Phase Contrast Imaging - Coherent Beams

School on X-ray Imaging Techniques at the ESRF

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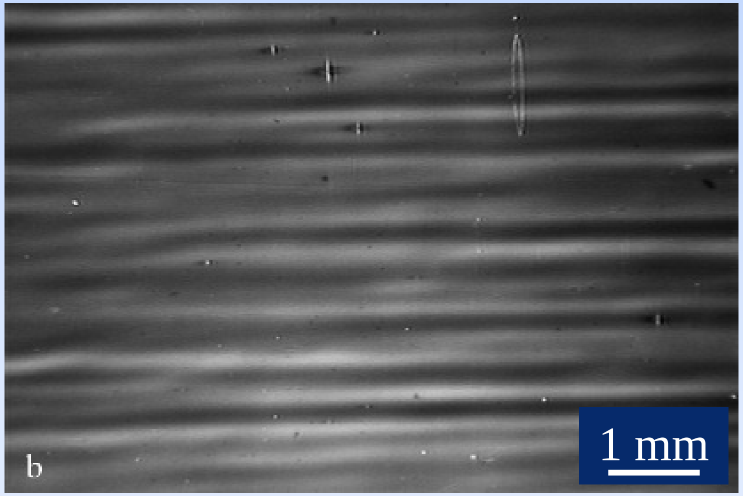
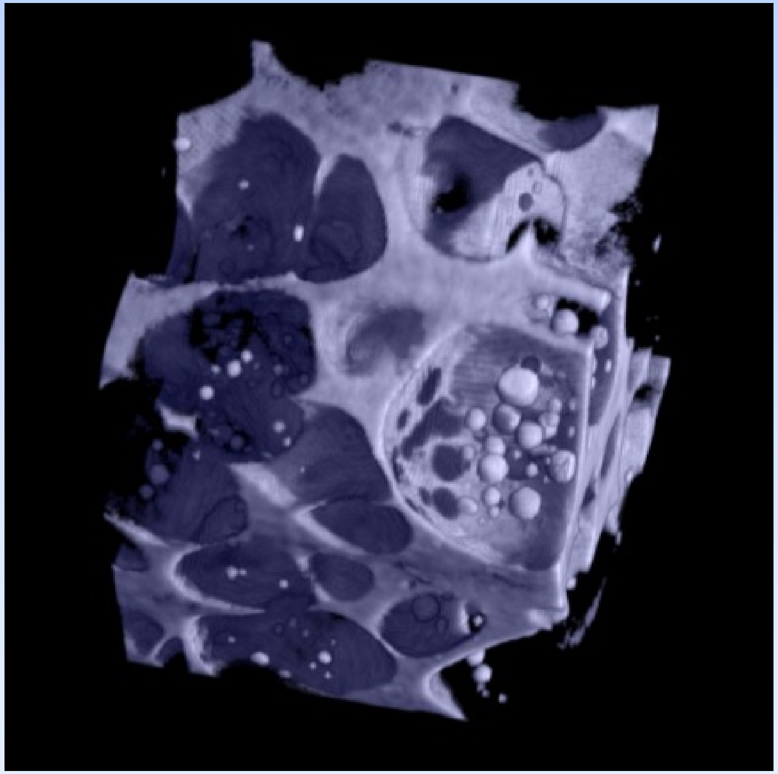
From artefacts to 3D phase contrast imaging



Unpolished beryllium window



Rendering of a semi-solid

Outline

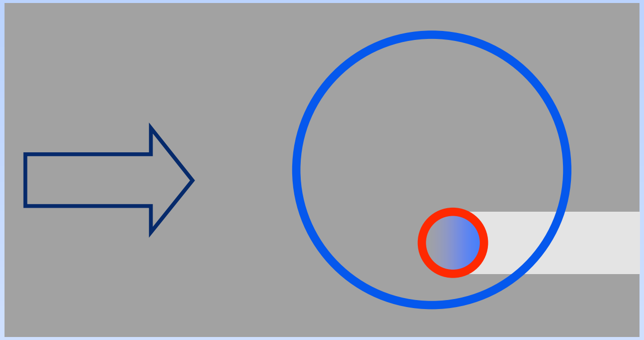
- Interest of phase contrast imaging
- Phase imaging techniques
- Spatial coherence
- Fresnel diffraction ⇔ direct problem

- Edge enhancement
- Phase retrieval
  Holotomography ⇔ inverse problem

Phase Contrast vs Absorption

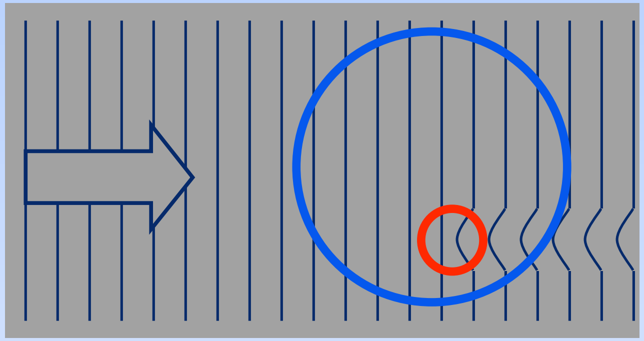
Simple transmission

Absorption



Sample

Phase



Sample

- Dream 1: **Zero Dose**

  Increase the energy

  Absorption contrast ↓ replaced by phase contrast

- Dream 2: Improve the **Sensitivity**

  Absorption contrast too low high spatial resolution

  light materials

  similar attenuation

Absorption vs Phase

- Weak interaction with matter
- Refractive index *n* (X-rays):

$$\boxed{n = 1 - \delta + i\,\beta}$$

$\delta >> \beta$

10^{-6} 10^{-9}

β – Absorption index

- photo-electric effect
  Compton scattering
- strong energy dependence
- $\beta = (\lambda / 4\pi).\mu$

