delta) / \exp(ik\Delta)$$

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

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

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

Refractive Index



Refraction

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

Scattering

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

$d\psi_S^P = \left(\frac{e^{i\,kR_0}}{R_0}\right)$ incident wave

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

$\left(-b\,\frac{e^{i\,kR_0}}{R_0}\right)$ spherical wave from one scatterer

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

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

Scattering picture:

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

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

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

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

$2kx^2/2Ro = kx^2/Ro$

include y direction:

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

amplitude at P:

phase factor

$d\psi_S^P \approx$

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

incident wave

number of scatters in volume element $\rho dxdy$

scattered wave from 1 scatterer

Refractive Index

$$\Psi_S^P = \int d\Psi_S^P = -\rho b\Delta\{\exp(i2kRo)\}/Ro^2 \bullet \underbrace{\int \exp(i\Phi(x,y))dxdy}_{\mathbf{i\pi Ro/k}}$$

[Ref.1]

Amplitude at P without slab:

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

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

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

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

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

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

<u>Total external reflexion (α'=0) for $\alpha = \alpha_c$:</u>

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

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

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

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

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

critical angle for Si

α_c = sqrt(2δ) = sqrt (4πρr_0/k^2)

<u>Silicon:</u> ρ = 0.699 e-/$Å^3$, λ = 1Å

α_c=sqrt(4π x 0.699 x 2.82e-5 x 1/$(2\pi)^2$)

= 0.0025 rad

Q_c = (4π/λ) sinα_c = 0.032 $Å^{-1}$

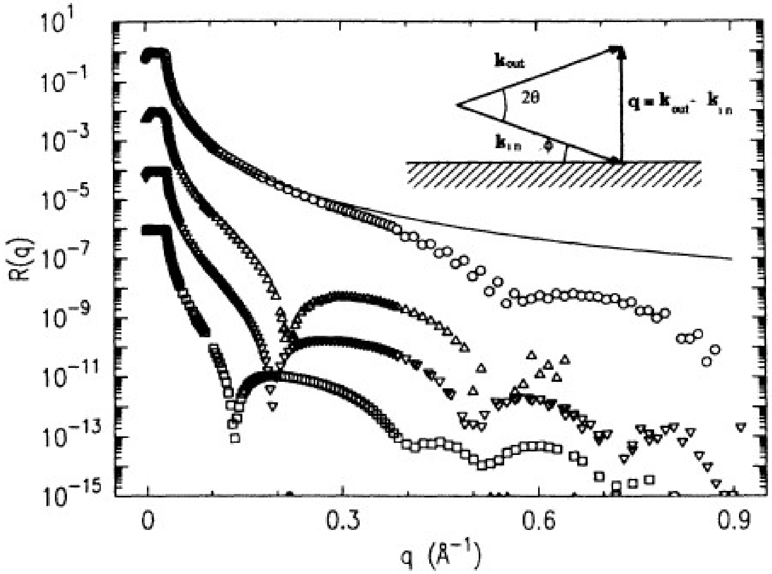
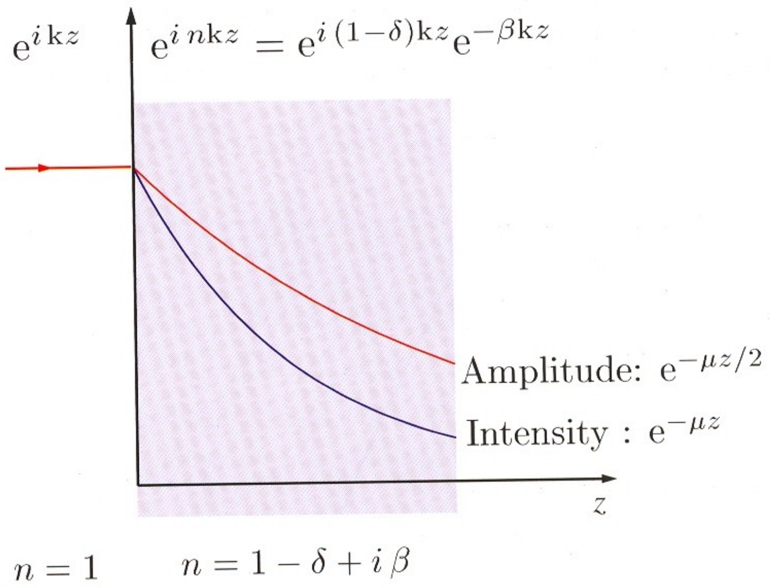


FIG. 1. Normalized reflectivity data from several samples. Successive data sets are displaced by 100 times and error bars omitted for clarity. (——) Theoretical reflectivity from an ideal step interface with bulk silicon density. (○) Uncoated silicon sample in helium; the "pairing" of points occurs for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

