PIER Graduate Week 2014
6 – 9 Oct 2014

Essentials of X-ray Physics

Scattering, Imaging, Spectroscopy and beyond

Part II

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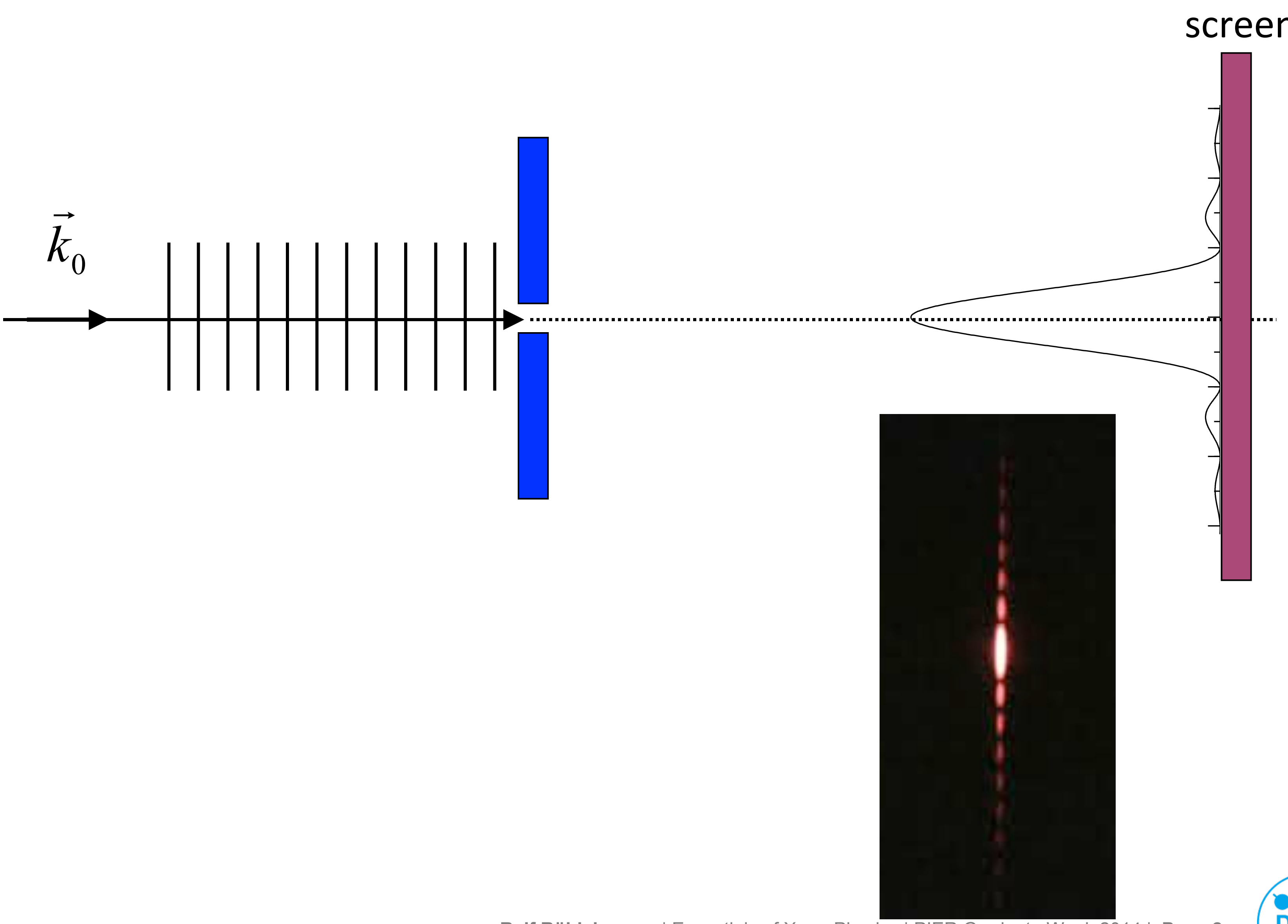
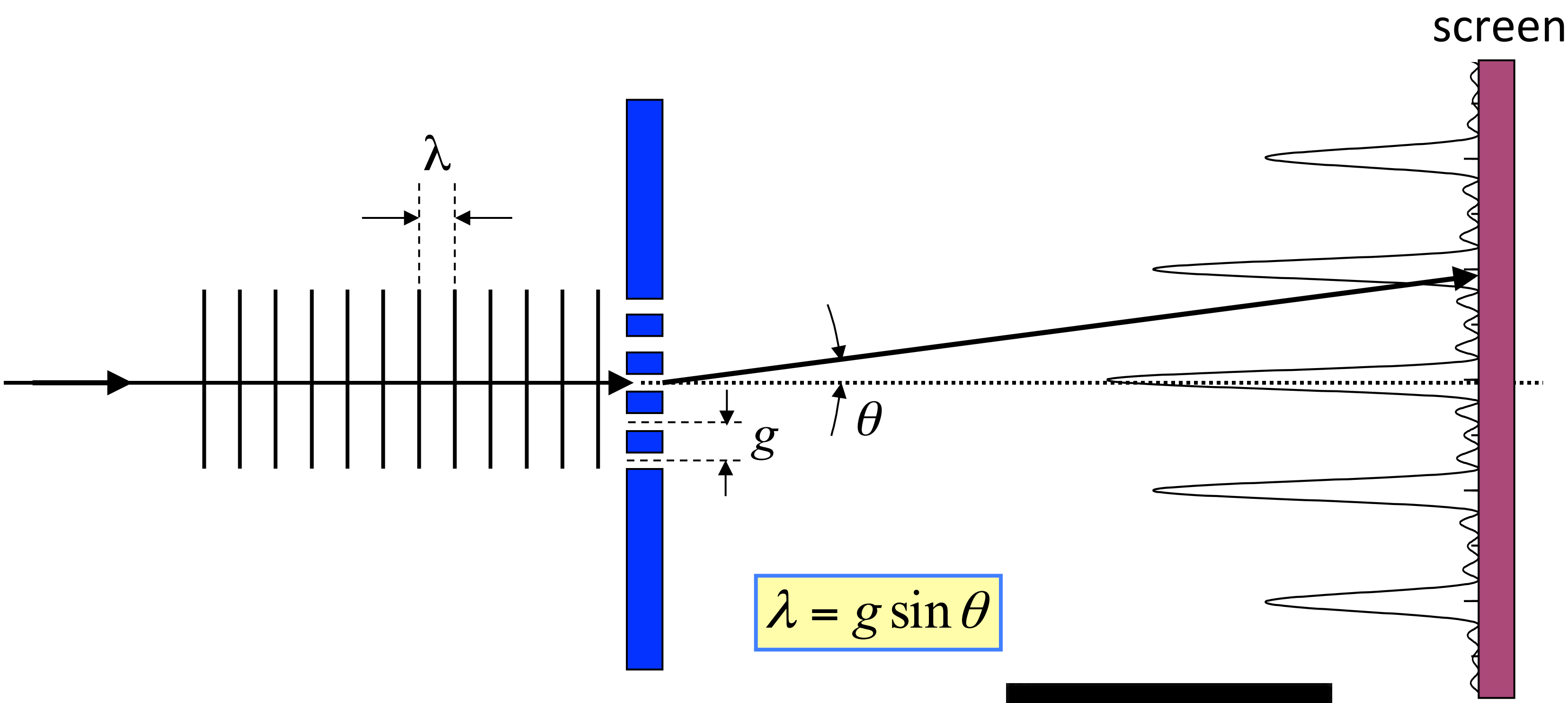
HELMHOLTZ ASSOCIATION

DESY

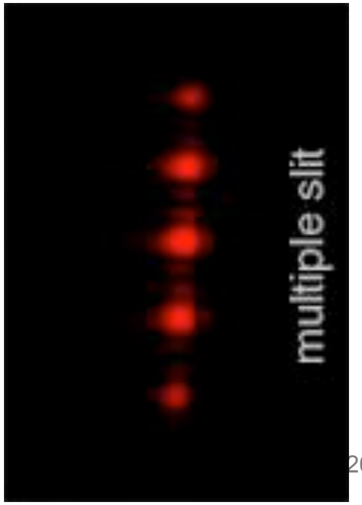
Structure Determination using Light: Diffraction at a Single Slit