  linear attenuation coefficient μ

$$= \frac{r_c \lambda^2}{2\pi V} \sum f_p''$$

δ – Refractive index decrement

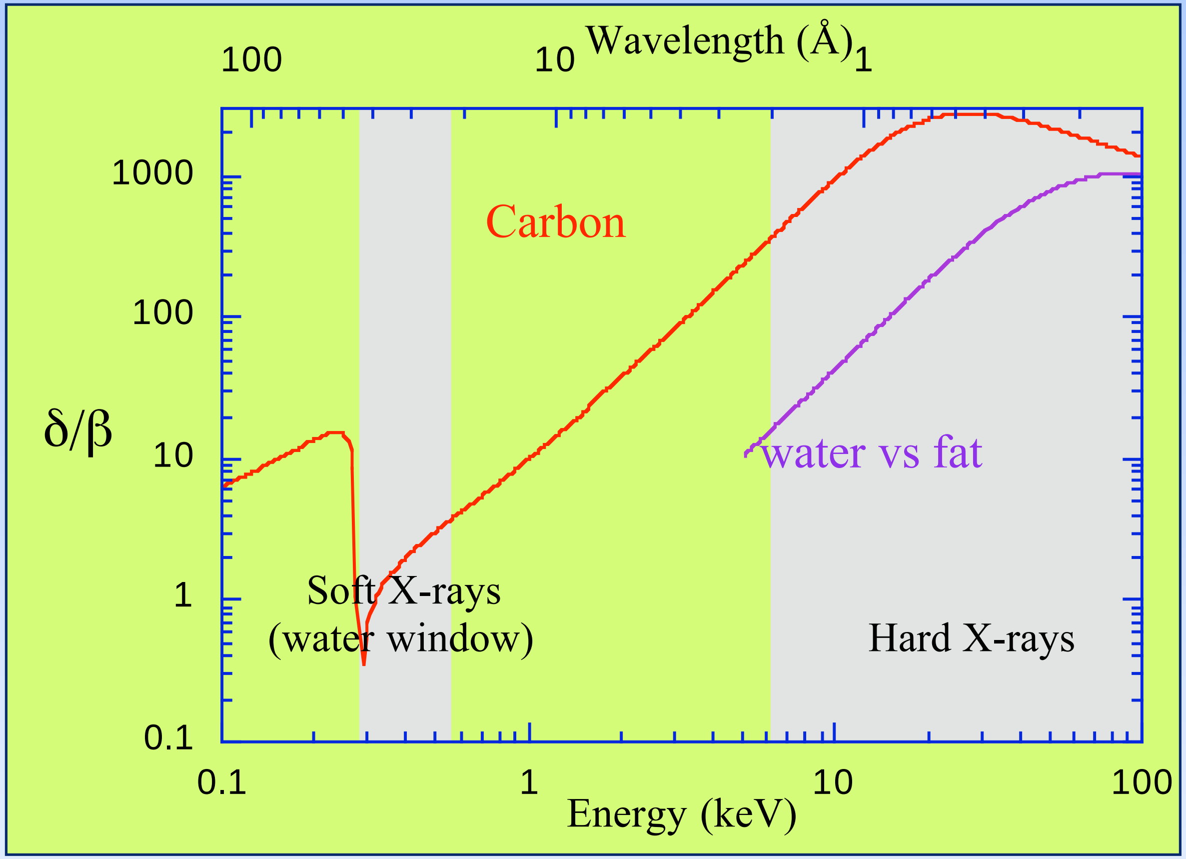
- proportional to
  electron density
- inversely proportional to
  energy^2
- $\delta = \frac{r_c \lambda^2}{2\pi V} \sum \left(Z_p + f_p'\right)$

$\approx 1.3\ 10^{-6}\ \rho\ \lambda^2$

ρ in g/cm^3, λ in Å

XOP: http://www0.esrf.fr/computing/scientific/xop2.1/

Phase vs Absorption

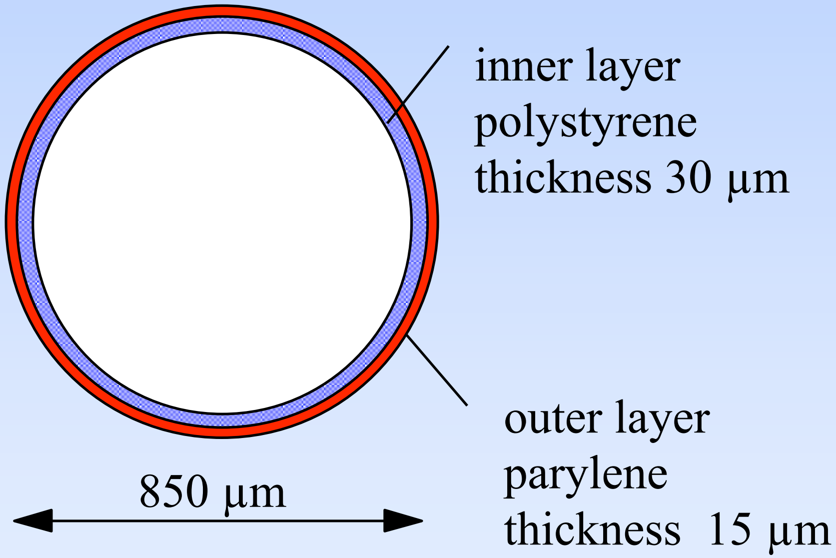


Gain of 100 or 1000 !

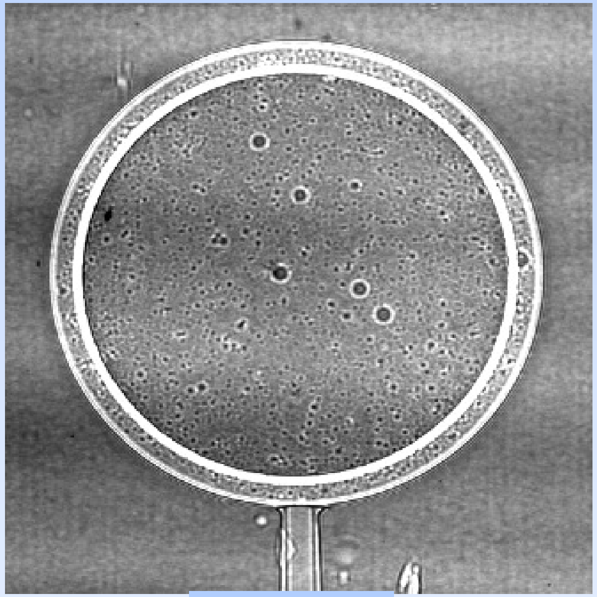
http://www-cxro.lbl.gov/optical_constants/

Absorption vs Phase

Polymer sphere with two layers



Propagation

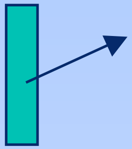


D = 83 cm

$\lambda = 0.7$ Å

200 μm

Transmission through a sample



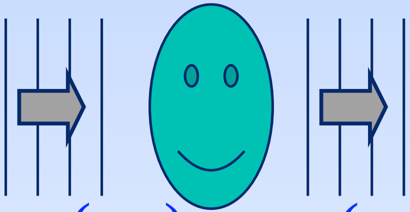
refractive index $n = 1 - \delta + i\beta$

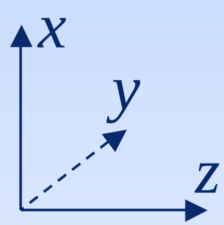
Δz

$$e^{ik_{\text{medium}}\Delta z} = e^{i\frac{2\pi}{\lambda}\boxed{n}\Delta z} = e^{i\frac{2\pi}{\lambda}\Delta z} . e^{-i\frac{2\pi}{\lambda}\delta\Delta z} . e^{-\frac{2\pi}{\lambda}\beta\Delta z}$$