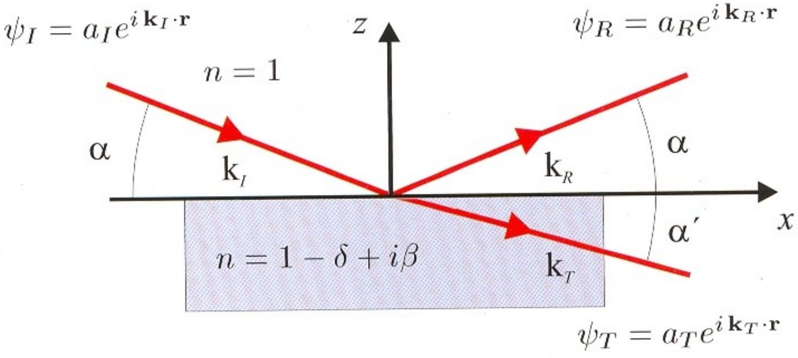
(when intensity drops according to exp(-µz))

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

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')

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

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

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

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

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

<u>Fresnel equations:</u>

$$\boxed{\begin{aligned} r &= a_R/a_I = (\alpha-\alpha')\,/\,(\alpha+\alpha') \\ t &= a_T/a_I = 2\alpha\,/\,(\alpha+\alpha') \end{aligned}}$$

r: reflectivity t: transmittivity

Snell's law and the Fresnel equations (2)

Note: α' is a complex number

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

Consider z-component of transmitted wave:

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

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

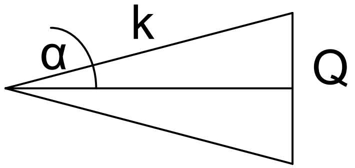
exponential damping

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

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

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

use wavevector notation:



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

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

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

use dimensionless units:

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

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

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

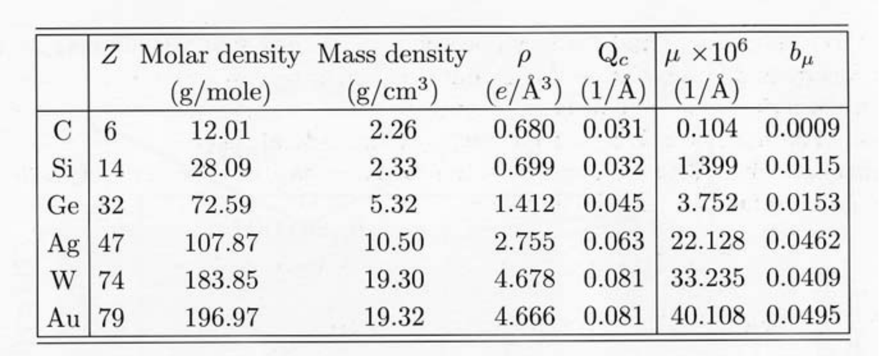
$b_u = (2k/Q_c)\beta = (4k^2/Q_c^2)\mu/2k = 2k\mu/Q_c^2$

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

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/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:

$$\boxed{\begin{aligned} r(q) &= (q - q') / (q + q') \\ t(q) &= 2q / (q + q') \\ \Lambda(q) &= 1 / Q_c\, \mathrm{Im}(q') \end{aligned}}$$