Diffraction at a grating

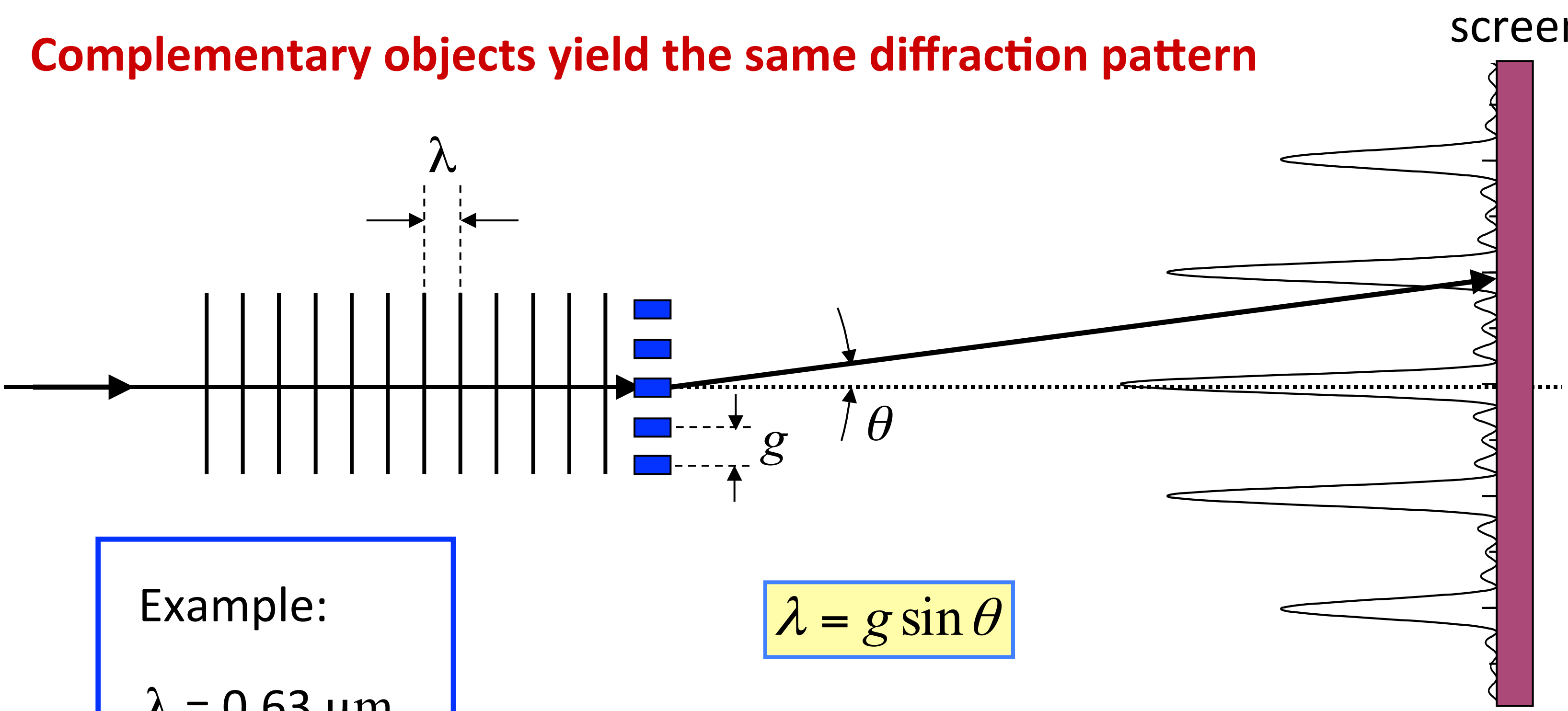


$$\lambda = g \sin\theta$$



Theorem of Babinet

Complementary objects yield the same diffraction pattern



Example:

$\lambda = 0.63\ \mu m$

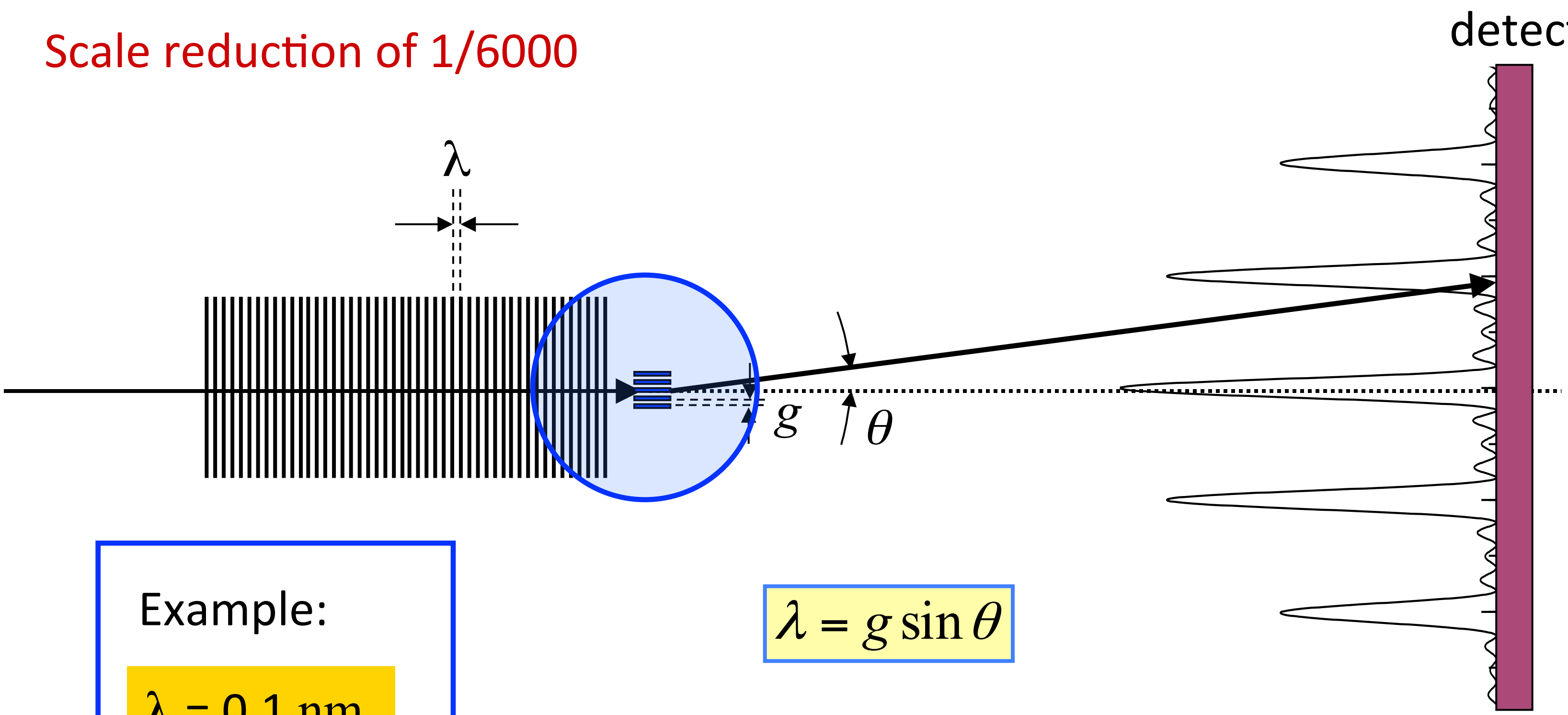
$\theta = 10^o$

$g = 3.6\ \mu m$

$$\lambda = g \sin\theta$$

Transition to x-rays

Scale reduction of 1/6000



Example:

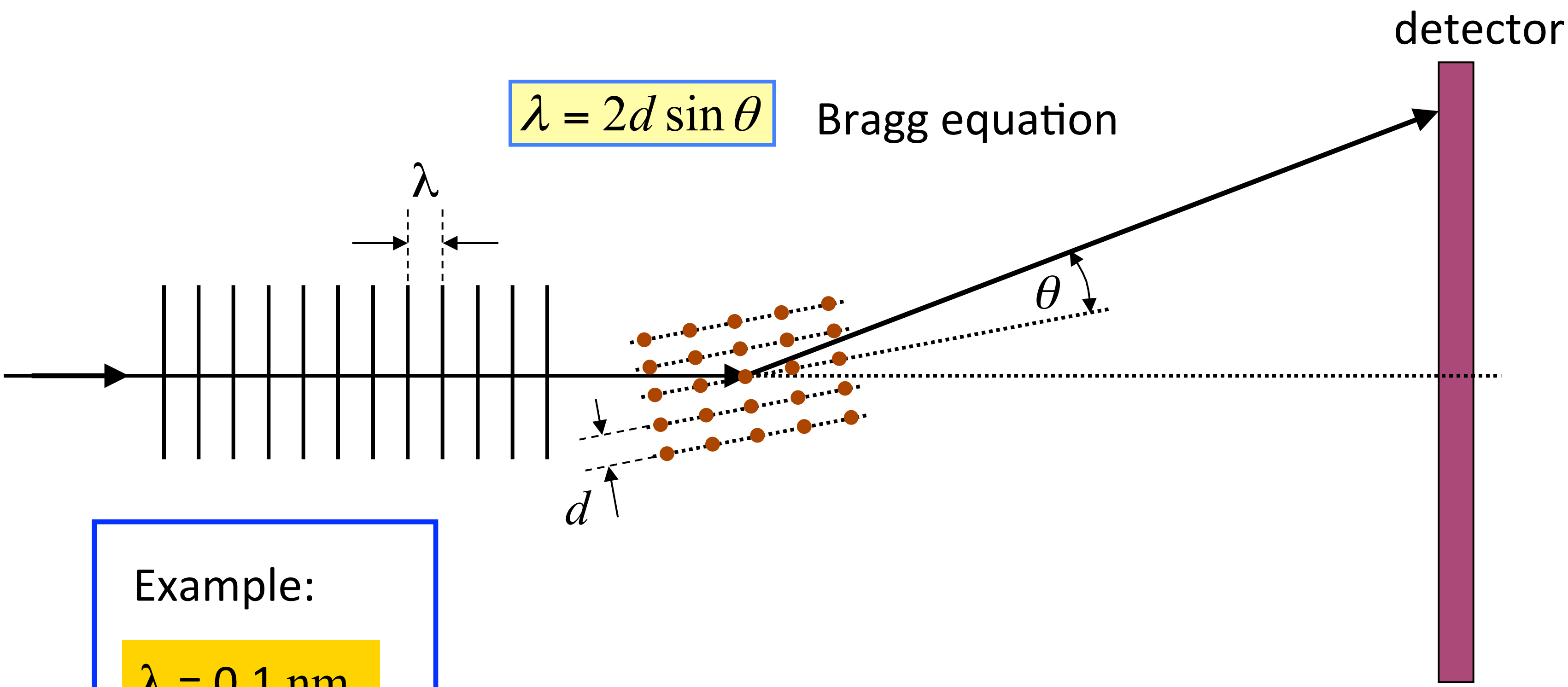
λ = 0.1 nm

θ = 10°

g = 0.6 nm → Interatomic spacings

$$\lambda = g \sin\theta$$

X-ray diffraction



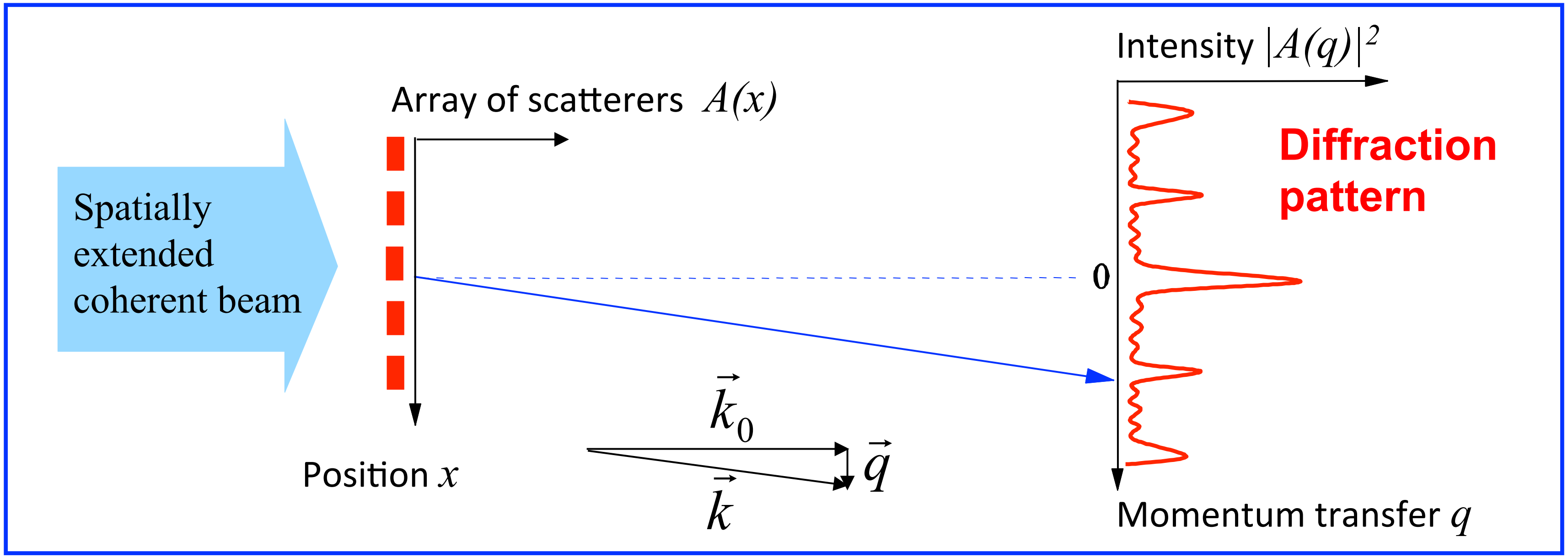
Example:

$\lambda = 0.1$ nm

$\theta = 10^{\circ}$

$g = 0.6$ nm → Interatomic spacings

Principles of structure determination



$\vec{q} = \vec{k} - \vec{k}_0$ momentum transfer

Relation between $A(x)$ and $A(q)$:

$$A(q) = \int A(x)\, e^{iqx}\, dx \quad (1)$$

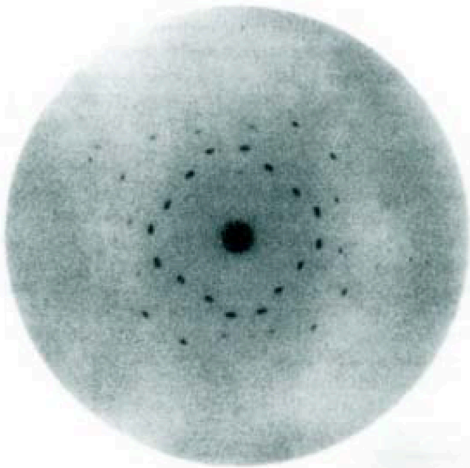
Task: Determine $A(x)$ from measured $|A(q)|^2$

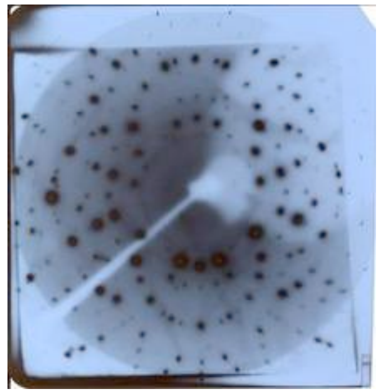
Problem: Eq. (1) cannot be simply inverted, because the phase is lost

(Phase problem of crystallography)

X-ray Diffraction from Crystalline Structures

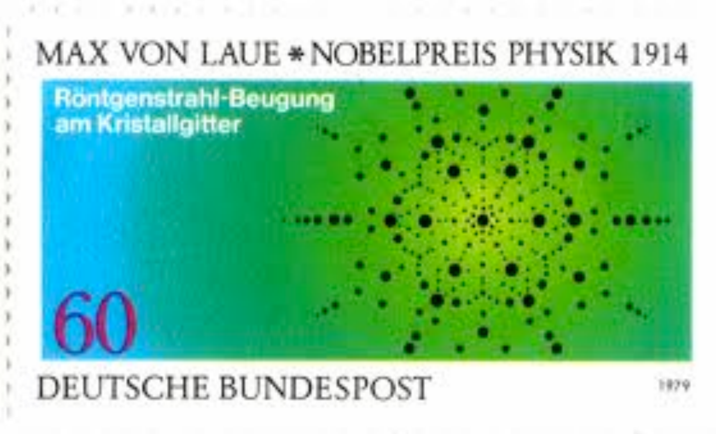
Apparently, x-rays are preferentially scattered in particular directions

