Berkeley Workshop on New Approaches to the Phase Problem for Non-Crystallographic Materials

17-19 May 2001

An Overview of Phase/Amplitude Retrieval from X-Ray Images

Stephen Wilkins, Tim Gureyev, David Paganin, Tim Davis, Sherry Mayo, Peter Miller,

D. Gao, D Parry, Andrew Pogany and Andrew Stevenson

CSIRO, Manufacturing Science & Technology

Clayton, Vic., Australia

X-Ray Technologies Pty Ltd

CSIRO

X-Ray Refractive Index

Generalized refractive index for x-rays :

$$n(\lambda) = 1 - \delta(\lambda) - i\,\beta(\lambda)$$

Absorption:

$$\beta(\lambda) = \frac{\lambda}{4\pi}\,\mu(\lambda) \sim O(\lambda^4) \sim O(1/E^4)$$

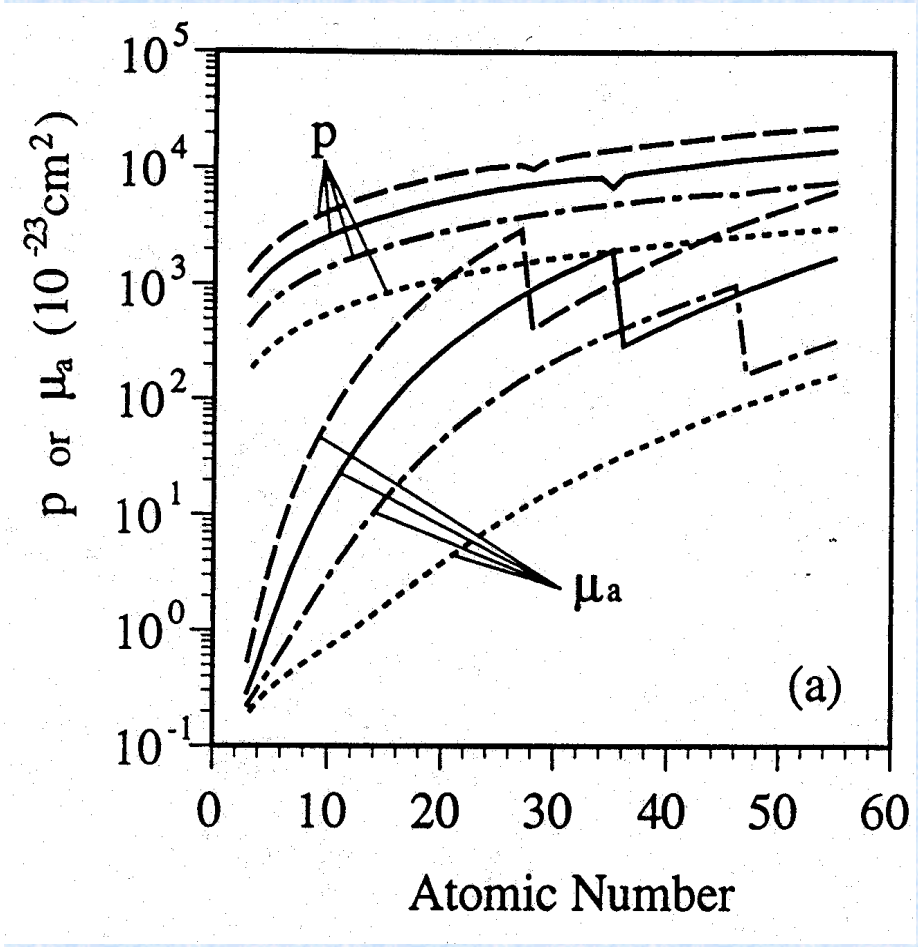
Pure refraction :

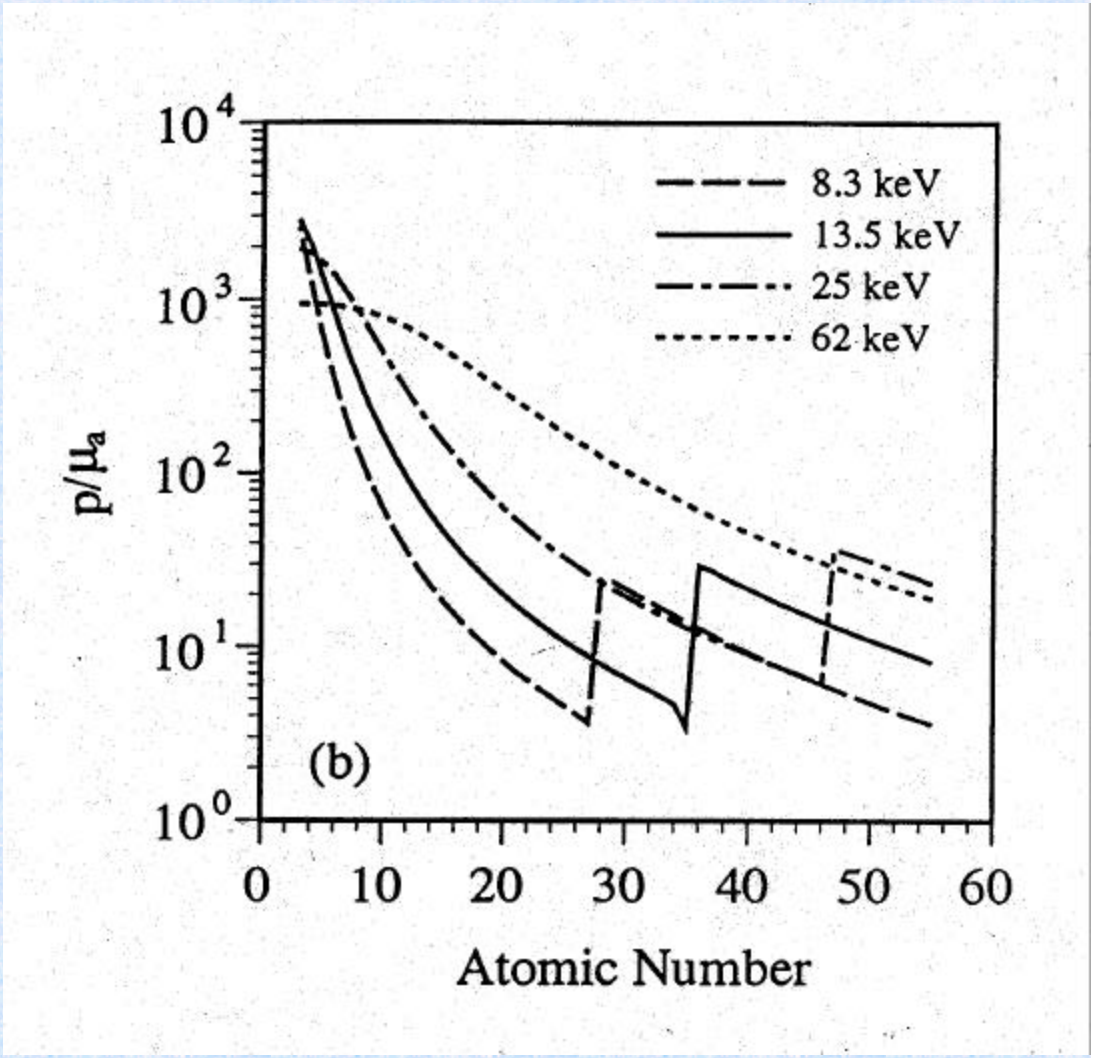
$$\delta(\lambda) = \frac{r_o \lambda^2}{2\pi} N_o f_R \sim O(\lambda^2) \sim O(1/E^2)$$

λ is the x-ray wavelength

$\delta \sim < 10^{-6}$!!

Absorption and Phase Cross-Sections





Calculated values for phase-shift cross-section p and absorption cross-section μ_a.as a function of atomic number (b) ratios of p to μ_a (from Momose & Fukuda,Med Phys. 1995, **22**, 375).

Phase and Sample Properties

Relationship for phase

$$\phi(x,y,z,k) = -k \int \delta(x,y,z';k)\, dz' = \frac{2\pi r_e}{k} \int \rho(x,y,z')\, dz' = O(\lambda)$$

where

$k = 2\pi/\lambda$

r_e - classical electron radius

ρ = electron density

Interferometric approaches to X-ray phase-contrast imaging

Bonse & Hart,

Appld Physics Letters, 1965, **7** , 99)

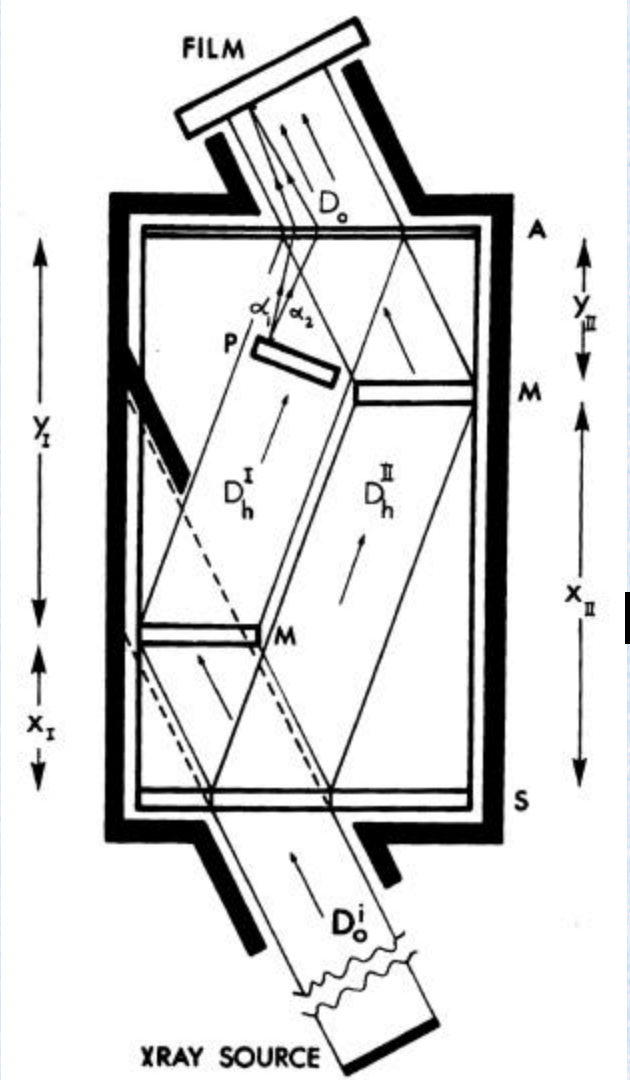


Fig. 2. Beam configuration. S—beam splitter, M—separated transmission mirrors, A—analyzer. Note the focusing effect of $K\alpha_1$ and $K\alpha_2$ if topographs are taken with the D_0 beam.

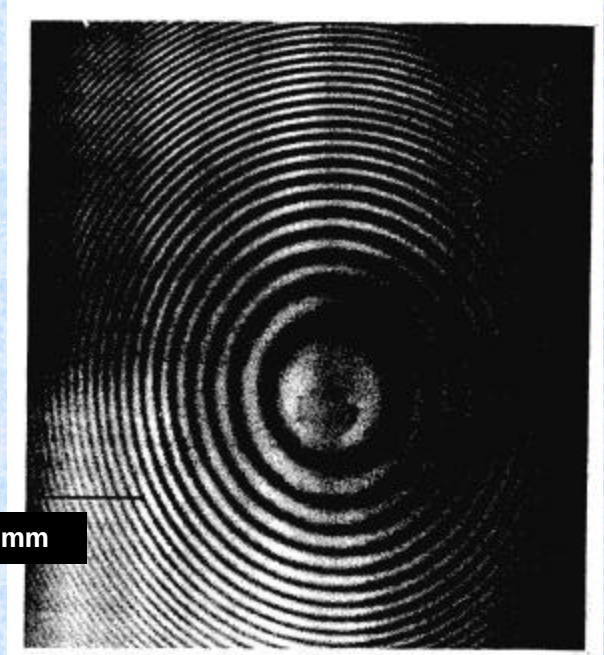
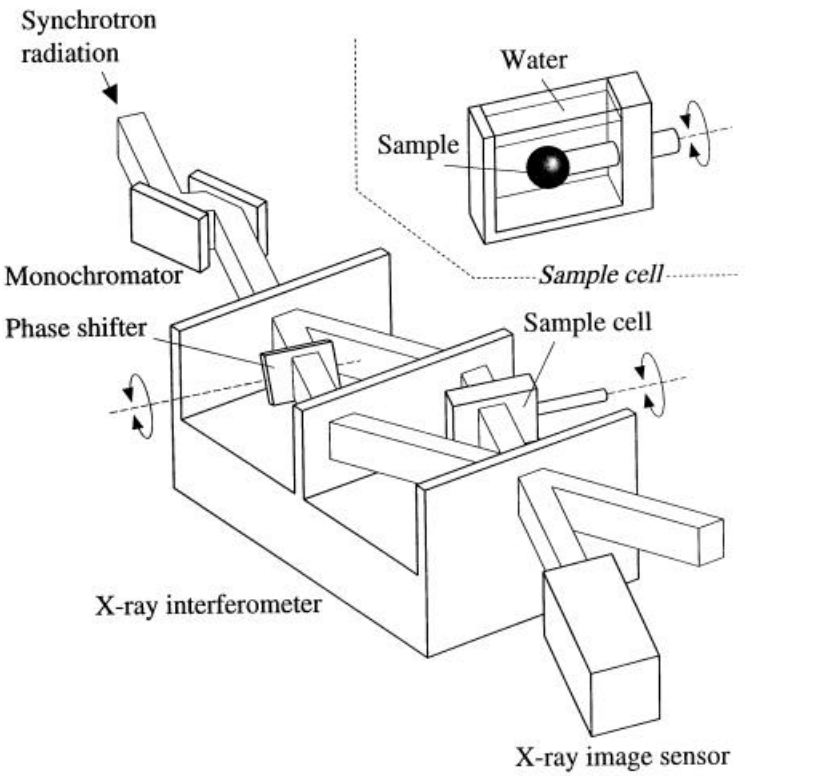