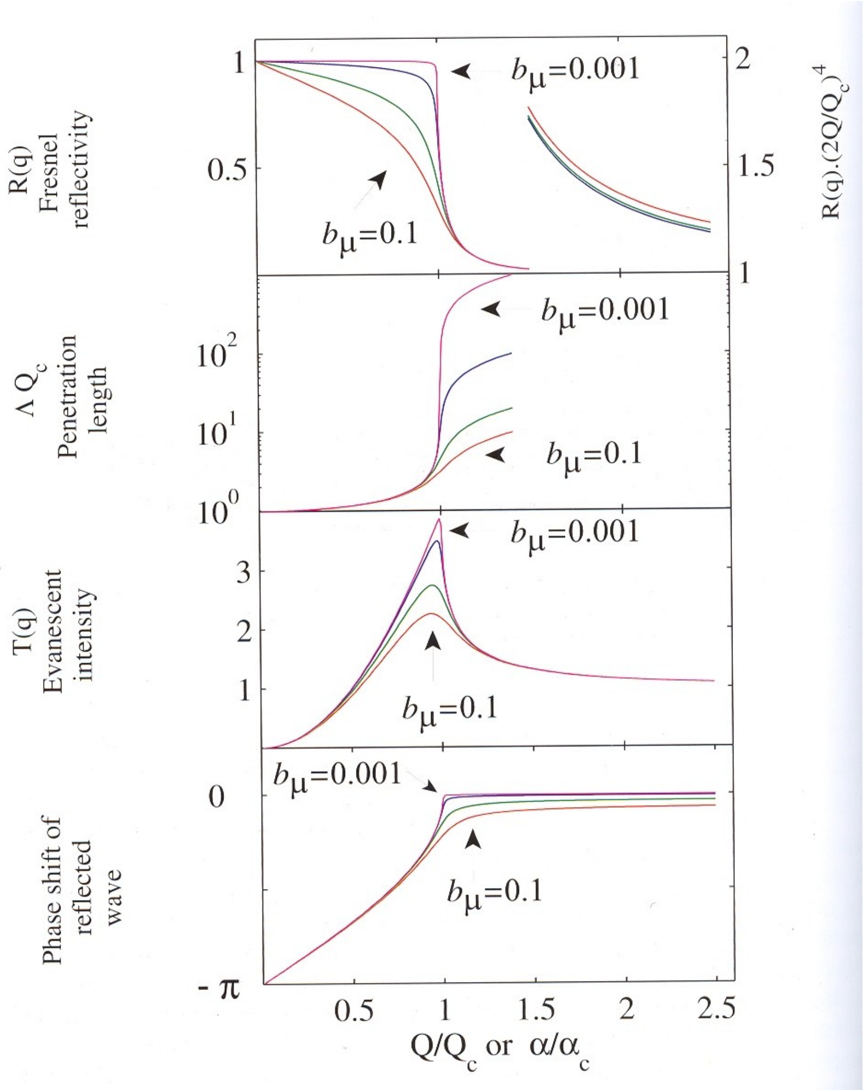
Snell's law and the Fresnel equations (4)

Fresnel equations:

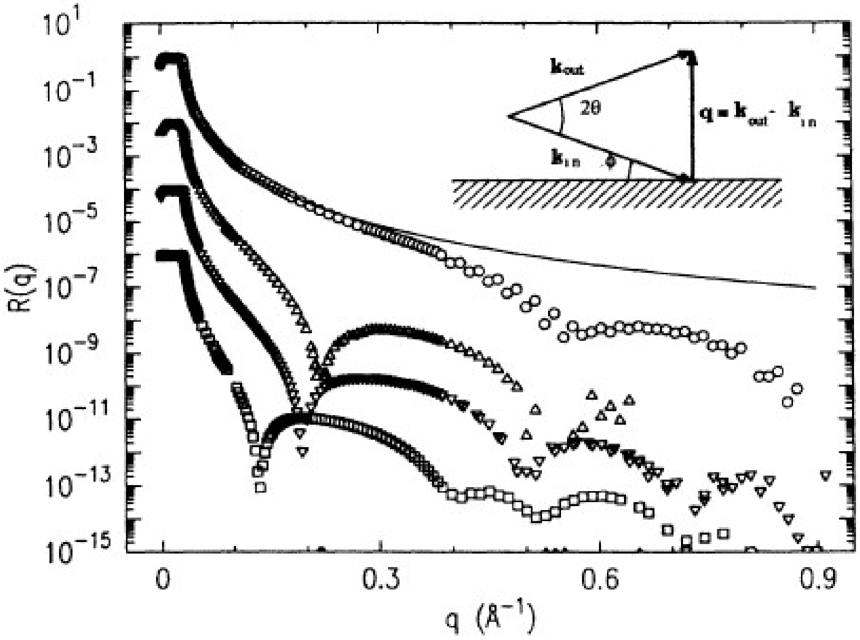
q>>1: $R(Q) \sim 1/q^4$,
$\Lambda \approx \mu^{-1}$,
$T \approx 1$,
no phase shift

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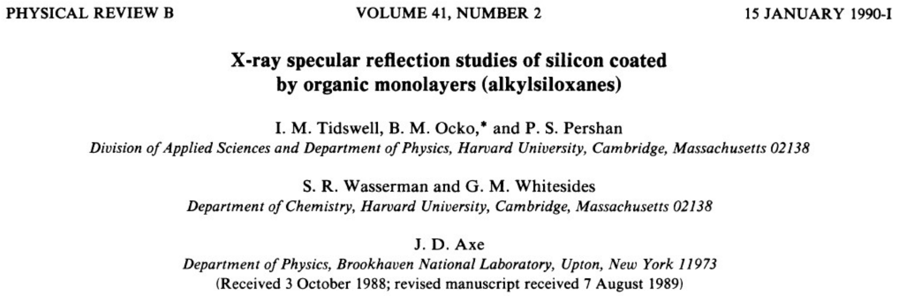
PHYSICAL REVIEW B VOLUME 41, NUMBER 2 15 JANUARY 1990-I

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

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