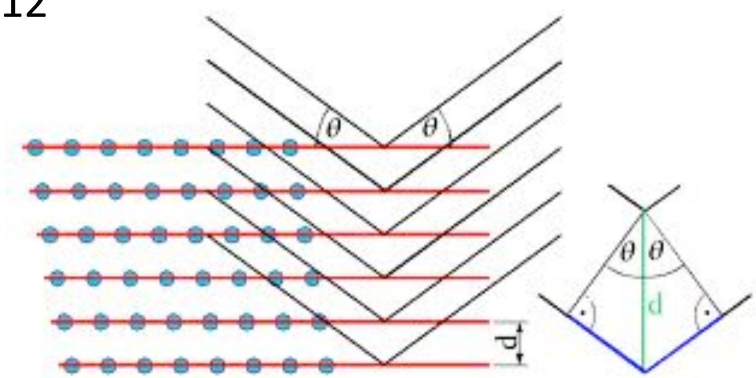




First diffraction patterns obtained by Max v. Laue in 1912

Max von Laue (1879 – 1960)

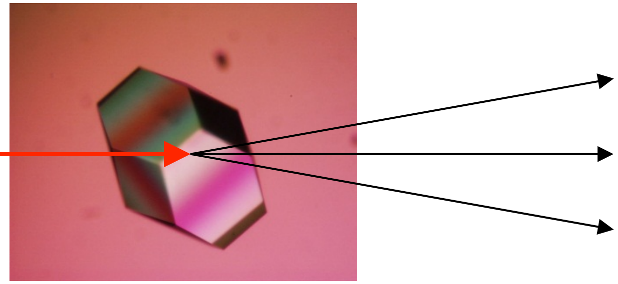




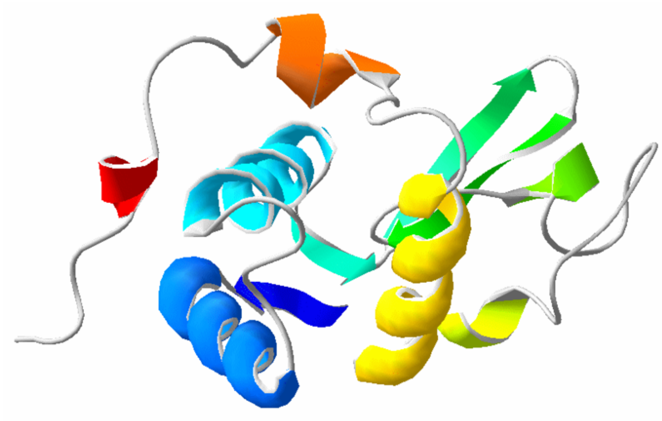
Today: X-ray diffraction of synchrotron radiation for structure determination

Structure Determination of Proteins

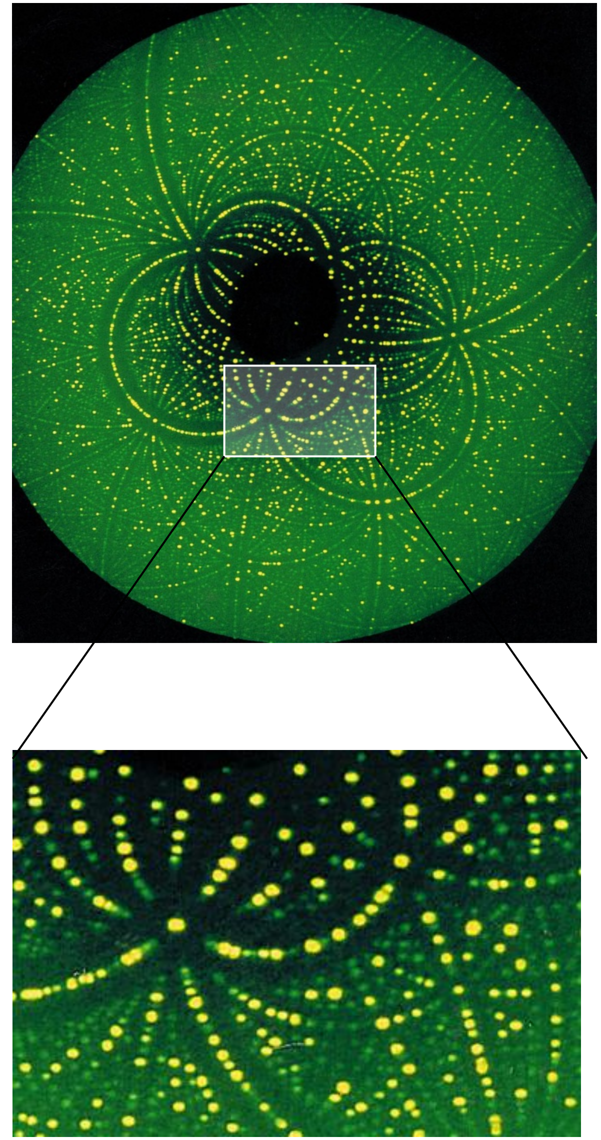
X-rays



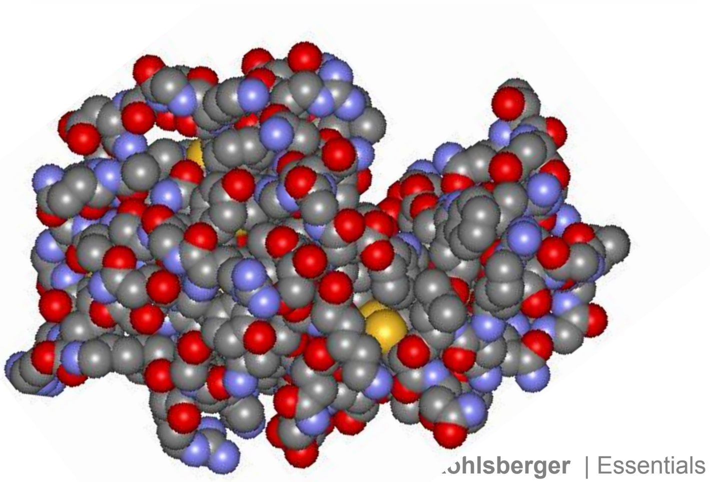
Protein crystal:
Lysozyme
(enzyme from egg white)