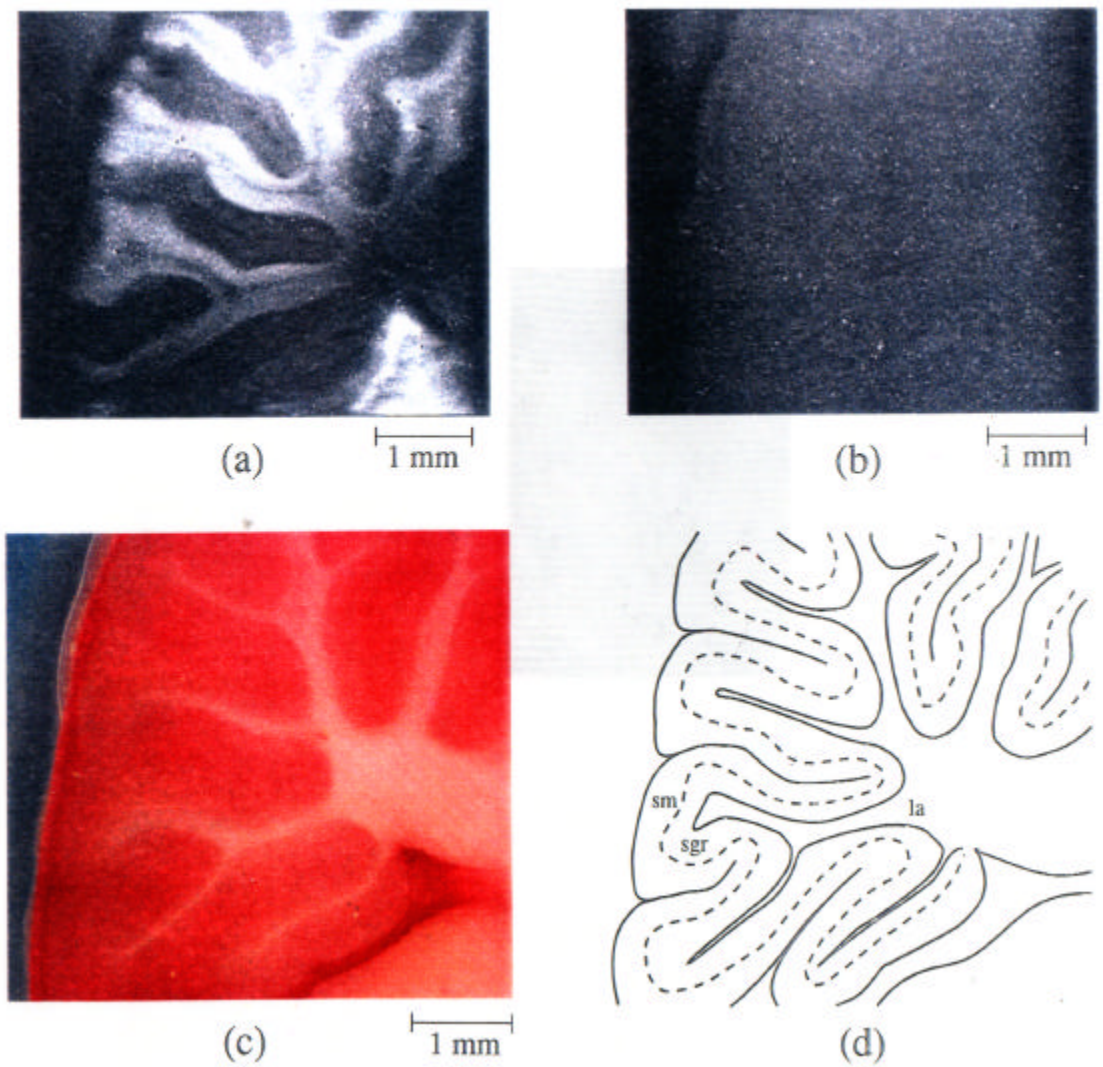
Fig. 4. Phase picture of plano-concave epoxy plate. Note the hole in the center of the plate. Scale mark is 1 mm.

2p ambiquity !

X-ray interferometry - ctd

Atsushi Momose et al, 1995-



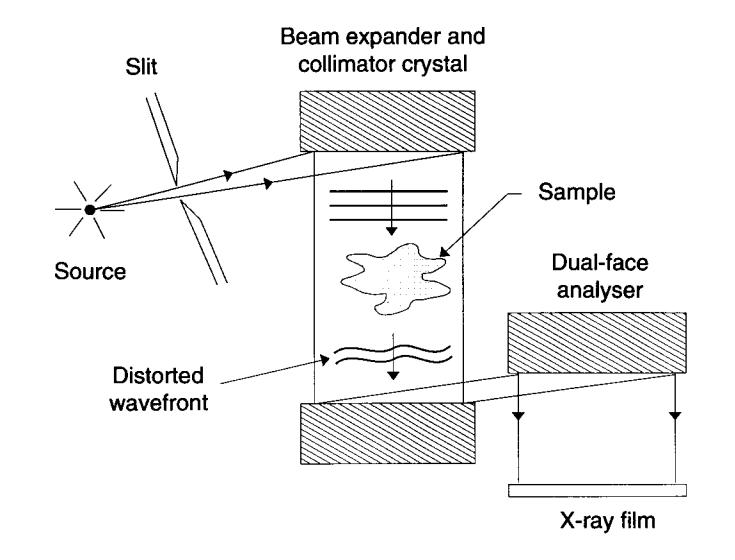


Very high sensitivity:

Dr / r » 10^{-9}

Crystal-Based approaches to X-Ray Phase-Contrast Imaging

Forster, Goetz & Zaumseil, *Kristal & Teknik* 1980, **15,** 937)



Davis, T.J. Gao, D. Gureyev, T.E Stevenson, A.W. & Wilkins, S.W. , *Nature 1995,* ***373,*** 595

Phase Contrast Imaging using perfect crystals (PCI) Chapman

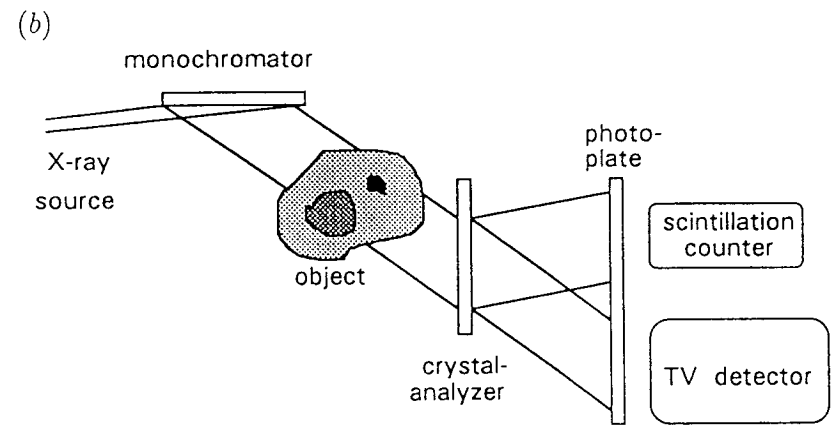


Figure 1. X-ray optic schemes of PDI: (*a*) triple-crystal and (*b*) double-crystal.

(Ingal, V.N. & Belyaevskaya, E.

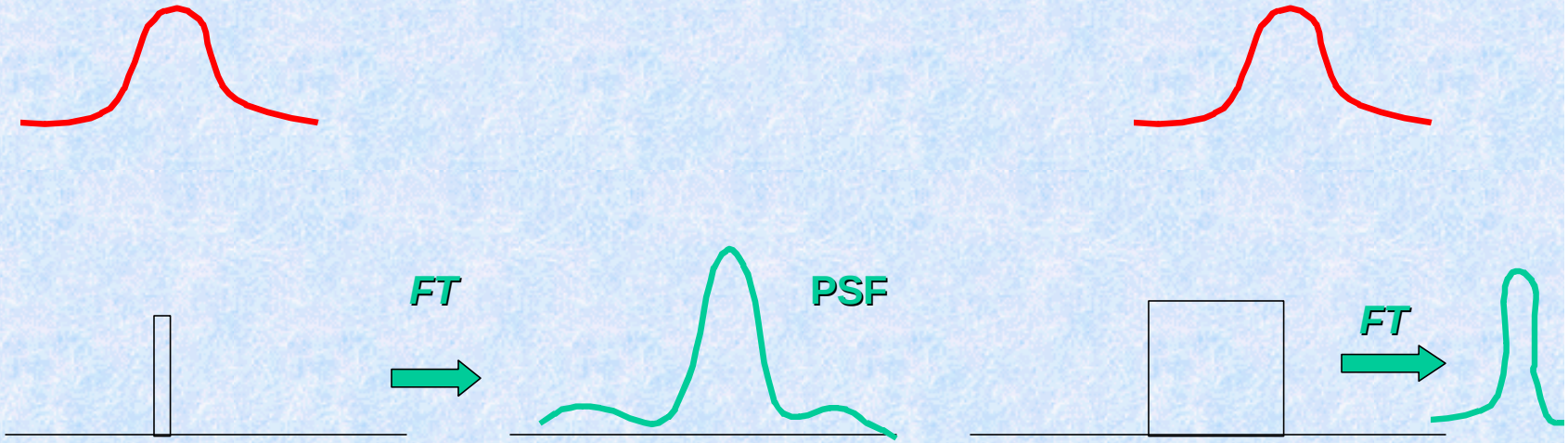
J Phys D: 1995, **28,**2314)

Phase Dispersion Introscopy (PDI) (Diffraction Enhanced Imaging = DEI, et al)

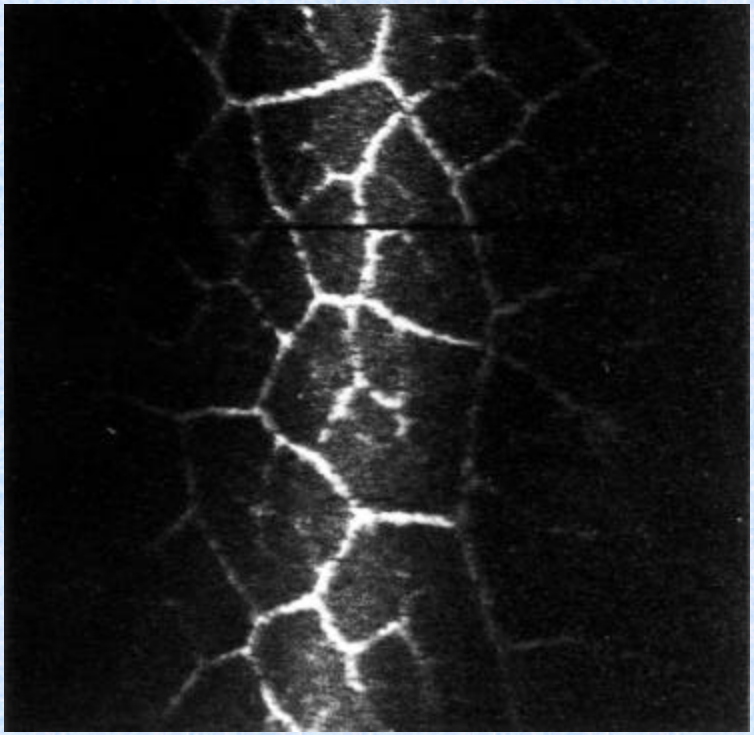
Regimes of X-Ray Phase-Contrast Imaging using Perfect Crystals

scattering
from sample:

ngular filter
analyzer xtal)
ocking curve:



“dark field”



eucalyptus leaf

(melliodora)

a “pure phase” object:

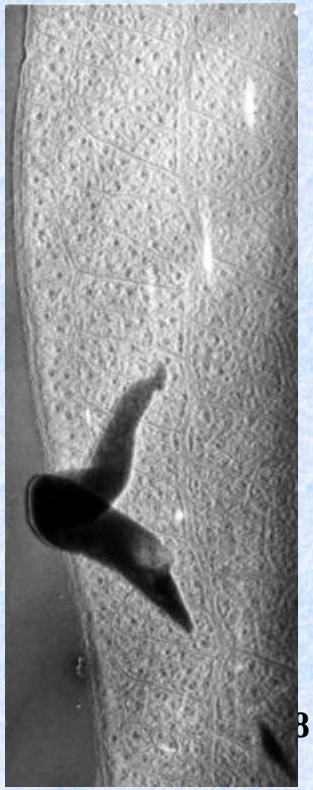
Ü E = 8keV

E =17keV Þ

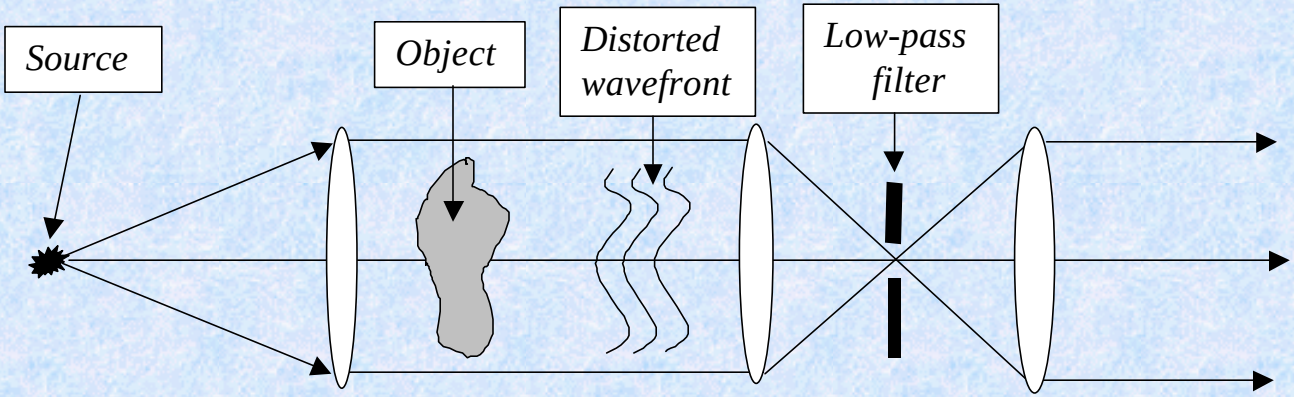
f

R(Ñf) » I/I$_o$

Recorded by
E Belyaevskaya =>



Optical analogy for double-crystal approach to PCI

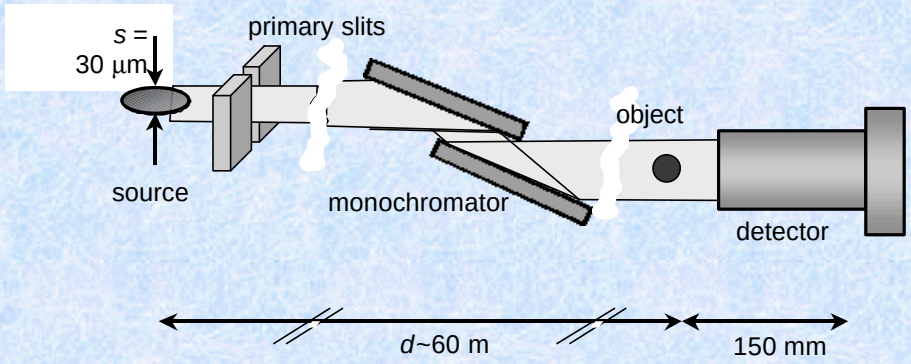


Optical analogy

Propagation-Based approaches to X-Ray Phase-Contrast Imaging

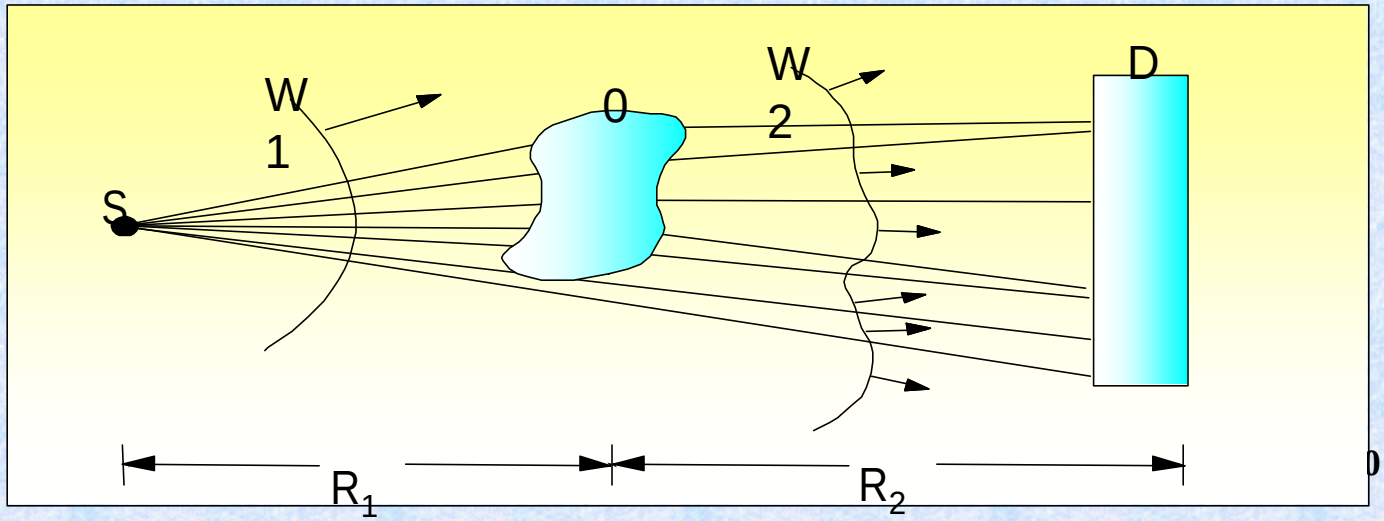
Snigirev et al using SR sources

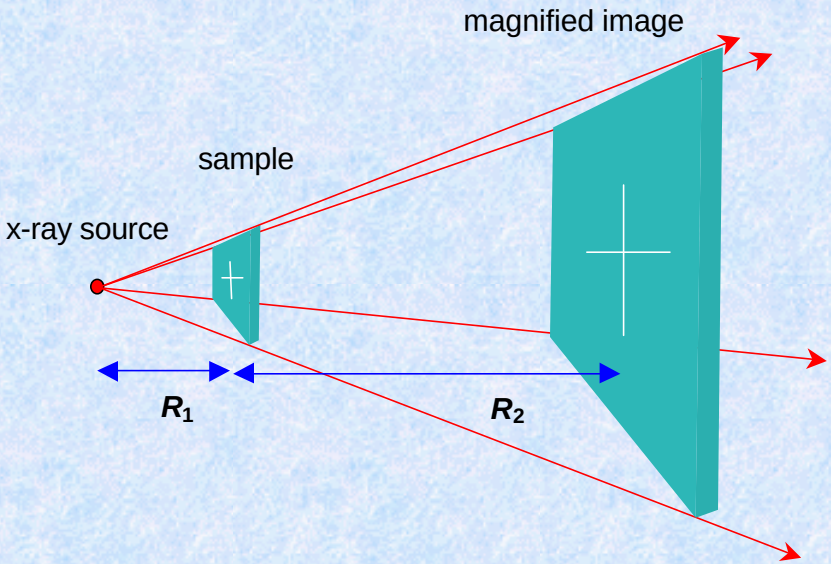
(1995)



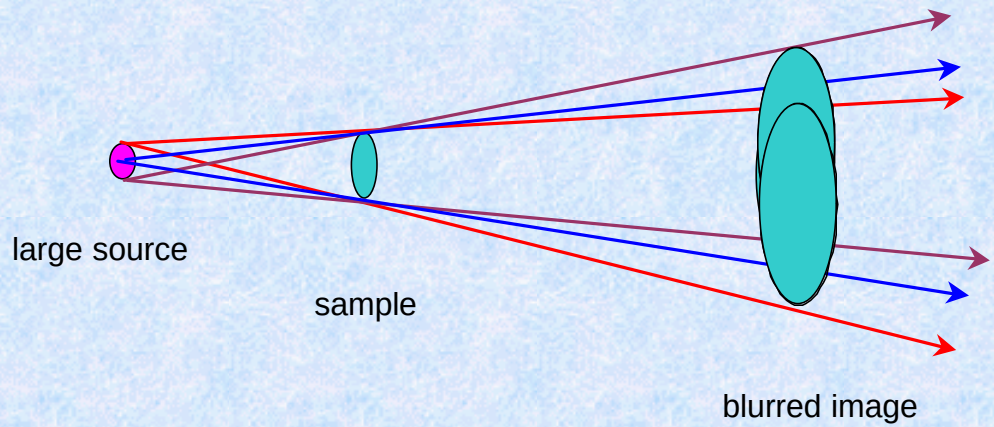
CSIRO group using lab-based (polychromatic) sources

(1996)

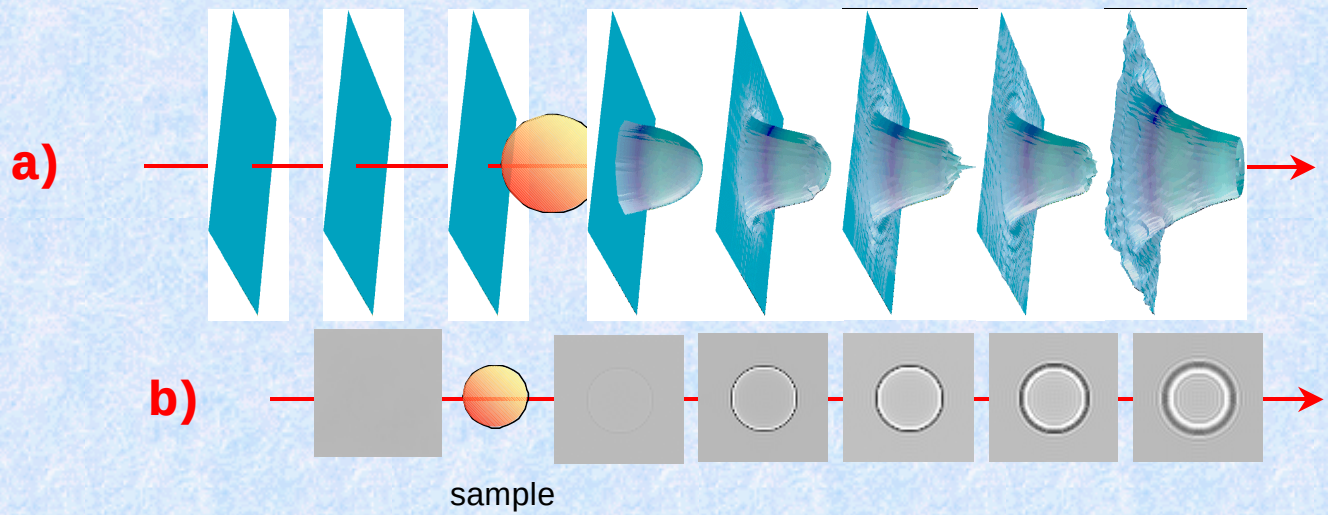




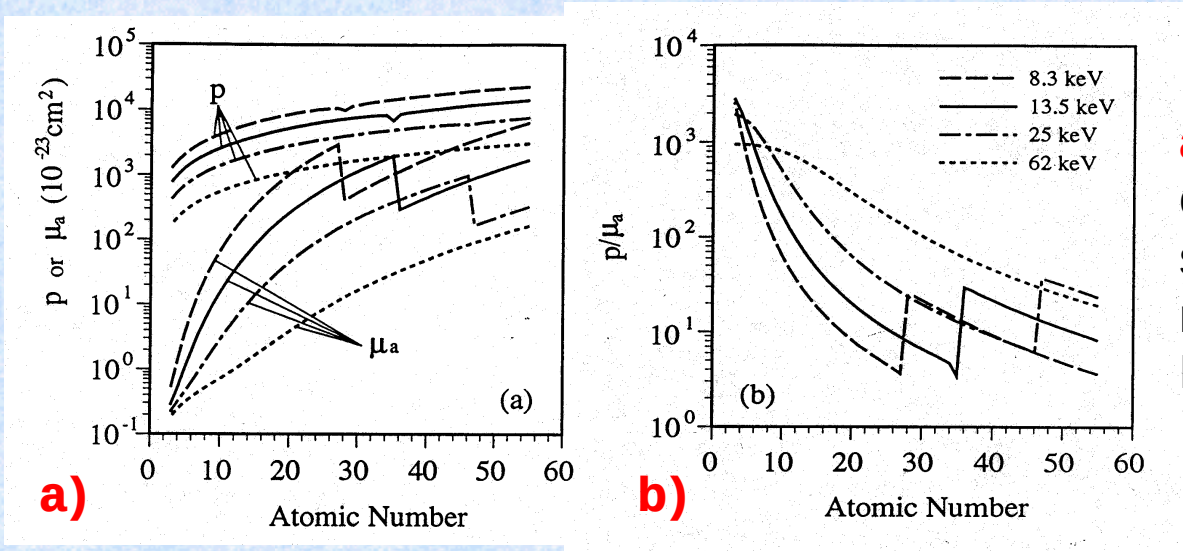
A schematic diagram of the point projection x-ray microscope.



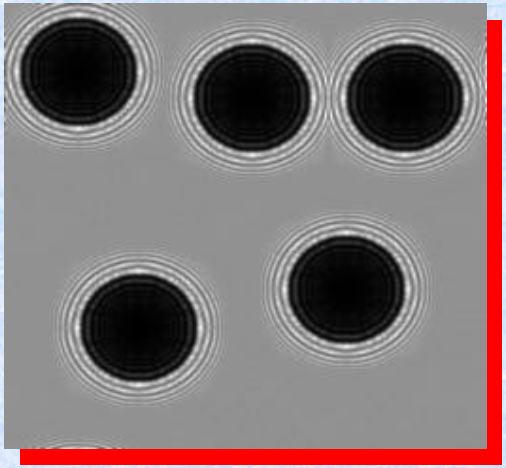
The size of the source determines the resolution of the projection microscope.



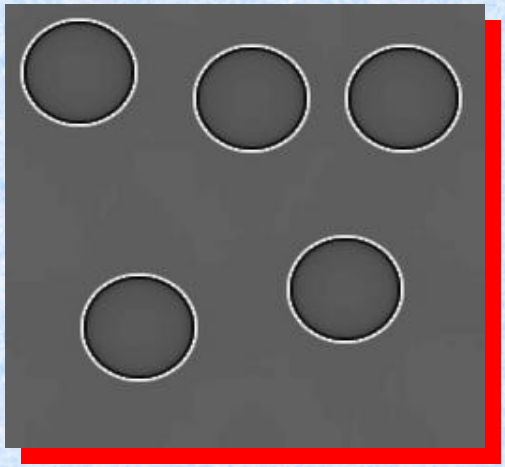
The development of the interference pattern of a wave after passing through a refracting sphere. **a)** the development of the phase profile; **b)** the development of the intensity.



a) Calculated values for phase-shift cross-section p and absorption cross-section μ_a.as a function of atomic number. **b)** ratios of p to μ_a (from Momose et al).



a)



b)

Energy dependence of XUM images of 5 micron carbon spheres

a) Simulated XUM image of 5 micron carbon spheres using 10 Å (1.24 keV) x-rays and R' = 1mm.