Transmission function

projection of the refractive index distribution





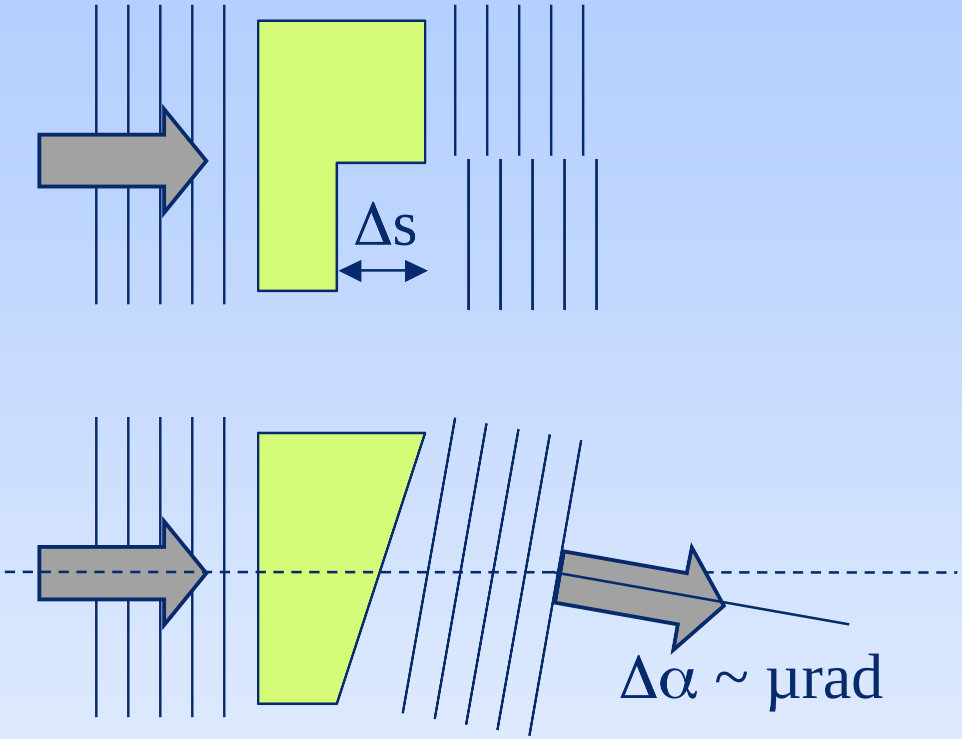
$u_{\text{inc}}(x,y)$ $\quad$ $u_0(x,y) = T(x,y).\, u_{\text{inc}}(x,y)$

Amplitude $\quad A(x,y) = e^{-\frac{2\pi}{\lambda}\int \beta(x,y,z)\mathrm{d}z} = e^{-\frac{1}{2}\int \mu \mathrm{d}z}$

$T(x,y) = A(x,y).e^{i\varphi(x,y)}$

Phase $\quad \varphi(x,y) = \varphi_o - \dfrac{2\pi}{\lambda}\int \delta(x,y,z)\mathrm{d}z$

Phase Sensitive Techniques



Phase Retardation

$$\Delta\varphi = -\frac{2\pi}{\lambda}\delta.\Delta s$$

Deflection

$\Leftrightarrow$

Phase gradients

$$\Delta\alpha = -\frac{\lambda}{2\pi}\frac{\partial\varphi}{\partial x}$$

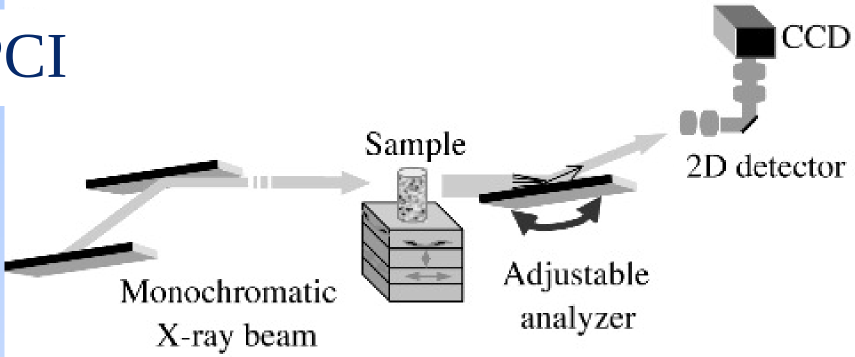
At zero distance:

Intensity $I_0 = |u_0|^2 = I_{\mathrm{inc}}.\exp\left(-\int \mu \mathrm{d}z\right)$

$\Rightarrow$ all phase information is lost

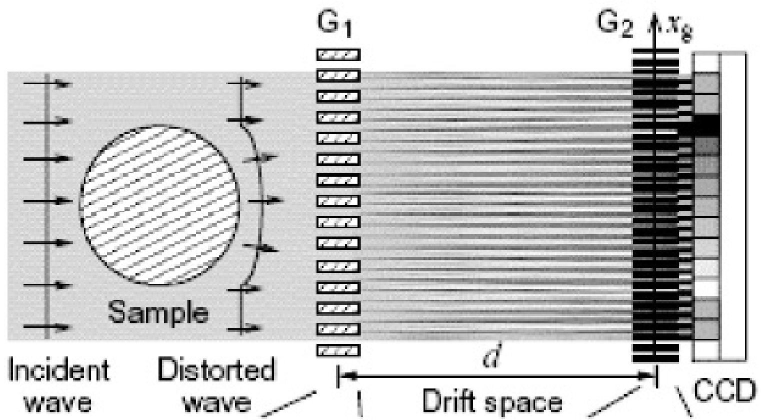
Phase Contrast Imaging methods

Analyzer-based PCI



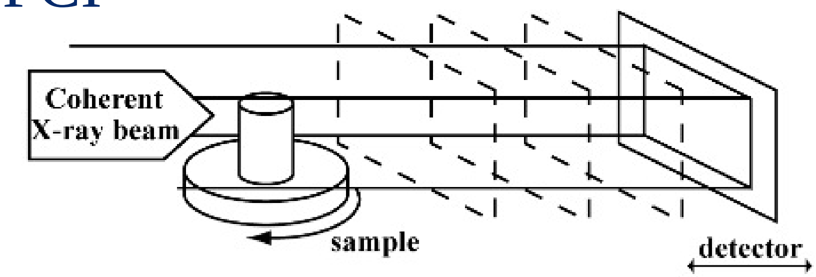
ID17
see A. Bravin's talk
Medical Imaging

Grating-based PCI



BM05
wavefront sensor
Ch David, F Pfeiffer, SLS
T Weitkamp, Anka

Propagation-based PCI

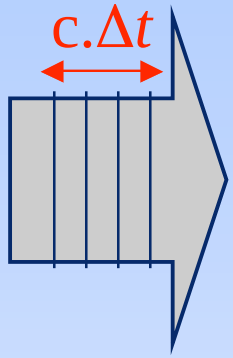


ID19
Edge enhancement
Holotomography

Coherence

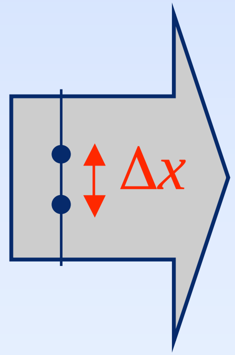
Coherence of a beam

Temporal Coherence
correlation in time $u(t)\ u(t+\Delta t)$



Monochromaticity: $\Delta\lambda/\lambda$
Longitudinal coherence length: $\lambda^2 / \Delta\lambda$