Diffraction pattern

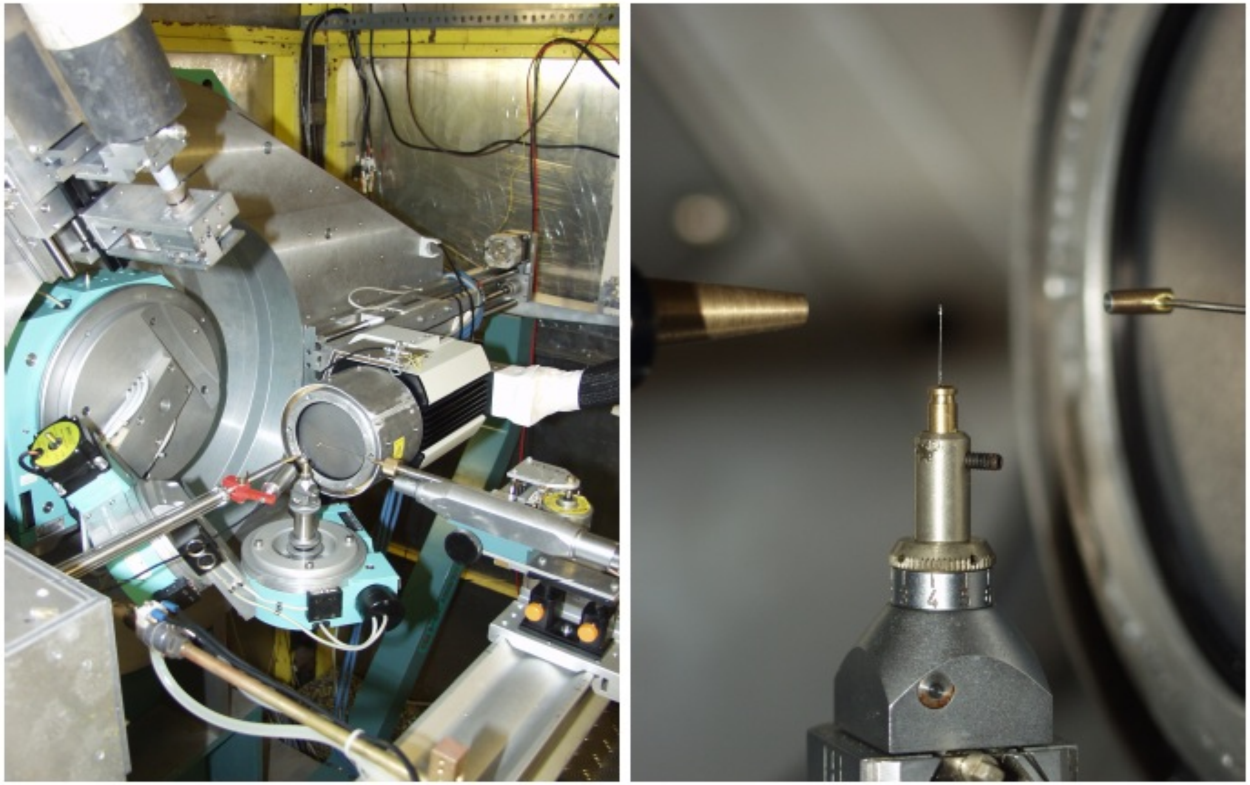


Carbon: Grey
Nitrogen: Blue
Oxygen: Red
Sulphur: Yellow



Structure determination of Proteins: Instrumentation

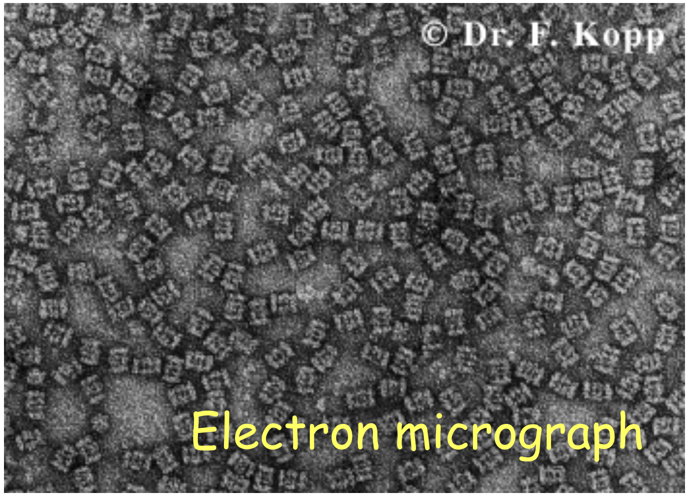
Single crystal diffractometers

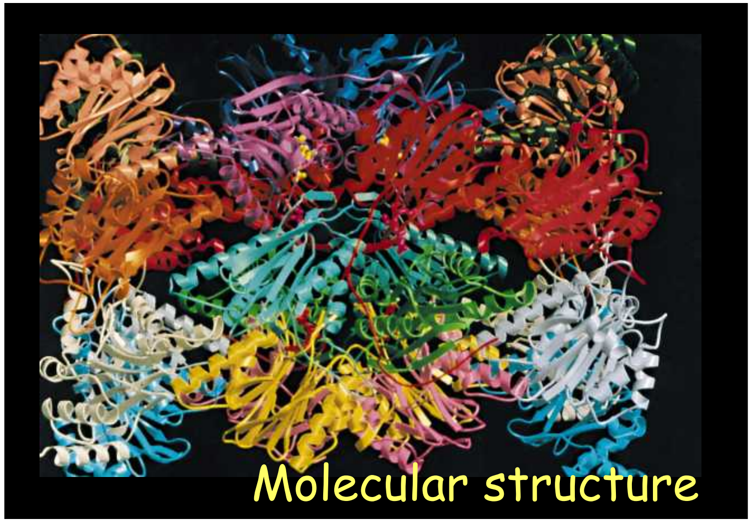


Single crystal diffractometer in κ-geometry with CCD and scintillation counter. Crystal mounted on a glass fiber. The κ-diffractometer has 3 rotations for the crystal and one for the detector.

The Proteasome

(cuts proteins into peptides and amino acids)



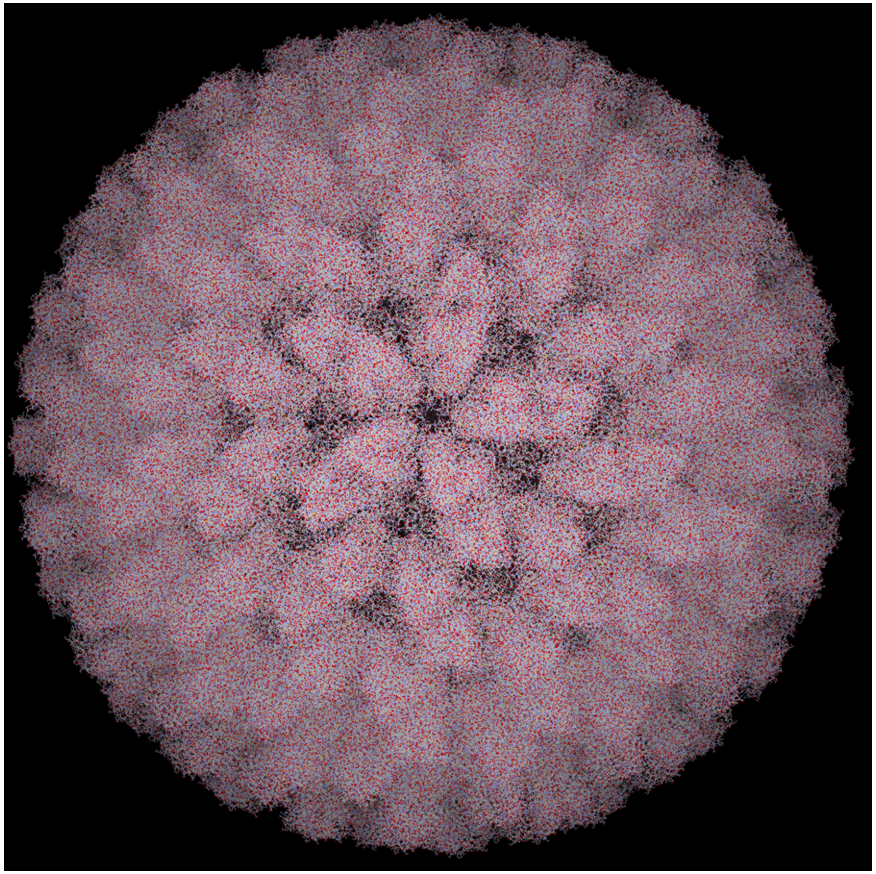


The Ribosome

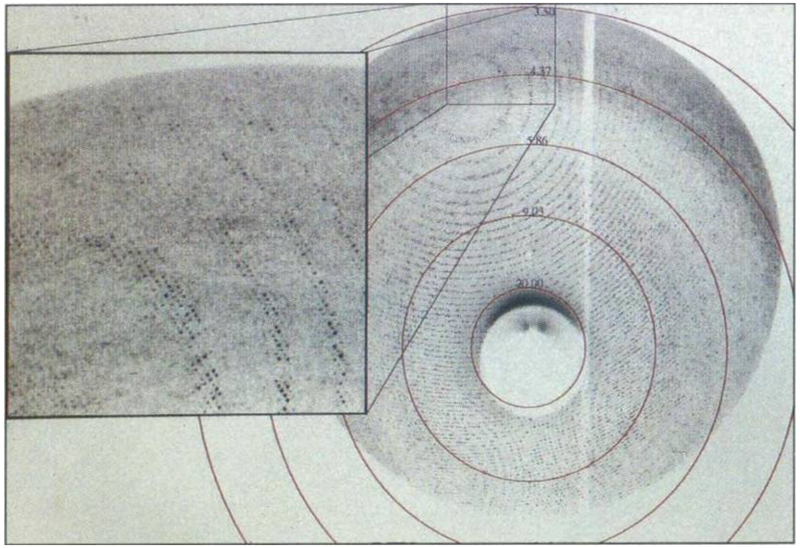
(synthesis of proteins)

The 30S subunit of the ecoli ribosome

Very Large Biomolecules (e.g. Viruses)