Other parameters:

δ= 0.32 10^{-3}, β = 0.20 10^{-4},

ϕ= -20021 rad/cm, μ = 2561 cm^{-1},

$t_{2\pi}$ = 3.14 um (2π phase thickness).

b) Same sample for 1 Å (12.4 keV) x-rays and R' = 1mm.

Other parameters:

δ= 0.30 10^{-5}, β = 0.1776 10^{-8},

ϕ= -1917 rad/cm, μ = 2.232 cm^{-1},

$t_{2\pi}$ = 32.8 um (2π phase thickness)

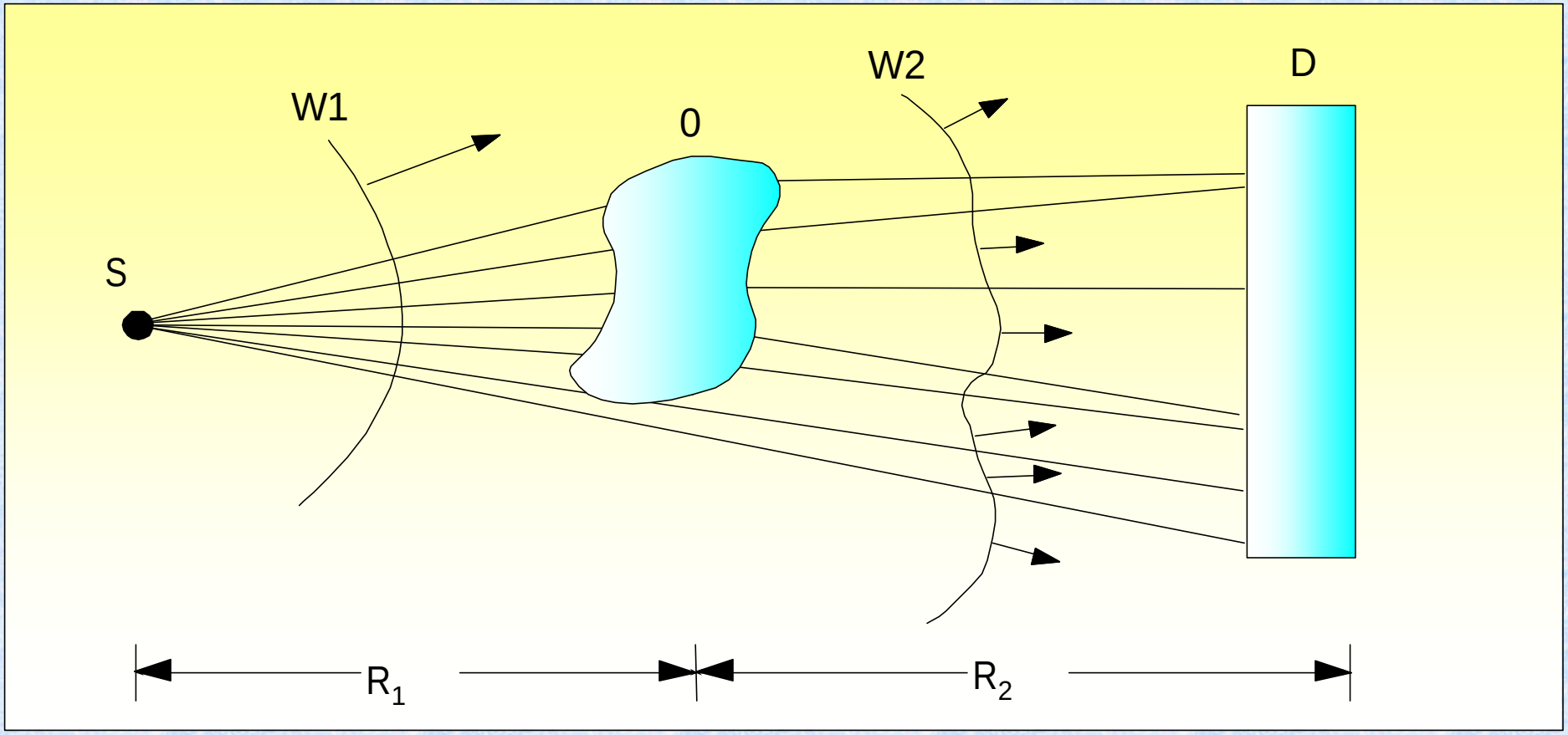


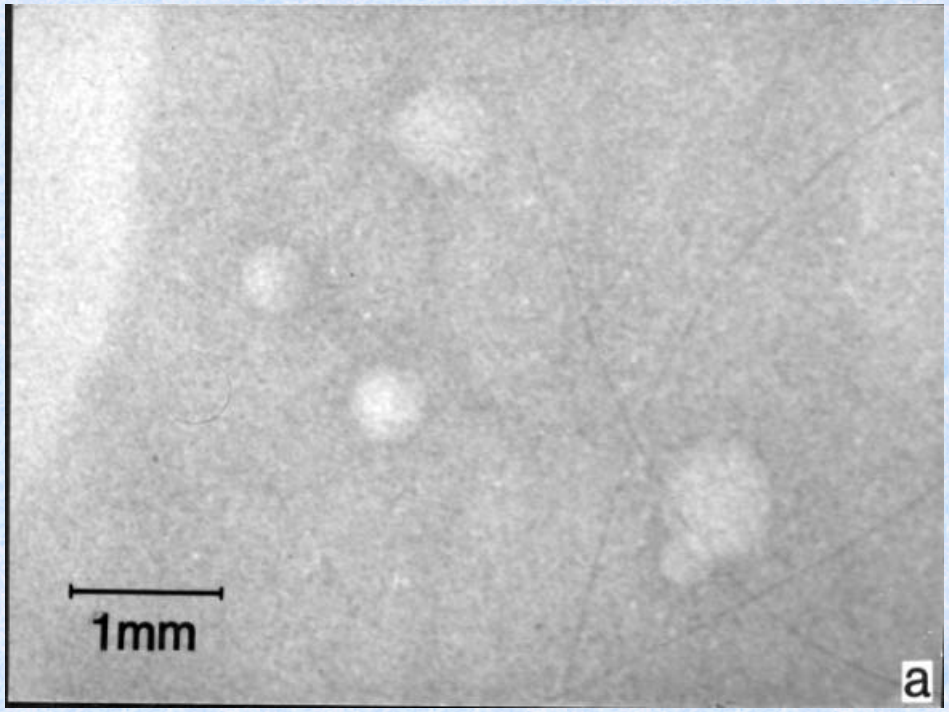
Fig. 1. Experimental geometry using the polychromatic "in-line" method, where *S* is a Kevex microfocus X-ray source (10 ! m); **O** the object; **D** the imaging detector; $\mathbf{R_1}$ the source-object distance; $\mathbf{R_2}$ the object-image distance.

Point Projection Imaging with a Microfocus Source

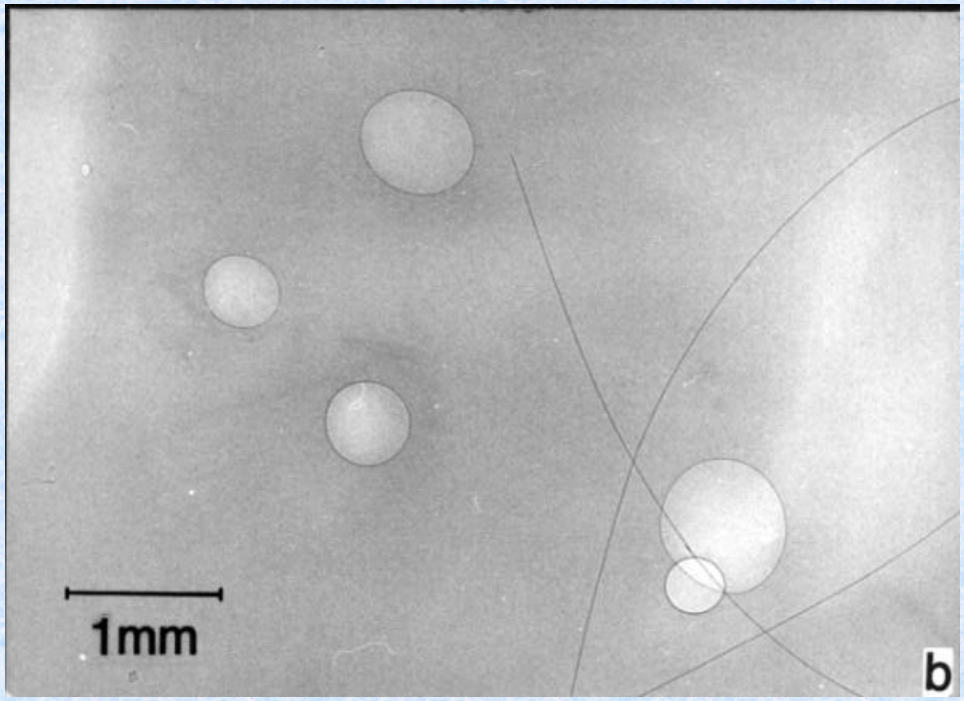
1. Have magnification therefore don't need high spatial resolution detectors
2. Don't need x-ray optics or high precision mechanics
3. Don't need (very high) chromatic coherence

Phase-Contrast Radiography (PCR)

Images of a polymer glue containing 10 mm fibres and bubbles



contact image



phase-contrast image

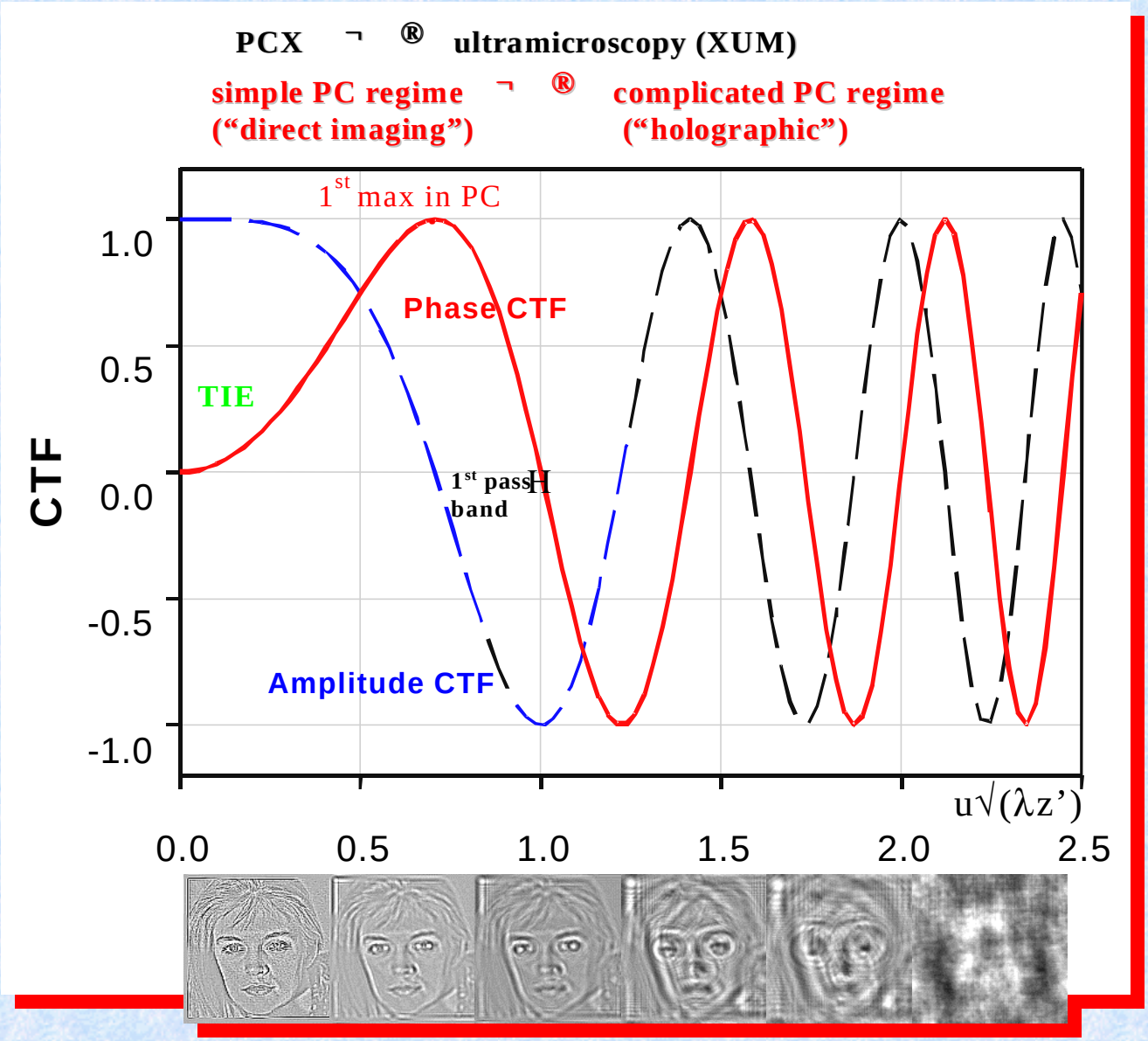
The Weak (Phase) Object Approximation

Fourier optics approach - "phase grating"