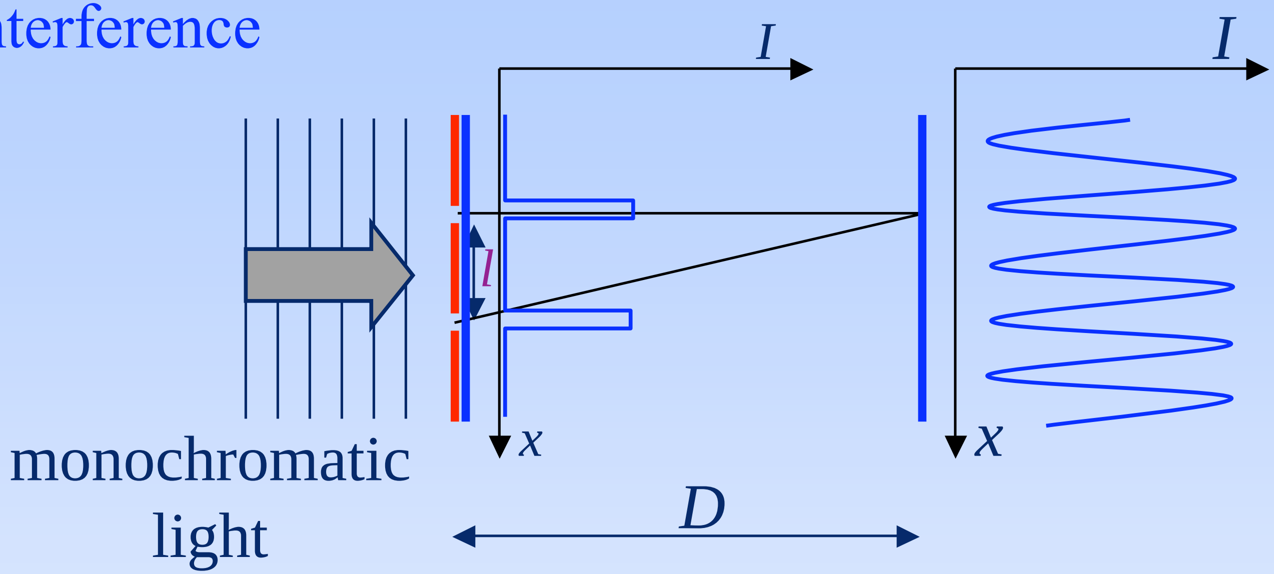
Spatial Coherence
correlation in space $u(x)\ u(x+\Delta x)$



Angular source size: α
Transverse coherence length: $\lambda / 2\alpha$

Spatial Coherence

- Interference



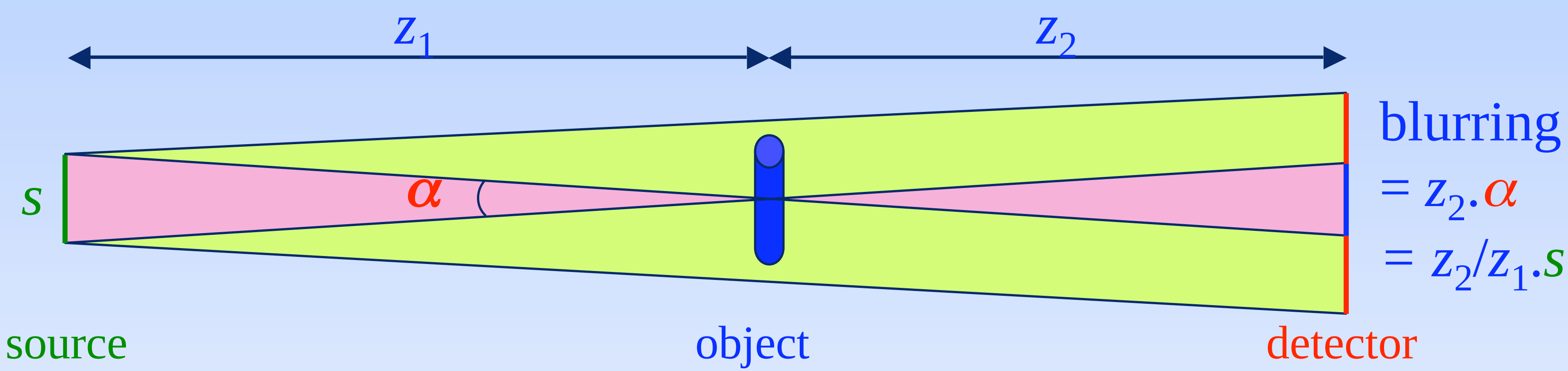
condition: *l* smaller than *transverse coherence length*

visibility is given by the complex degree of coherence $\gamma(x_1,x_2)$

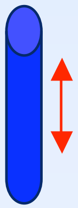
- Applications with X-rays
  - Phase Contrast Imaging / Coherent Diffraction Imaging
  - Speckle experiments
  - Extreme Focusing

Spatial Coherence

- Hard X-ray / neutron sources are ~ incoherent
- Wave is partially coherent when the source is small and far



- Transverse coherence length



$$l_{coh} = \frac{\lambda}{2\alpha} = \frac{\lambda.z_1}{2s}$$

Laboratory: $l_{coh} < 1\ \mu\text{m}$

ESRF, ID19: $s = 25\ \mu\text{m}$, $z_1 = 145$ m

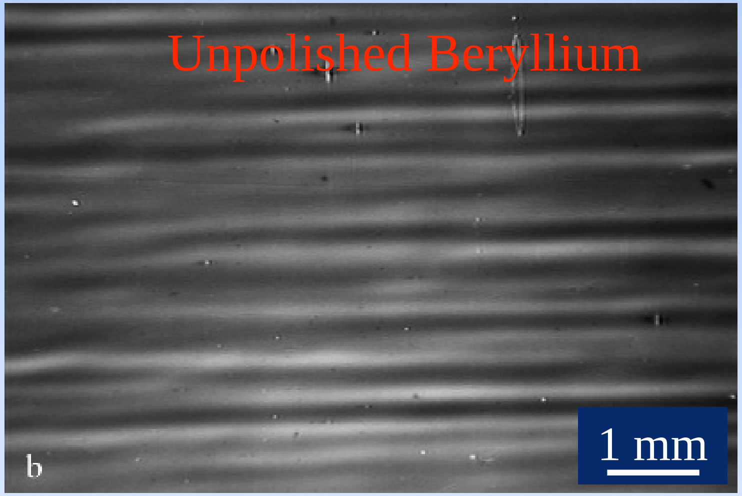
$\alpha < 0.2\ \mu\text{rad}$ $l_{coh} \sim 250\ \mu\text{m}$