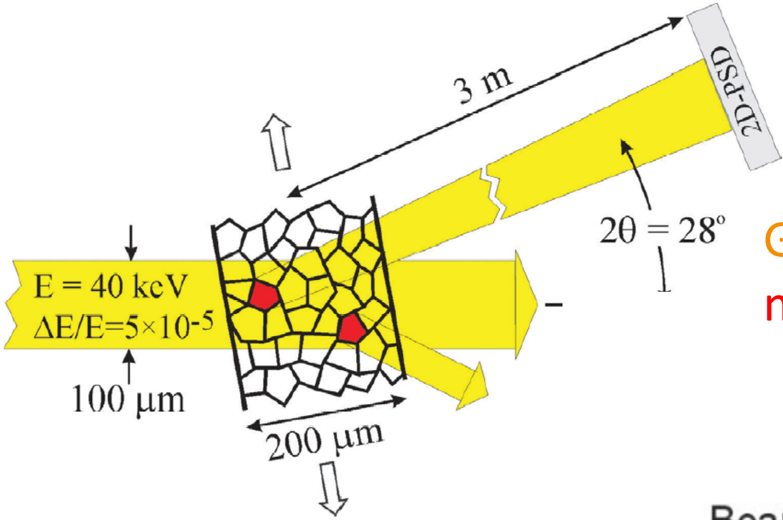


Example: Blue Tongue Virus



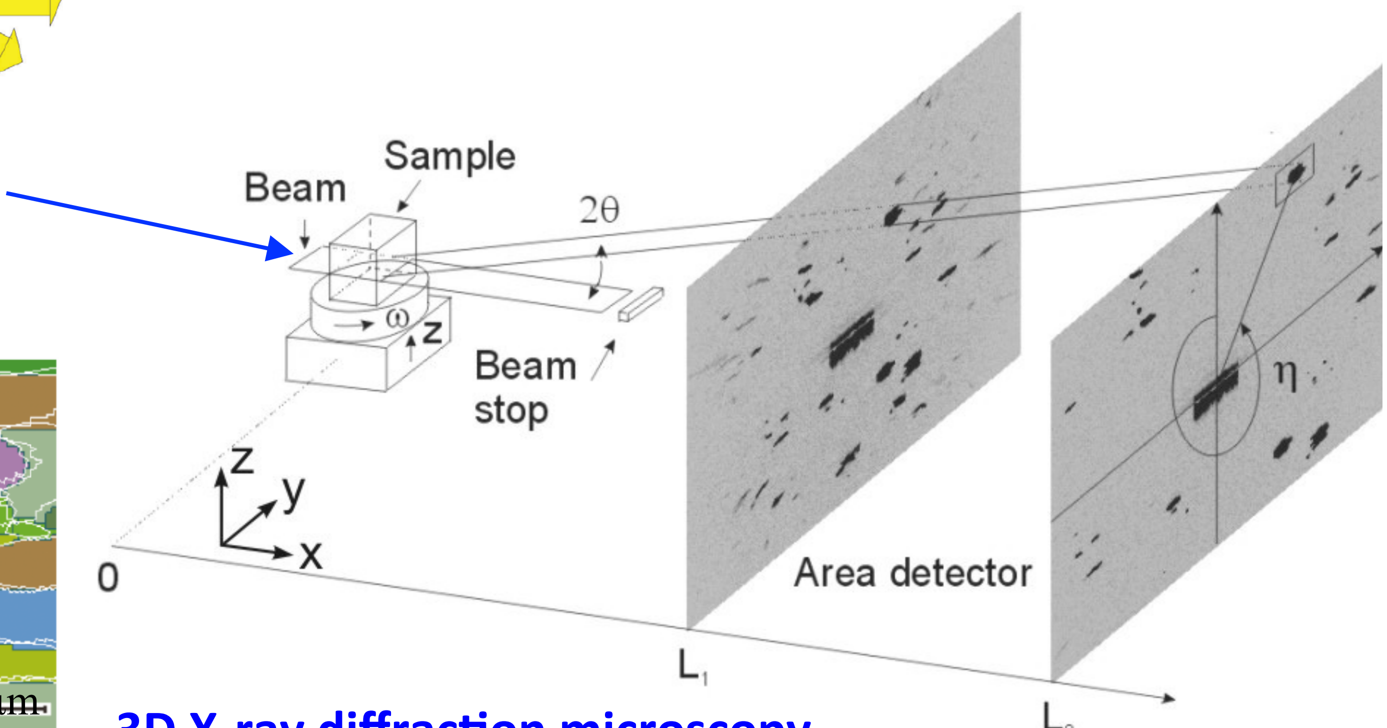
J.M. Grimes et al., Nature 395, 470-478 (1998)

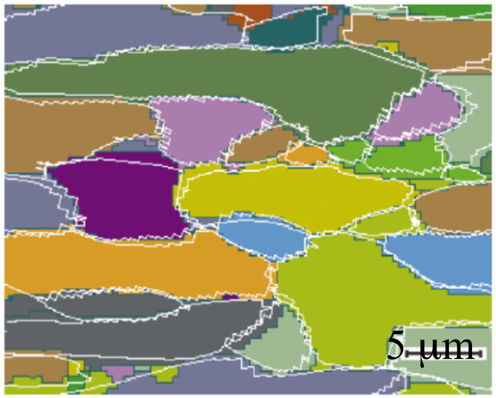
Materials Science: Grain Structure of Metals and Alloys



How does the microstructure of a material change upon mechanical load and deformations ?

Grain properties to be determined: position, morphology, orientation, deformation, composition





3D X-ray diffraction microscopy

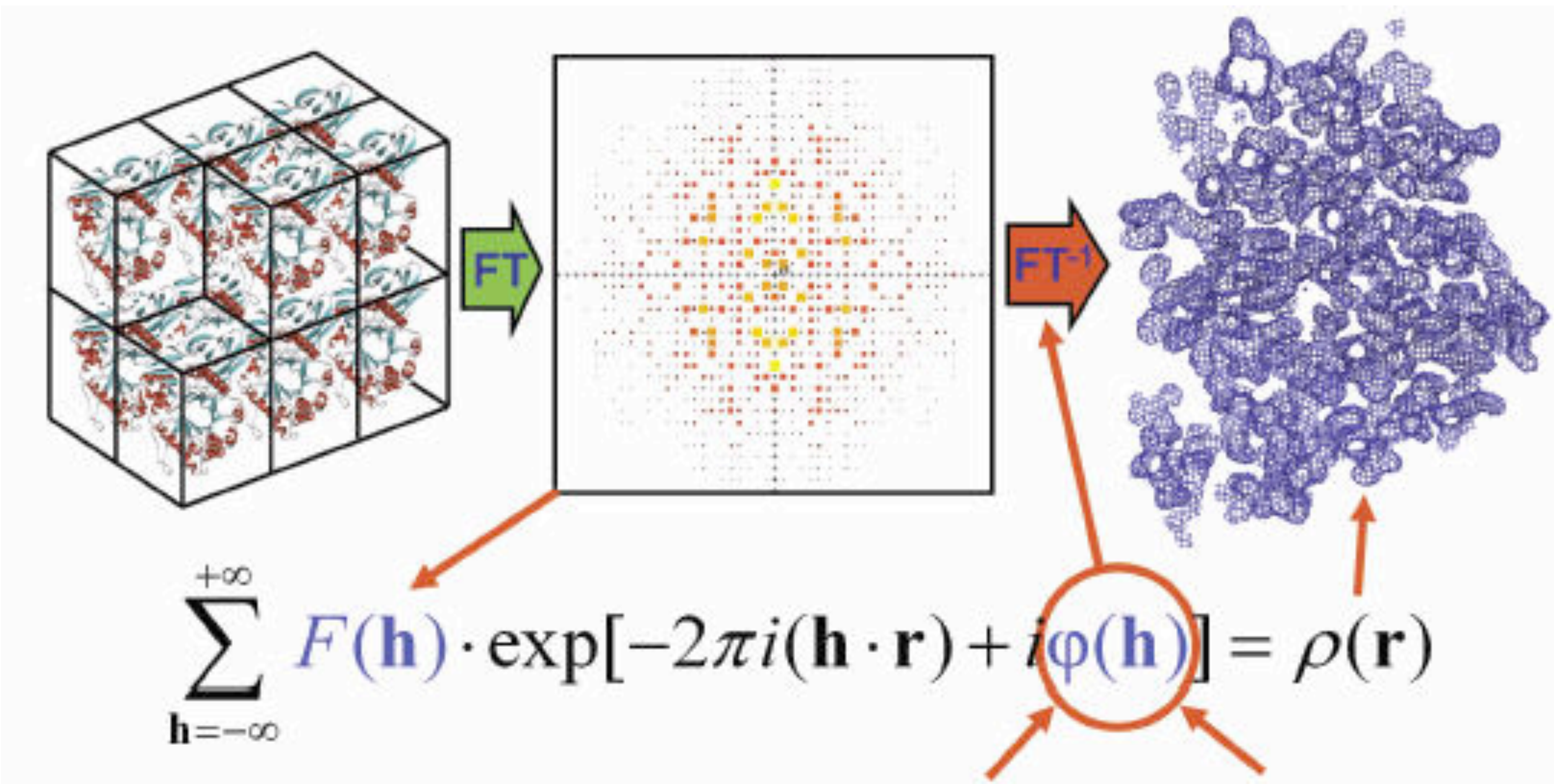
H. F. Poulsen et al., J. Appl. Cryst. 34, 751 (2001)