(see Cowley & Moodie, 1960)

$$\exp(-i\,\mathrm{f} - \mathrm{m}t) \approx 1 - i\,\mathrm{f} - \mathrm{m}\,t$$

Point source



Contrast Transfer Function (CTF) for phase and absorption information contained in the object. The thumbnail images of "Holly" taken as a pure phase object show the effect on image structure of imaging in different regimes. Note: all images might in principle be used to try to obtain the same information about the object ("Holly")

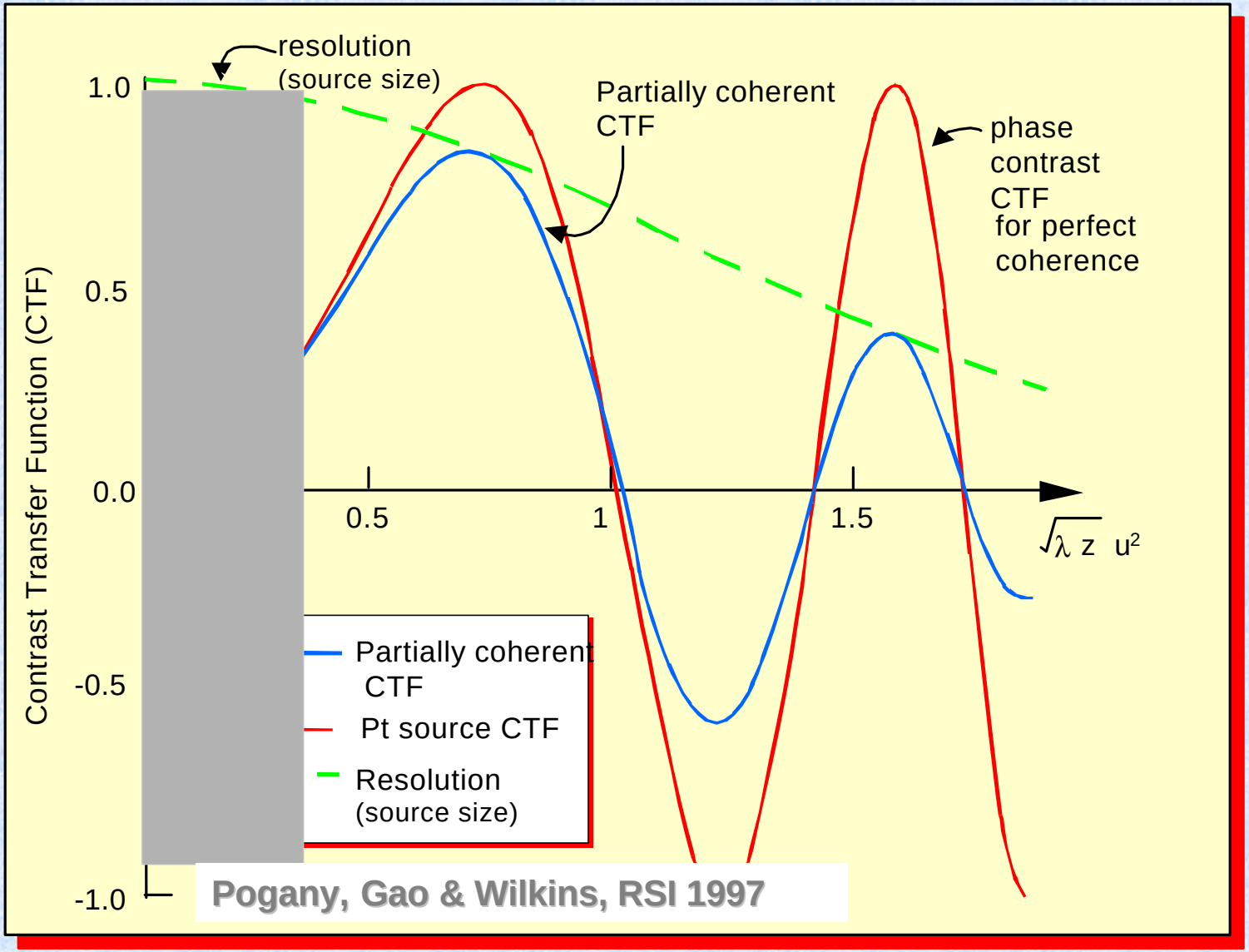
Transport of Intensity Equation (TIE)

$$k[I(\boldsymbol{r}_\perp, z+R) - I(\boldsymbol{r}_\perp, z)]/R \cong -\nabla_\perp \bullet [I(\boldsymbol{r}_\perp, z)\nabla_\perp j(\boldsymbol{r}_\perp, z)]$$

Zero absorption case:

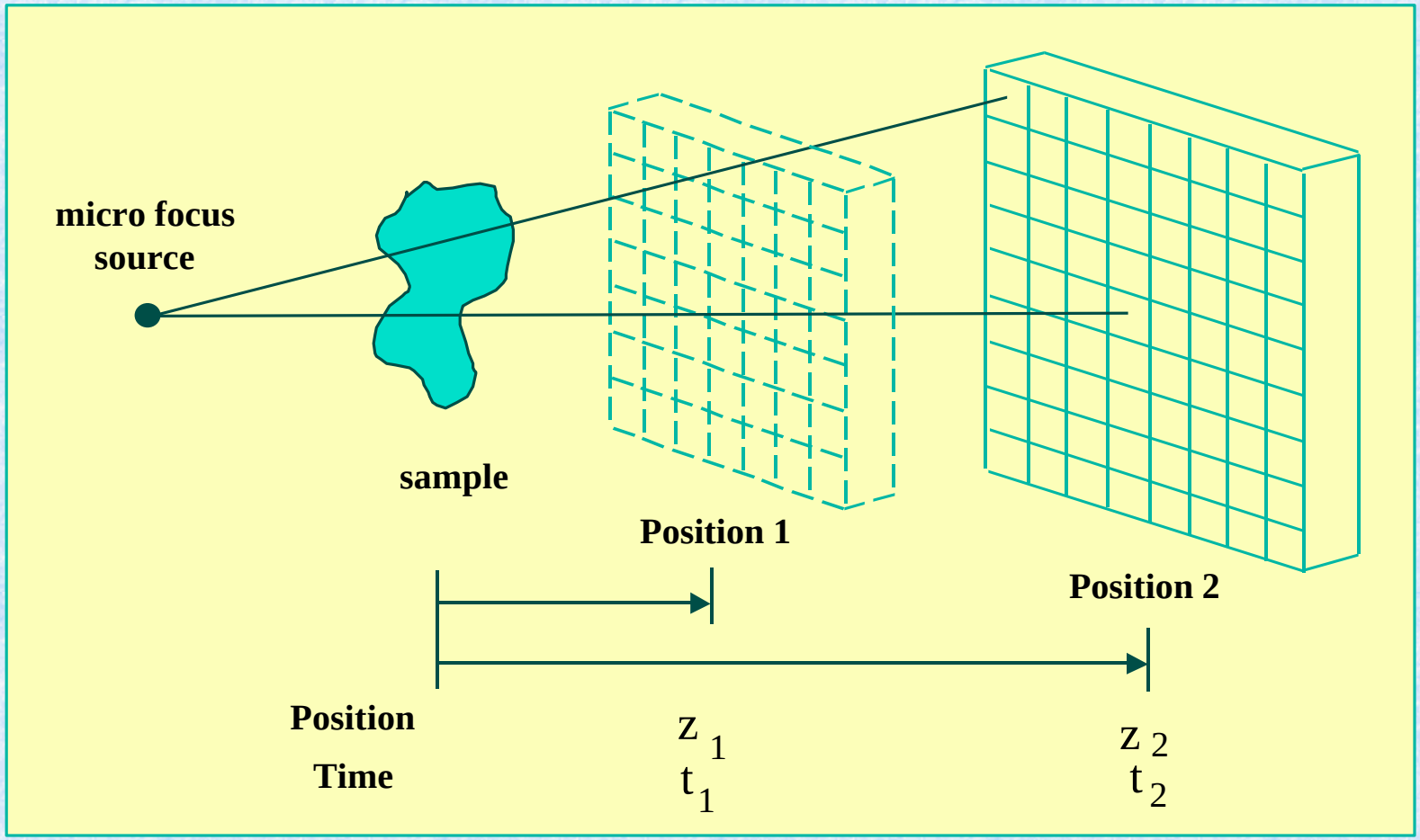
$$k[I(\boldsymbol{r}_\perp, z+R)/I(\boldsymbol{r}_\perp, z) - 1]/R \cong -\nabla_\perp^2 j(\boldsymbol{r}_\perp, z)$$

Here $I(\boldsymbol{r}_\perp,z)$ is intensity, $j(\boldsymbol{r}_\perp,z)$ is phase, $\boldsymbol{r}_\perp=(x,y)$, $k=2p/l$, R is the propagation distance and $\nabla_\perp=(\P_x, \P_y)$ is the 2D (transverse) gradient, $\nabla_\perp^2$ is Laplacian.



Contrast Transfer Function showing effect of damping term due to finite source size

The 2-Position Method of Determining Separate Absorption and Phase-Contrast Images



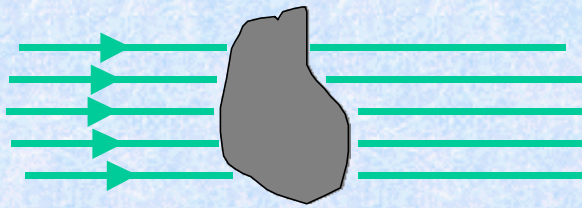
Geometrical Configurations for X-Ray Imaging

Reduced distance parameter in CTF:

$$z = R_1 R_2 / (R_1 + R_2)$$

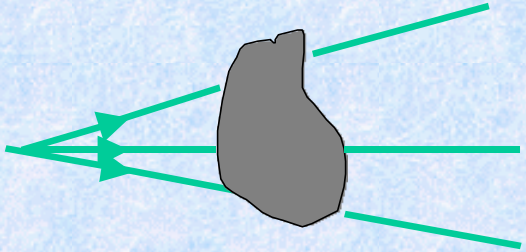
1. Plane wave case (e.g. synchrotron):