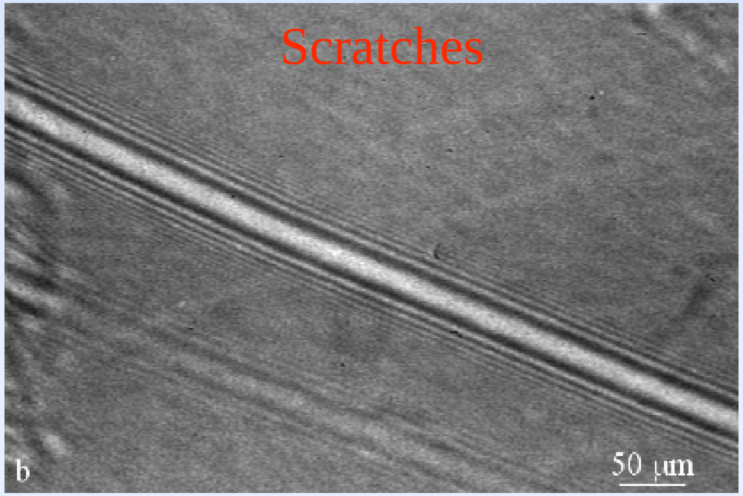
Image Degradation

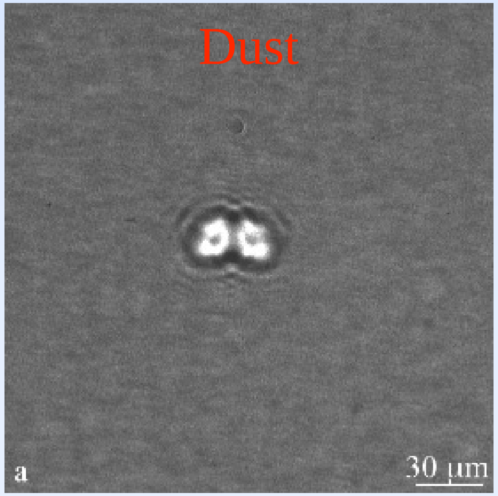
Everything in the beam can act as a phase object

- Stringent requirements on beamline optics: Polished windows, Monochromator surface, … Dust!

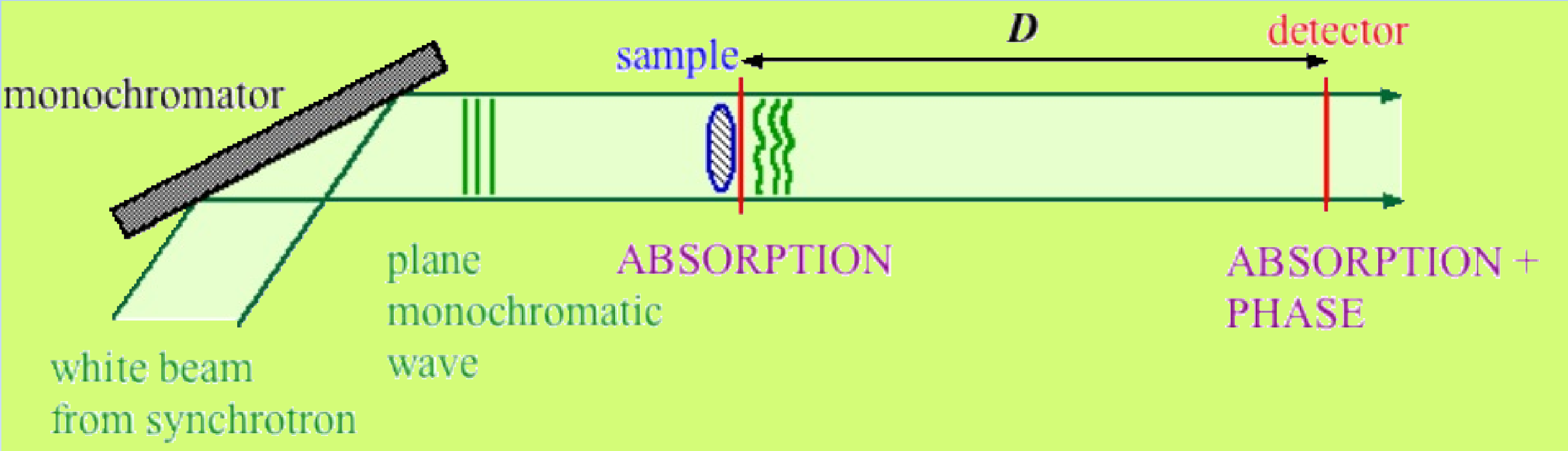
no thickness variations (surface)
no density fluctuations (volume)







Simple Propagation

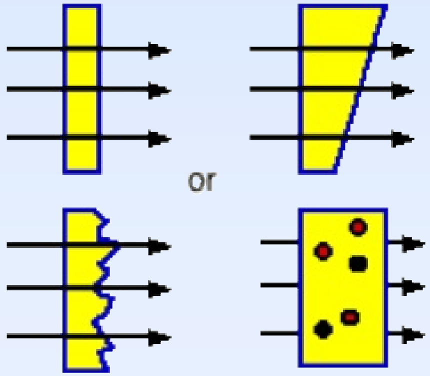


- Fresnel diffraction over a distance D (few mm to 1 m)

  Defocusing in electron microscopy

  In-line Gabor holography

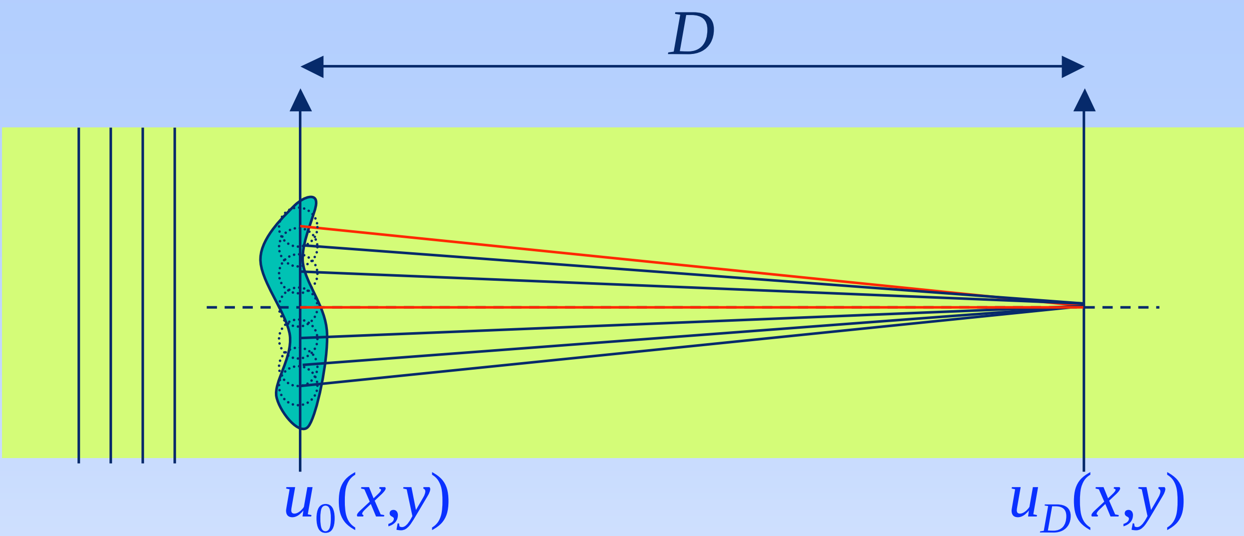
- At least $\boxed{\frac{d^2\varphi}{d^2x} \neq 0}$



no contrast

contrast

Fresnel diffraction



- *In principle*: complete object contributes to a point of the image

  In practice: only finite region: first Fresnel zone

  radius $\boxed{r_F = \sqrt{\lambda D}}$

- First Fresnel zone determines the sensed lengthscale

  Distance to be most sensitive to object with size a: $\boxed{D = \frac{a^2}{2\lambda}}$