The phase problem of crystallography

Crystallized molecules

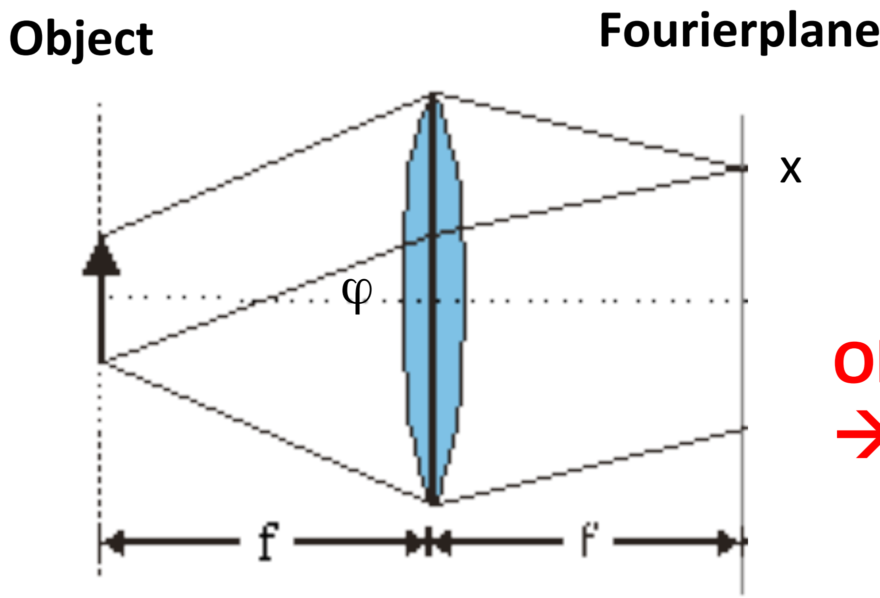
Diffraction pattern

Electron density of the molecule



Why don't we take a lens to obtain an image ?

Fouriertransformation (FT) with a lens



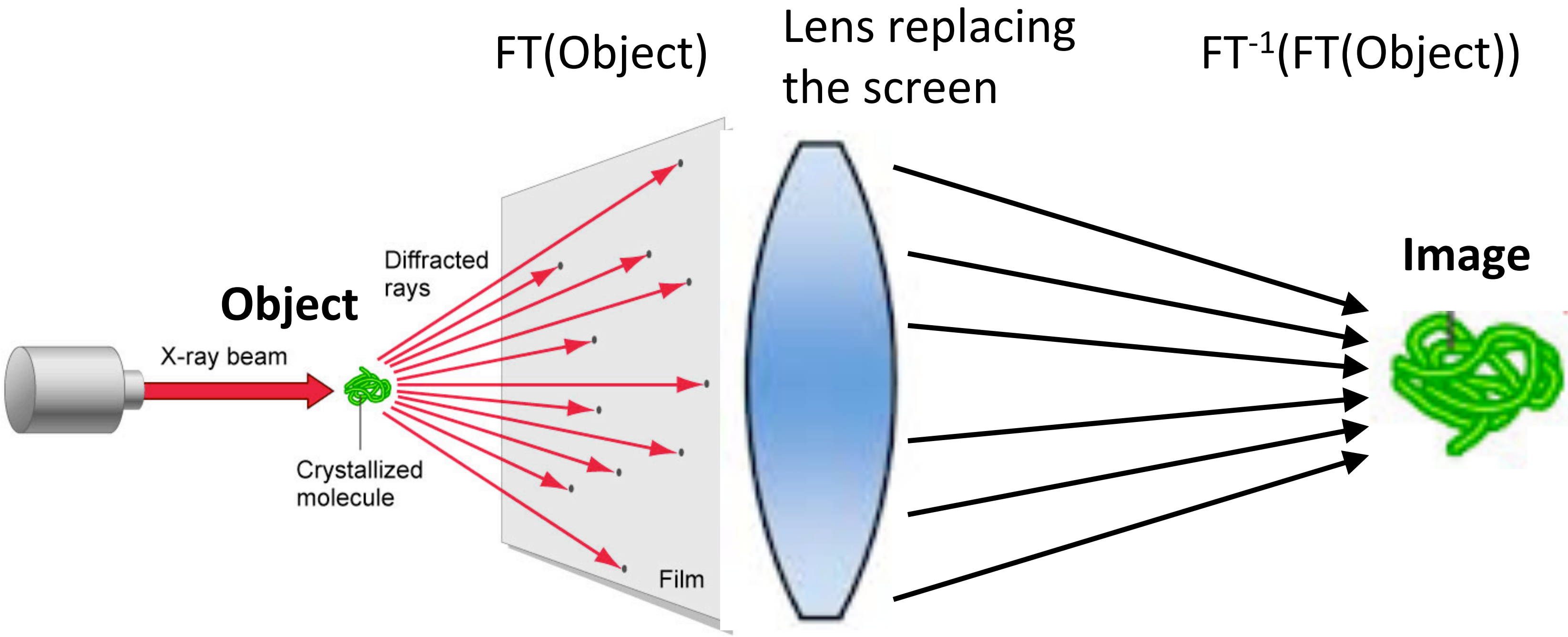
Object in the focal plane
→ FT(Object) in the Fourierplane

A lens focusses parallel rays from an object in the focal plane on a point in the Fourier plane

→ Mapping of angle φ to coordinate x

= Fouriertransformation of the object

Fouriertransformation with a lens



Can we apply this for x-rays ?

X-ray reflection from surfaces

Index of refraction

$$n = 1 - \delta$$

$$\delta = \frac{\rho_e \, r_0 \, \lambda^2}{4\pi}, \quad \rho_e \equiv \text{ electron density}$$

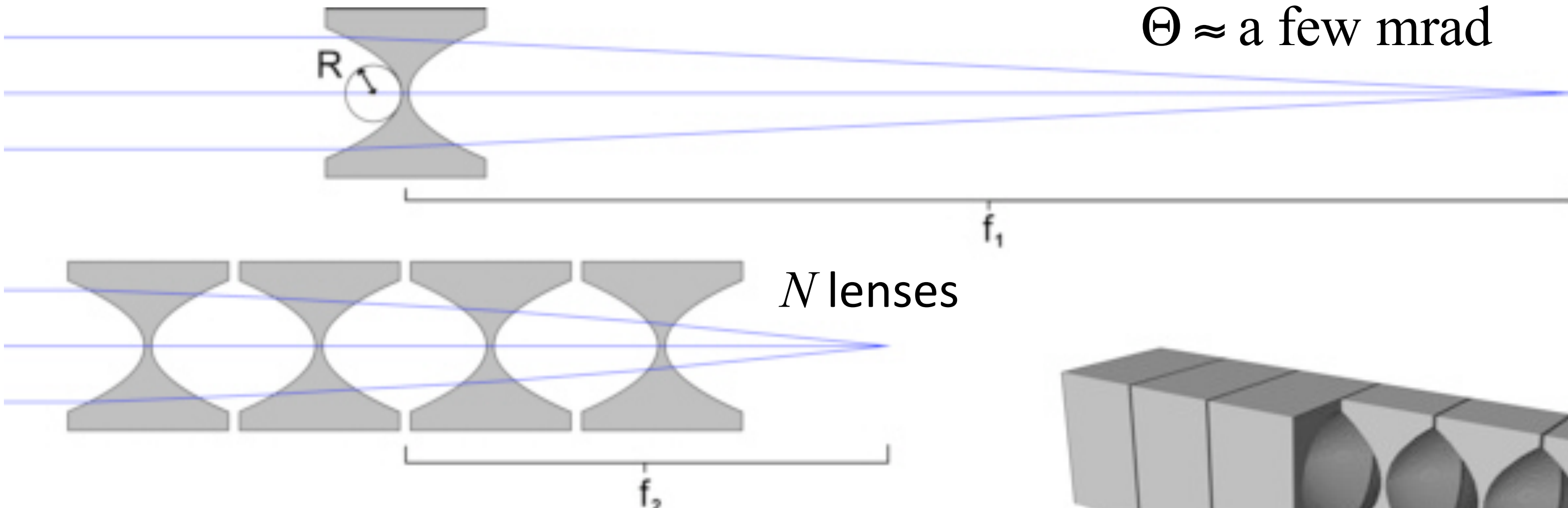
$$\approx 10^{-5} - 10^{-6} \quad \text{for} \quad \lambda = 0.1 \, \text{nm}$$

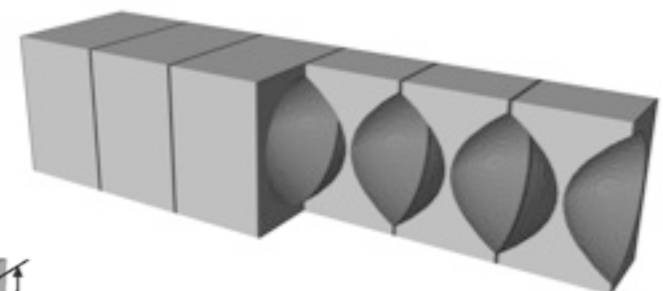
For x-rays, every medium is optically thinner than vacuum !