$$R_1 >> R_2 \quad \text{Þ} \quad z \;\text{»}\; R_2$$

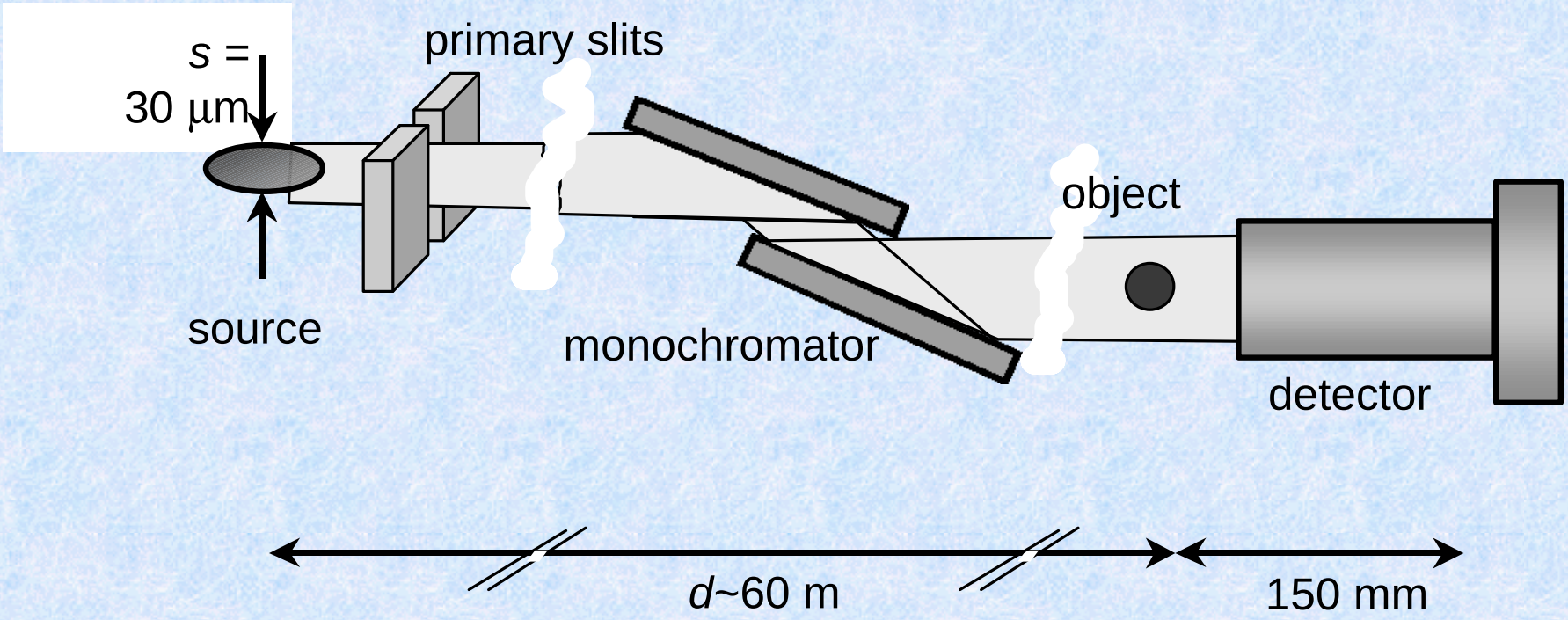


2. Point projection (microscopy) case:

$$R_2 >> R_1 \quad \text{Þ} \quad z \;\text{»}\; R_1$$



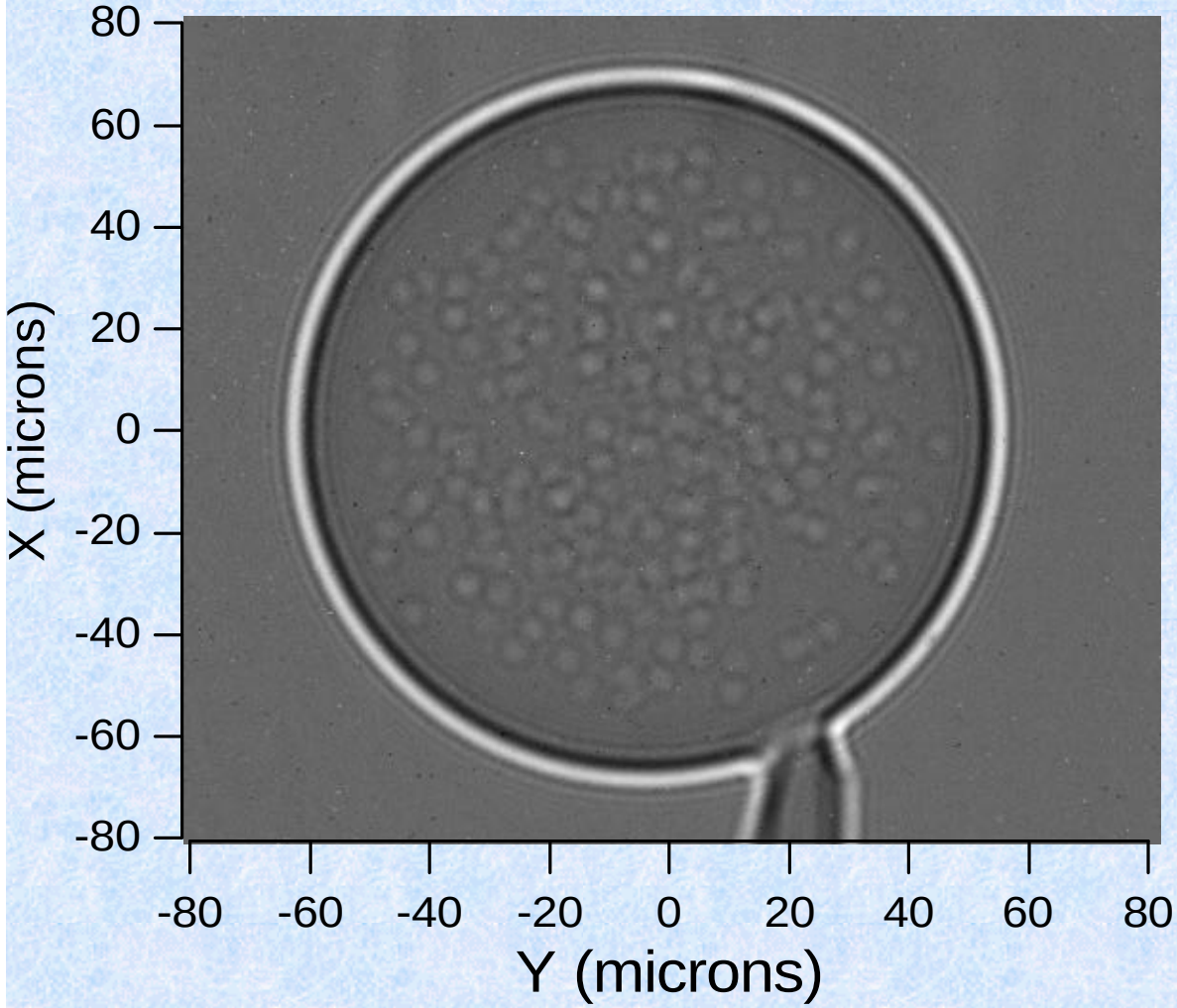
Plane-wave experiments on phase extraction using SR



ID-22 at ESRF - Snigirev

SR-based measurements of phase

118 micron polystyrene sphere



Carried out at ERSF- ID22:

Gureyev, Raven, Snigirev, Snigireva & Wilkins

J Phys. D: Appld Phys. 32 (1999), 865.

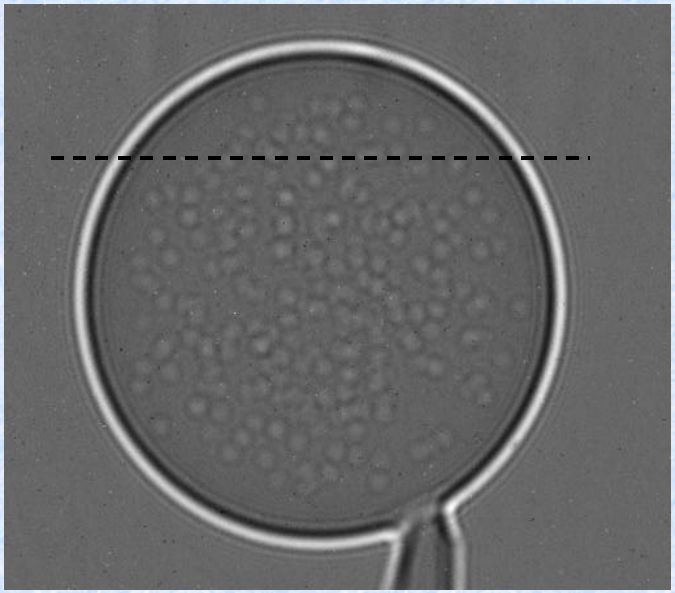
E = 19.6 keV

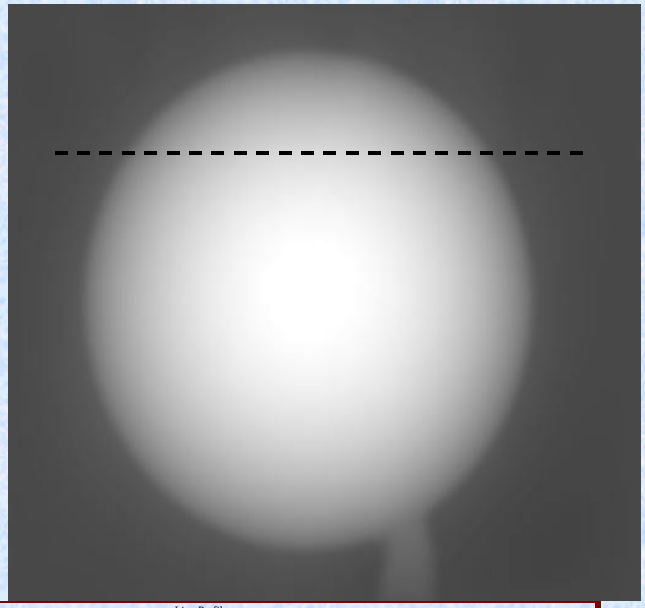
(absn ~ 0.25 %)

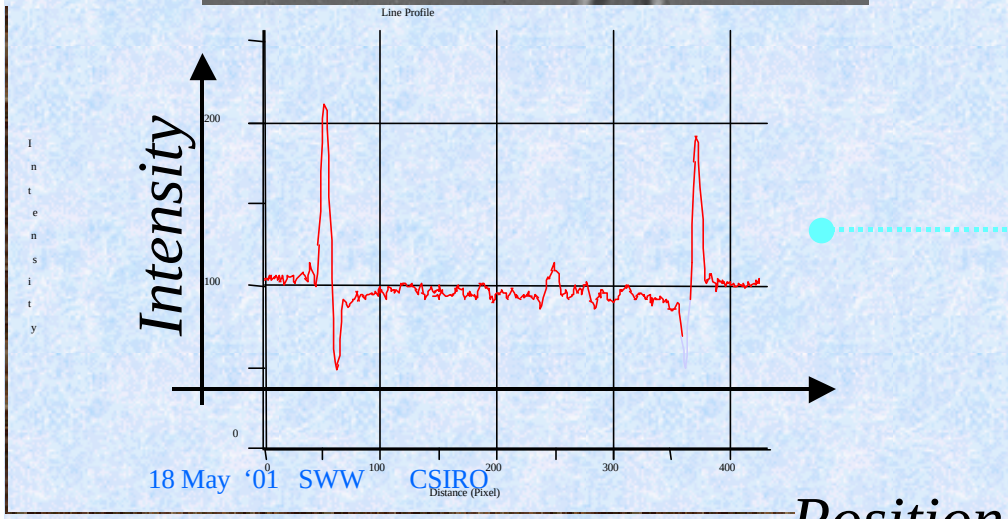
Fig. 3

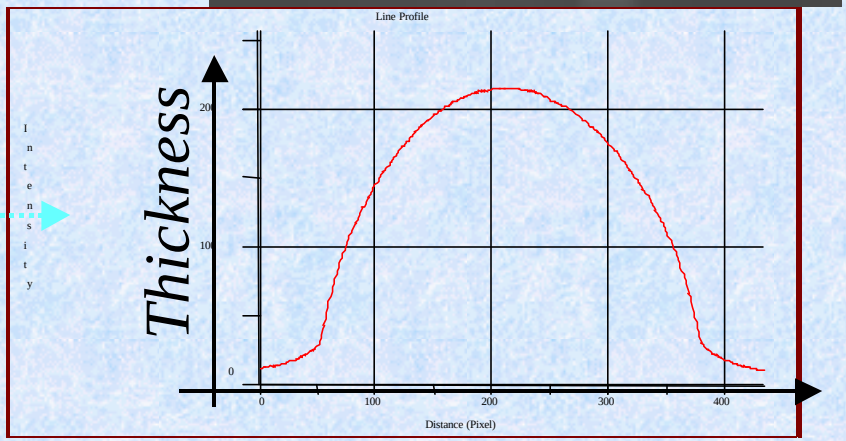
Role of Phase Retrieval in In-Line Imaging