  For example at $\lambda = 0.5$Å (25 keV)

  $a = 1\ \mu\text{m} \quad \Rightarrow \quad D = 10$ mm

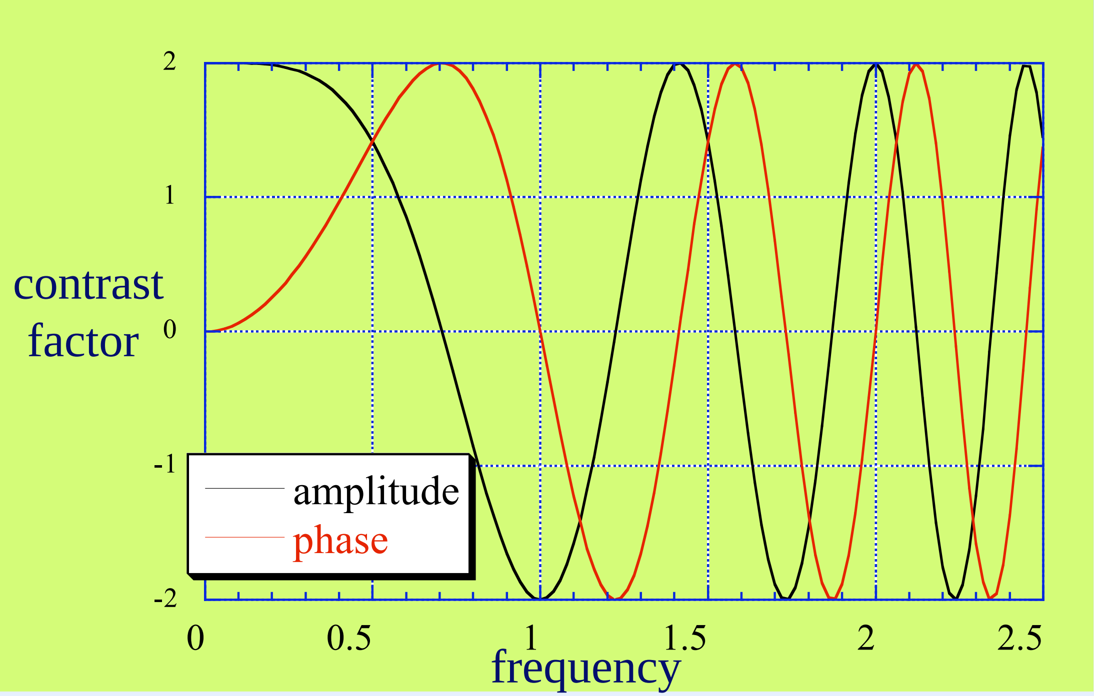
  $a = 40\ \mu\text{m} \quad \Rightarrow \quad D = 16$ m

Contrast Transfer Functions

- Fourier Transform of intensity and of phase are linearly related

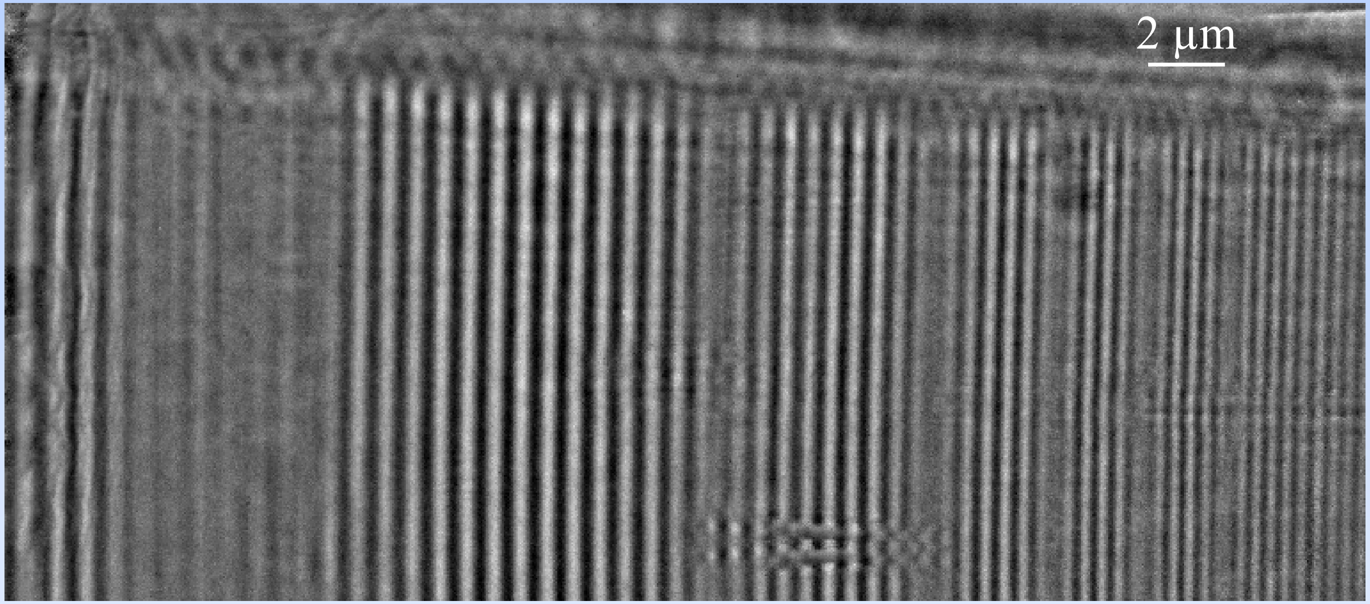
$$I_D(\boldsymbol{f}) = \delta_D(\boldsymbol{f}) + \underbrace{R_D(\boldsymbol{f})}_{\text{coherence \& detector}} \;.\; 2\,\underbrace{\sin(!\,\lambda D \boldsymbol{f}^{\,2})}_{\text{phase contrast factor}} \;.\; \varphi(\boldsymbol{f})$$

valid in case of a slowly varying phase



Variable period

Decreasing linewidth
Increasing spatial frequency



period " 720 nm

period " 530 nm

period " 610 nm

Object invisible !