X-ray Lenses

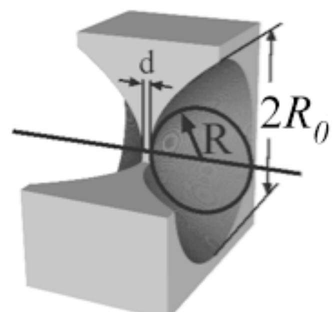
$n = 1 - \delta$ $\qquad$ $n < 1$ → Concave lenses are focussing:

$\Theta \approx$ a few mrad





Focal length : $f = \dfrac{R}{2\delta N}$



Numerical aperture $NA = n \sin \Theta$

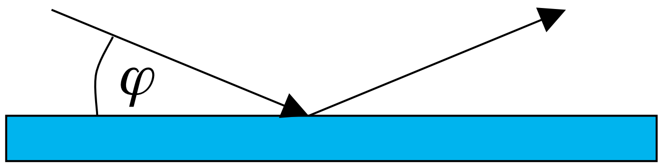
Resolution $d = \dfrac{\lambda}{2\, NA}$

Source: www.xray-lens.de

X-ray reflection from surfaces

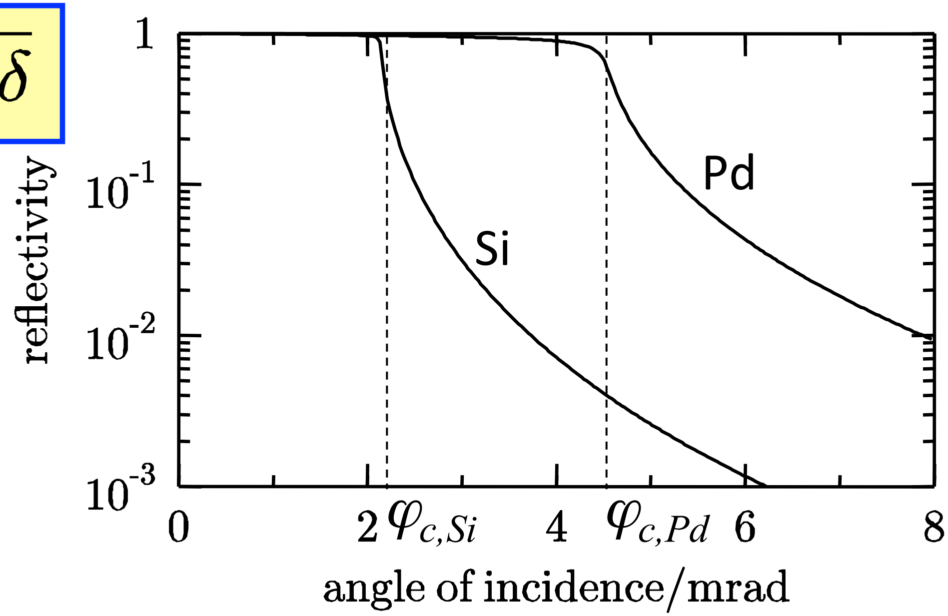
For x-rays, every medium is optically thinner than vacuum !

X-rays incident on a surface below the critical angle are totally reflected



Critical angle of total reflection

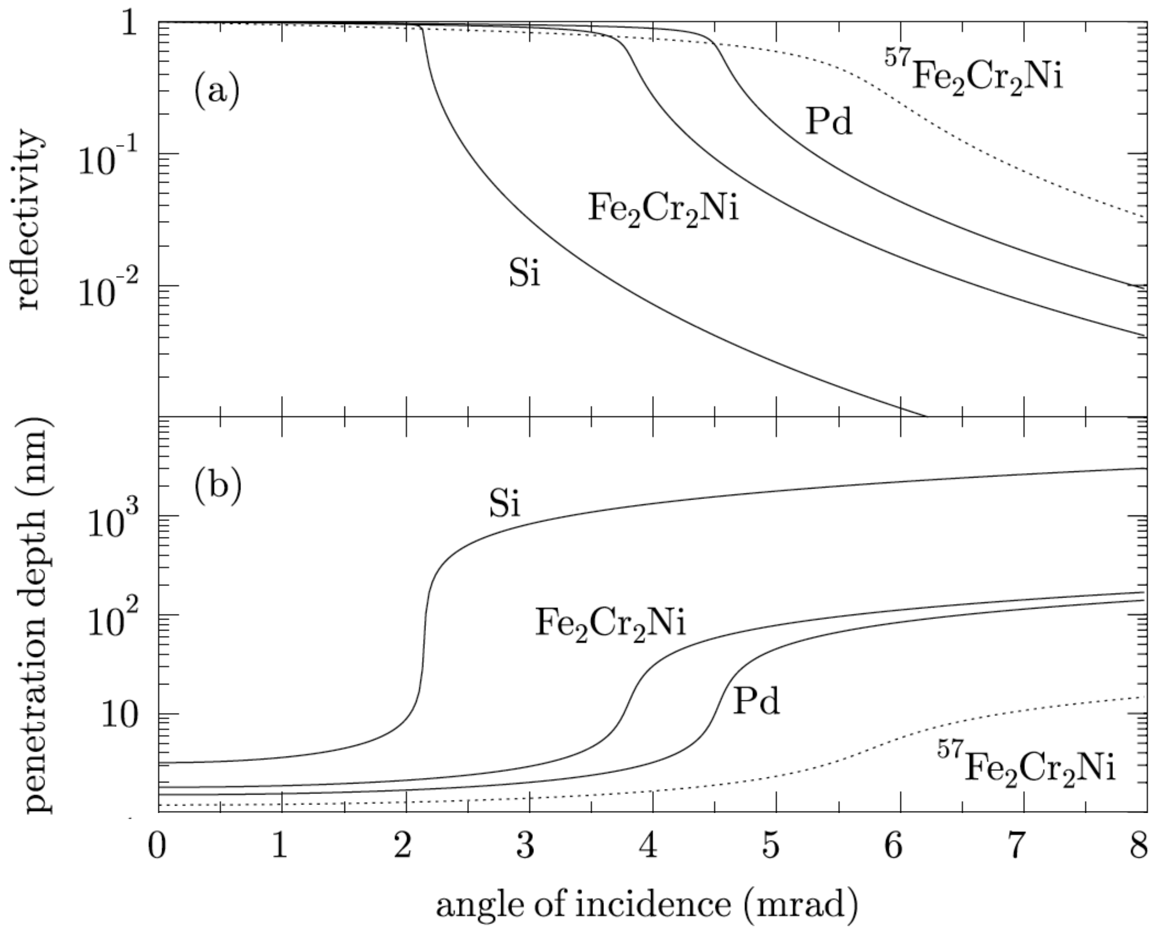
$$\varphi_c = \sqrt{2\delta}$$

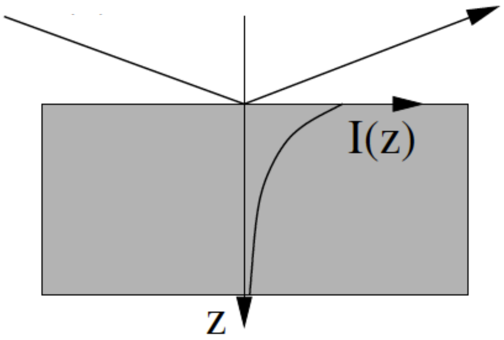


For angles $\varphi < \varphi_c$ the penetration depth of hard x-rays is only a few nm.

X-rays can be used for the study of structures at surfaces

X-ray Grazing Incidence and Penetration Depth





E = 14.4 keV