2. Restoration of the True Shape of an Object

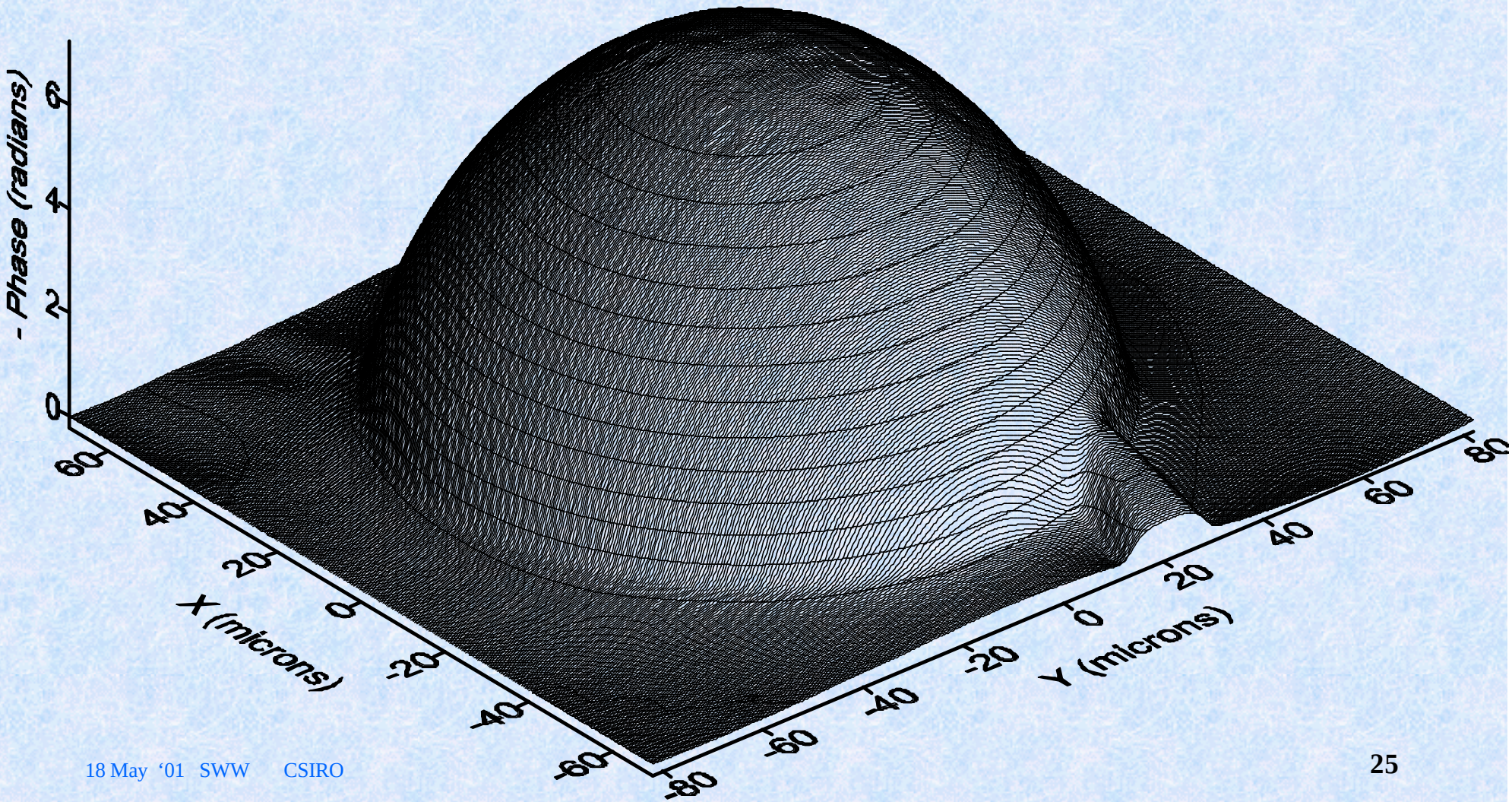








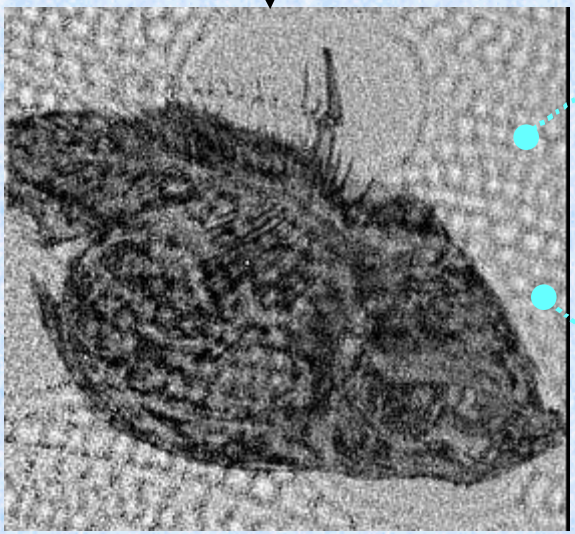
Retrieved Phase for Polystyrene Sphere

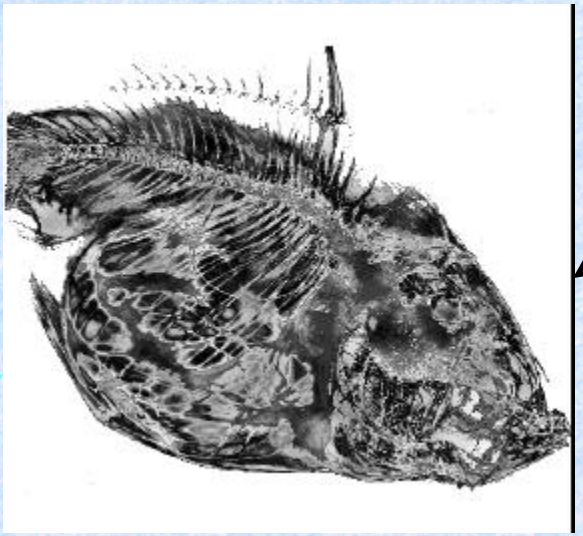


Role of Phase Retrieval in In-Line Imaging

1. Separation of Phase from Amplitude Contrast (Multi-Distance)

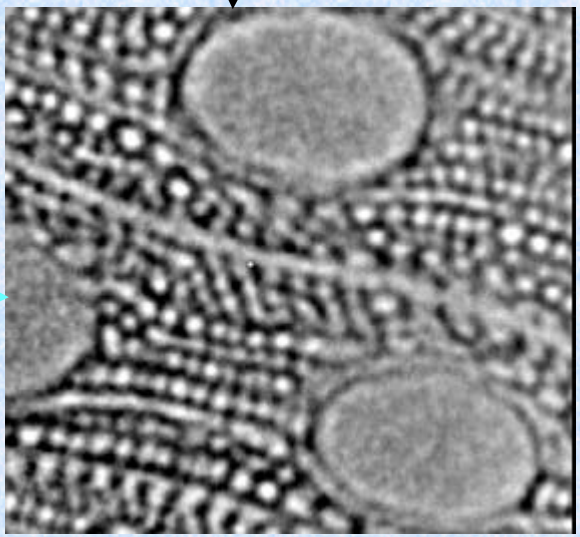
"Experimental" in-line image (amplitude/phase)



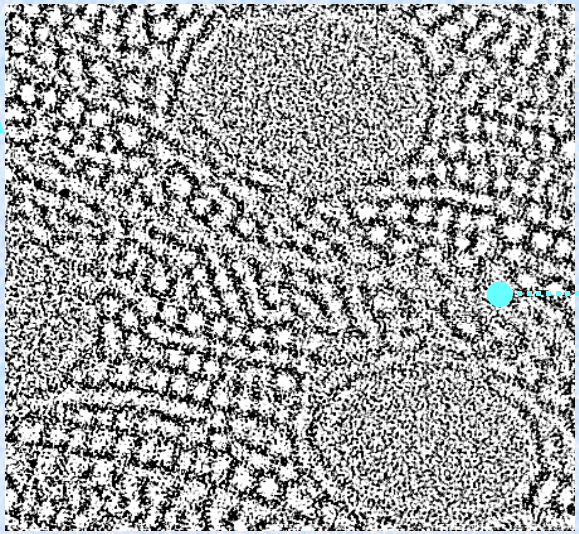


Extracted intensity $\exp[-\mu t(x,y)]$

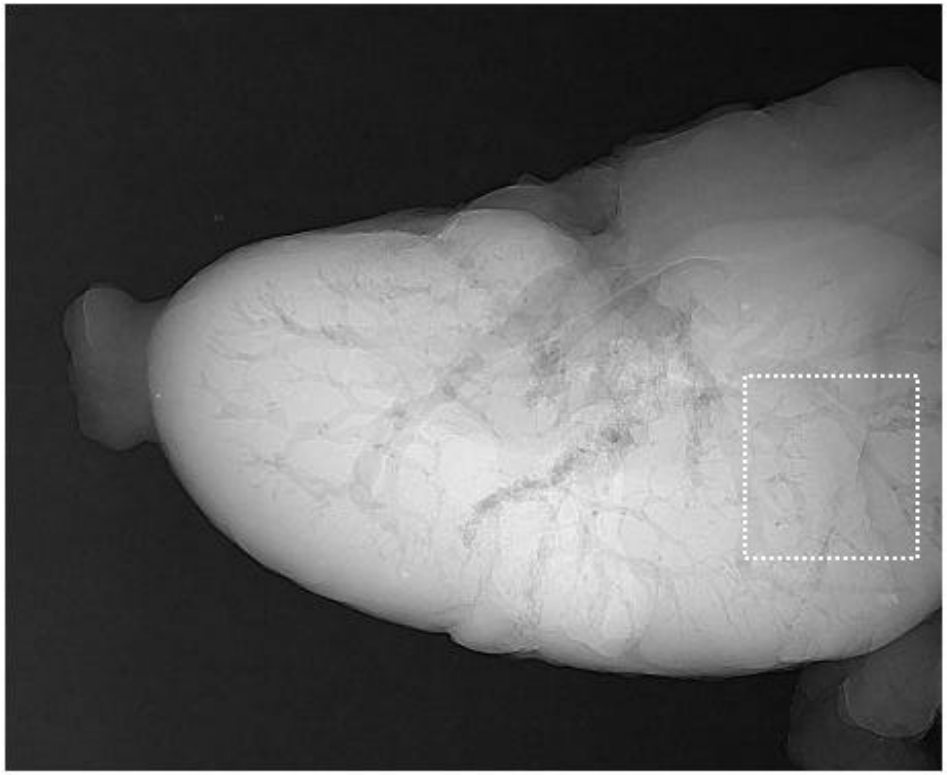
Extracted phase $\varphi(x,y)$



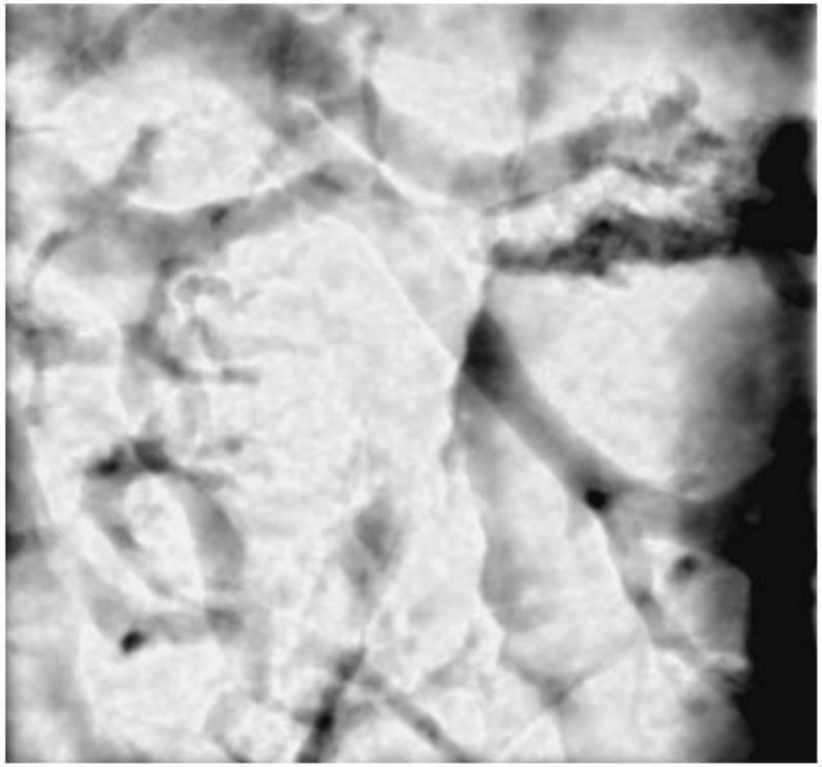
Extracted phase Laplacian $-\nabla^2\varphi(x,y)$



Quantitative Phase



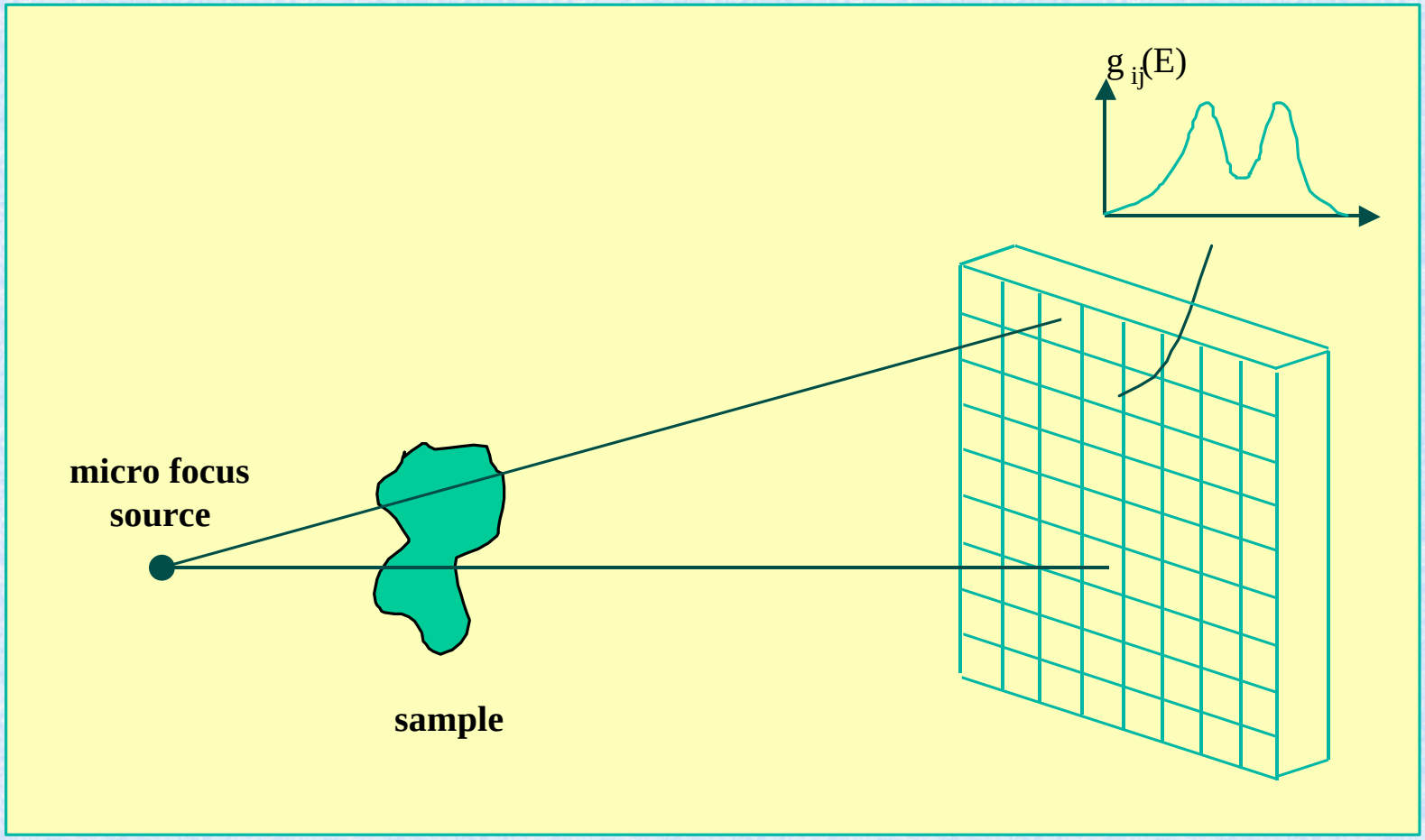
(a)



(b)

Excised mouse kidney - thickness determination

The Energy Sensitive 2-D Detector Method for Determining Separate Phase-Contrast and Absorption Contrast Images



Comparison of general features of the some specific Phase-Contrast Imaging techniques

Technique	Phase Quantity	Comment	Sensitivity ($\Delta r/r$)
1. Interferometry	f	modulo 2π	10^{-9}
2. Crystal-Based	$\tilde{N} f$	PDI/DEI regime	10^{-9} ?
3. Propagation-Based	$\tilde{N}^2 f$	TIE regime	?