Contrast depends strongly on period or spatial frequency

Obtained with KB-mirrors

Simulation

Known Object ⇒ Image

Direct Space | Reciprocal Space

OBJECT

multiplication wave with transmission function $T = A e^{i\varphi}$

convolution

PROPAGATION

diffraction integral

multiplication FT wave with propagator $P_D = \exp(-i\pi\lambda D \boldsymbol{f}^2)$

INTENSITY

$I_D^{\mathrm{coh}}(x,y) = |u(x,y)|^2$

auto-correlation

COHERENCE / DETECTOR

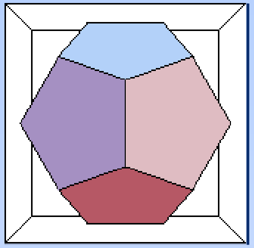
convolution intensity with
projected source
PSF detector

multiplication FT intensity with
degree of coherence $\gamma(\lambda D \boldsymbol{f})$
detector transfer function $R(\boldsymbol{f})$

Simulation

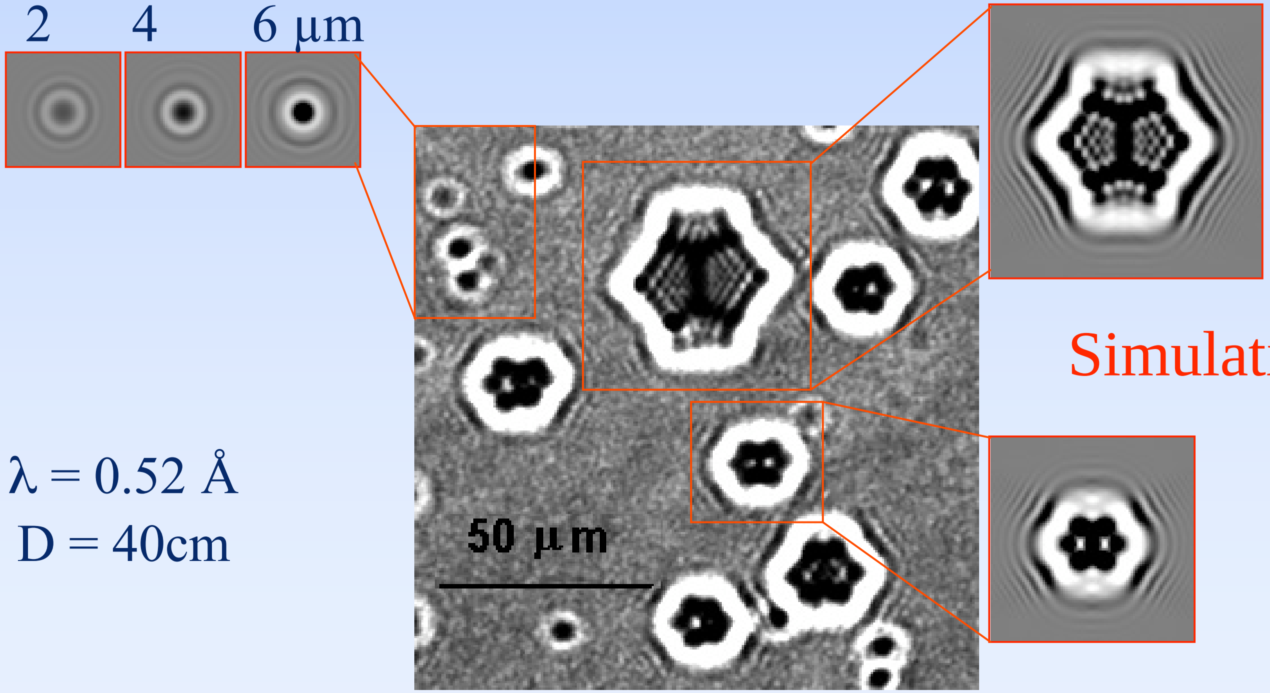
Known Object ⇒ Image

Porosity in Quasi-crystals



Hole =
dodecahedron seen
along the 2-fold axis

2 4 6 µm

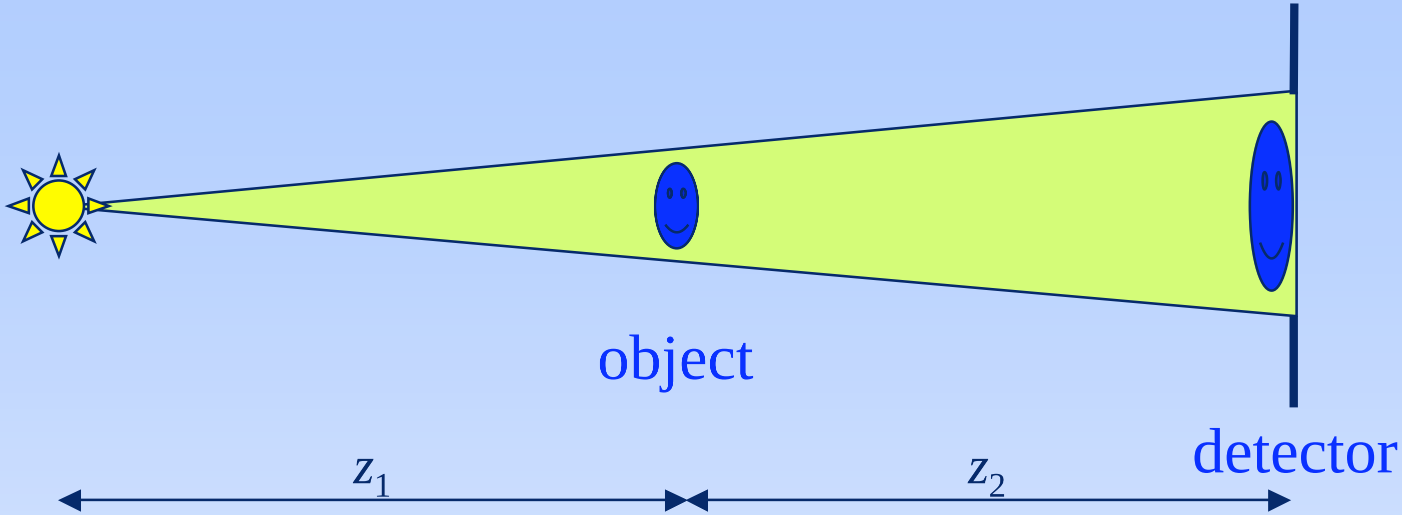


Simulations

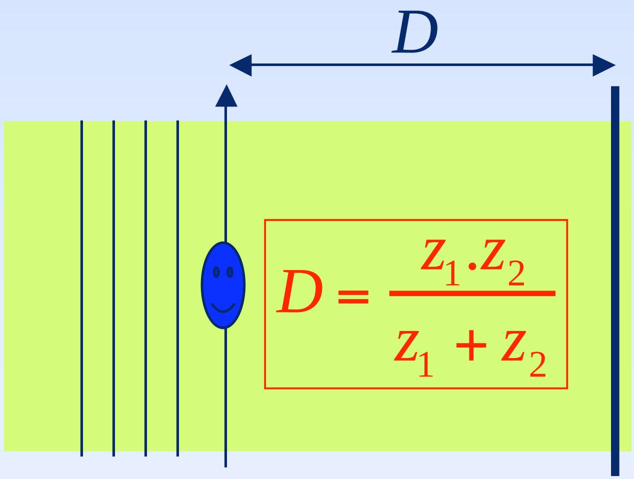