Lab Based X-ray Ultramicroscope

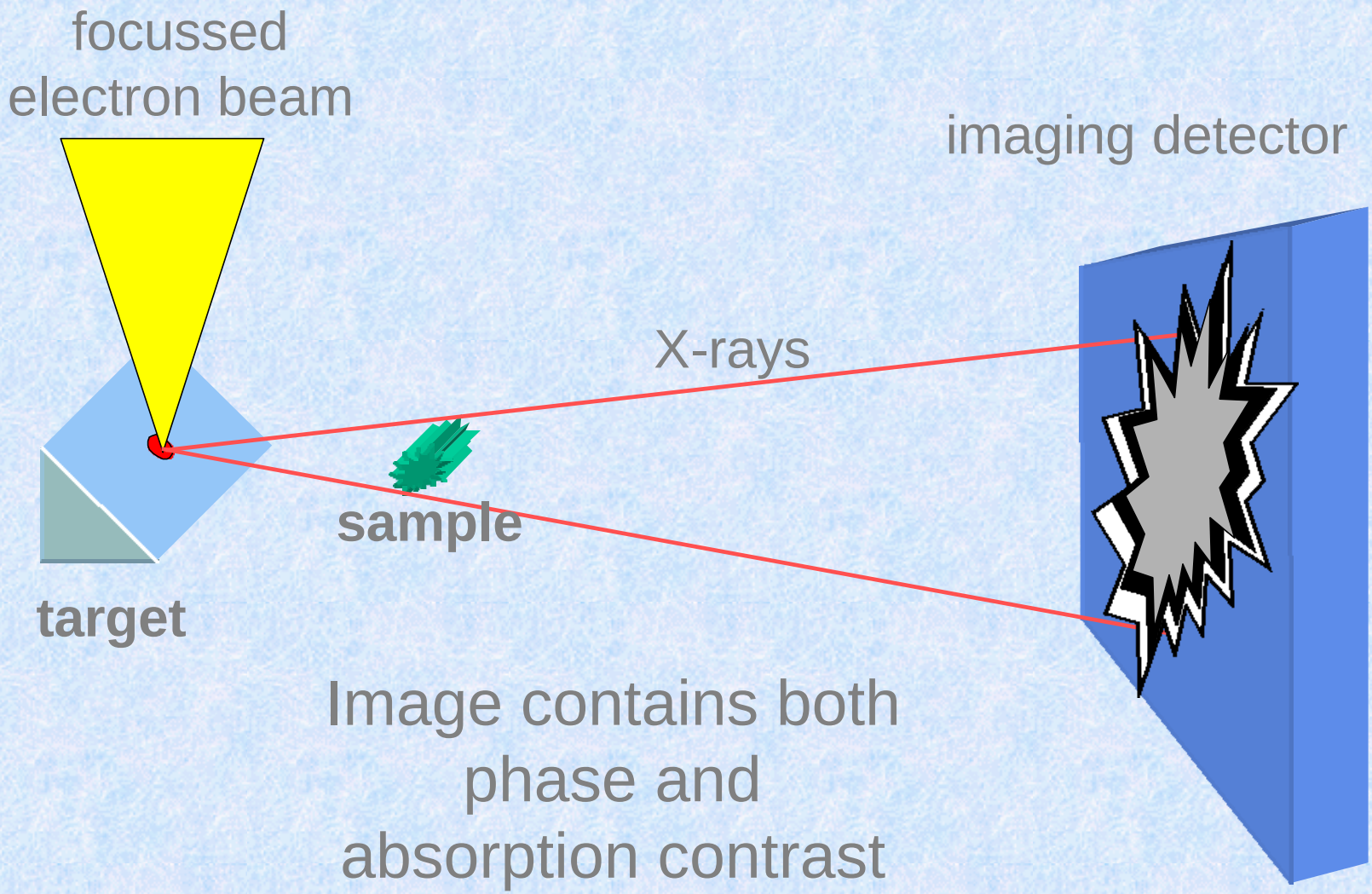


Image contains both
phase and
absorption contrast

X-RAY ULTRAMICROSCOPY

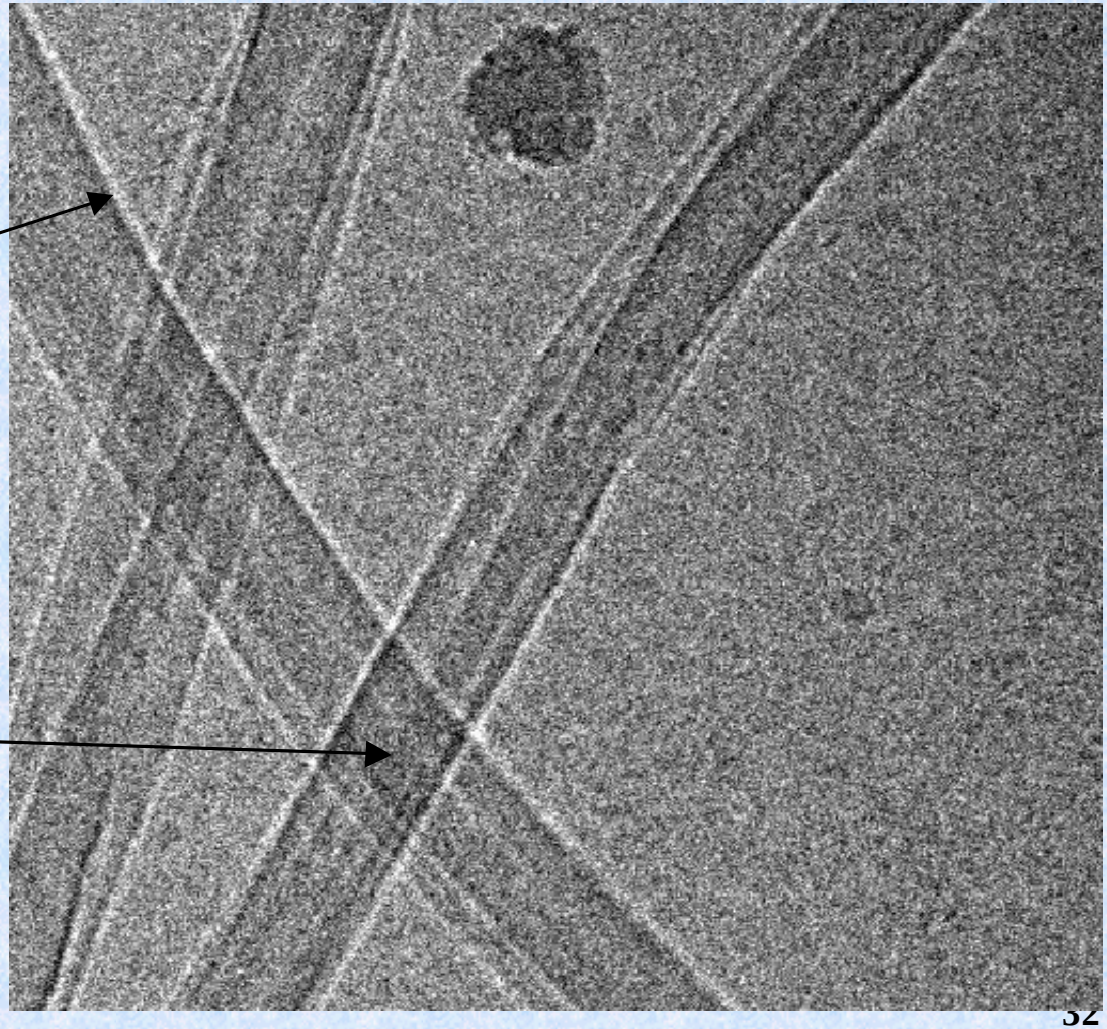
Advantages of XUM:

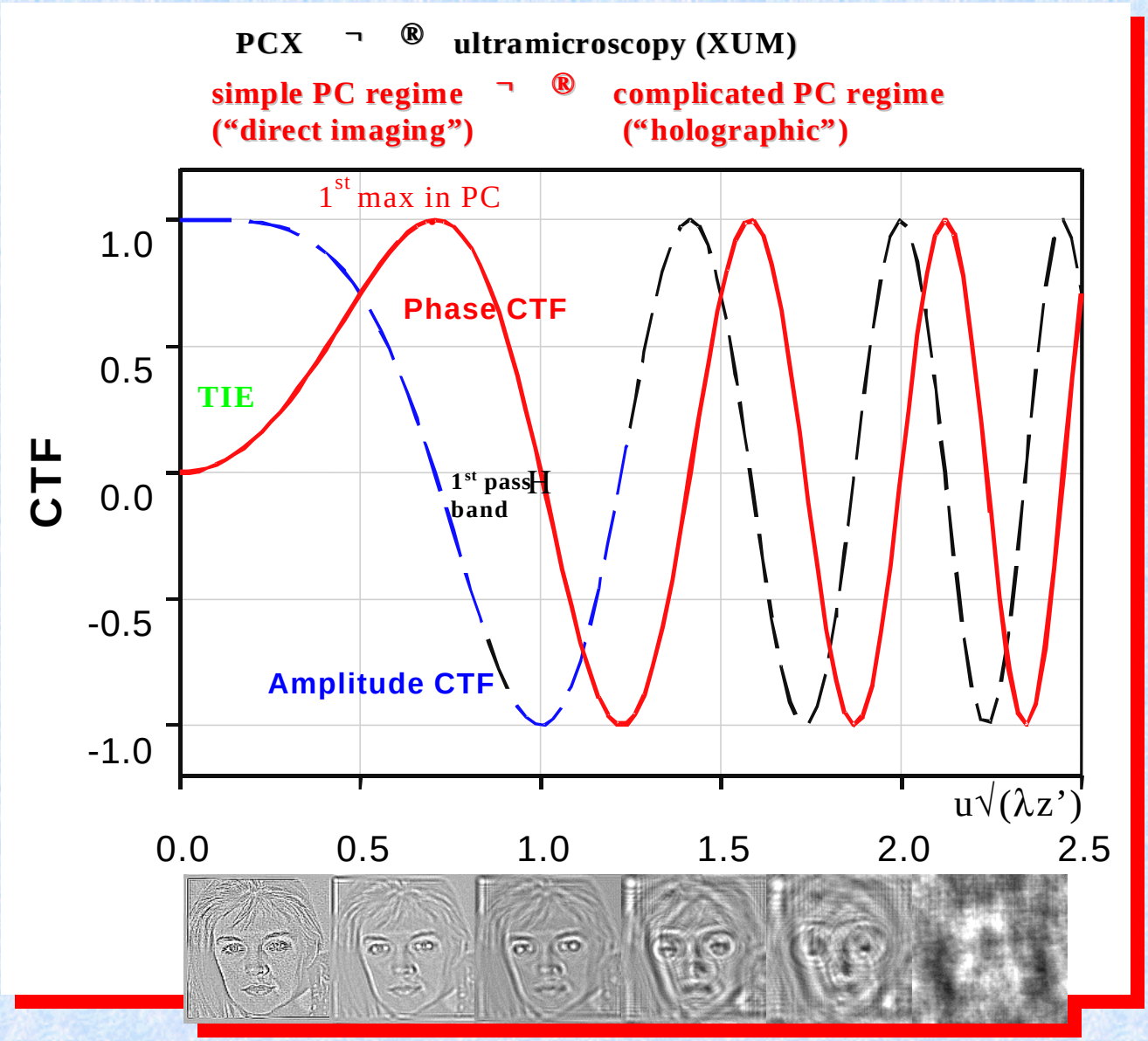
- resolution not limited by optics
- no (or simpler) aberrations
- versatile (many different types of sample cells)

Amplitude and phase contrast in in-line imaging

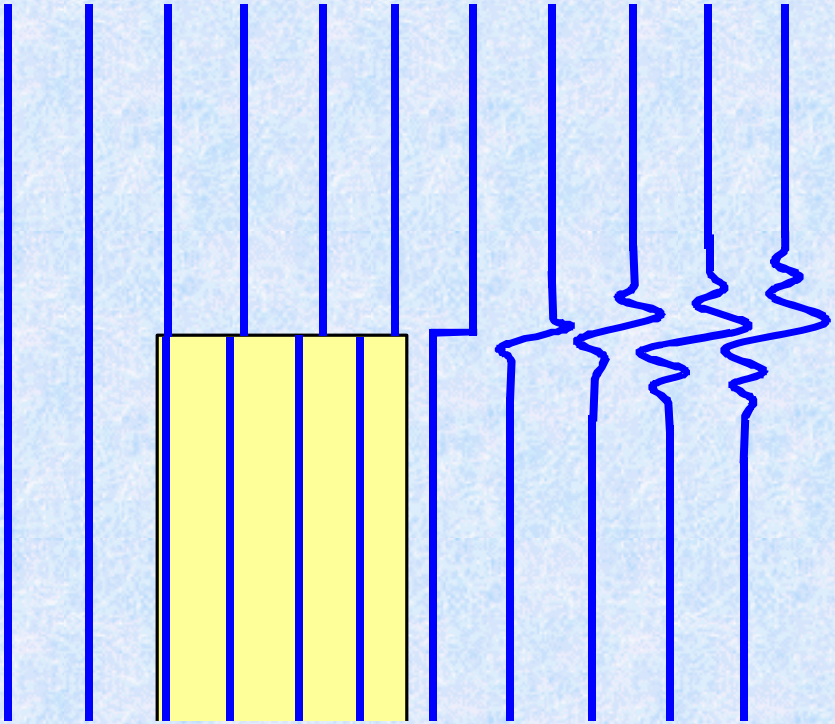
Phase contrast (sharp black/white stripes near the edges)

Absorption contrast (darker and lighter areas)





Contrast Transfer Function (CTF) for phase and absorption information contained in the object. The thumbnail images of "Holly" taken as a pure phase object show the effect on image structure of imaging in different regimes. Note: all images might in principle be used to try to obtain the same information about the object ("Holly")



Schematic illustration of the effect of loss of spatial resolution in an image due to diffraction effects. Immediately after the object the wavefront (phase) change is very sharp. However, on propagation this sharp feature becomes spread out laterally in space. Note that in the TIE approximation, intensity is related to Laplacian of phase.