$\lambda = 0.52$ Å
$D = 40$cm

S. Agliozzo (ESRF) / H. Klein / J. Gastaldi (CRMC2, Marseille)

Spherical wave illumination

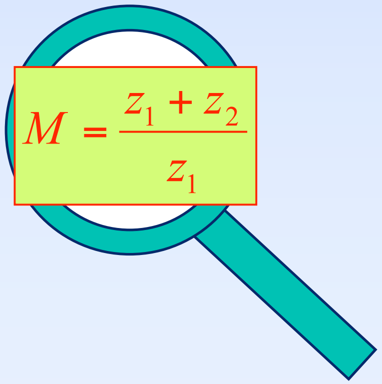


equivalent to



Plane wave illumination

+



Magnification

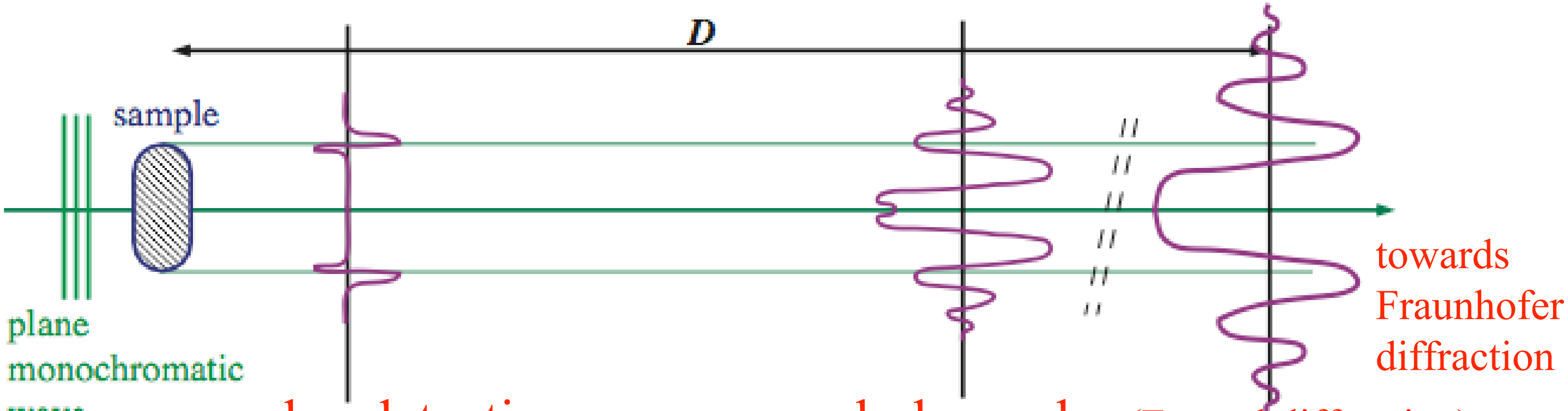
Limit cases

$z_1 >> z_2$

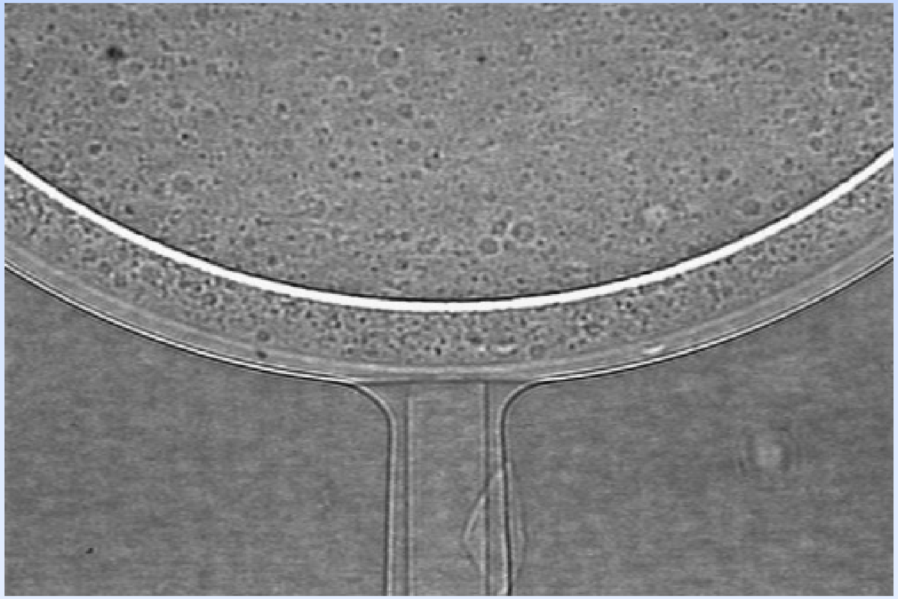
$D = z_2 \; ; M = 1$

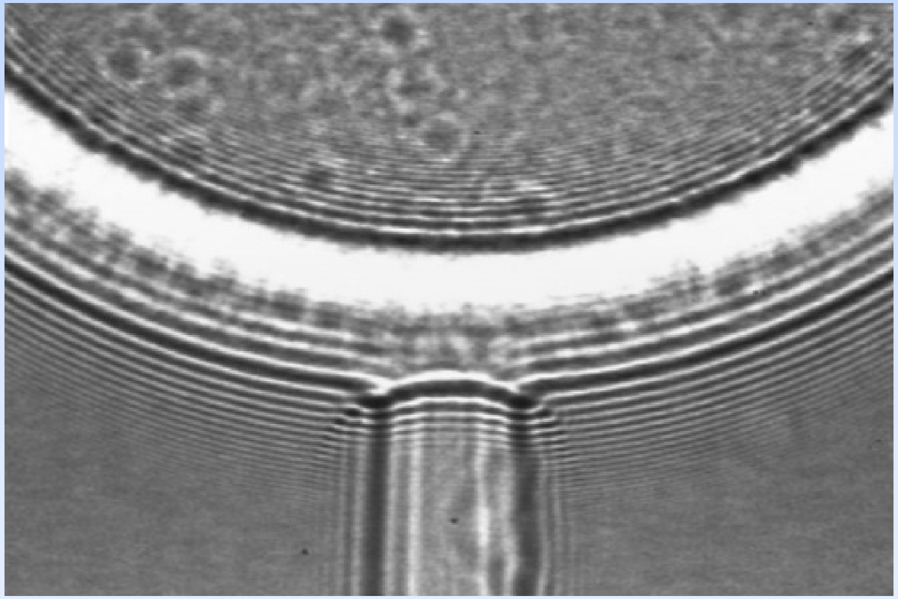
$z_1 << z_2$

$D = z_1 \; ; M = z_2/z_1$



edge detection versus holography (Fresnel diffraction)





D = 15 cm

each edge imaged independently
no access to phase, only to border

$$\boxed{\sqrt{\lambda D} << a}$$

$\lambda = 0.7$ Å

50 μm

D = 310 cm

deformed *image* of whole object
access to phase, if recorded at ≠ *D*'s

$$\boxed{\sqrt{\lambda D} \approx a}$$

Edge Detection

- Essentially edge enhancement
  Weak defocusing (and weak contrast!)

$$\boxed{\sqrt{\lambda D} << a}$$

- Radiography (2D)

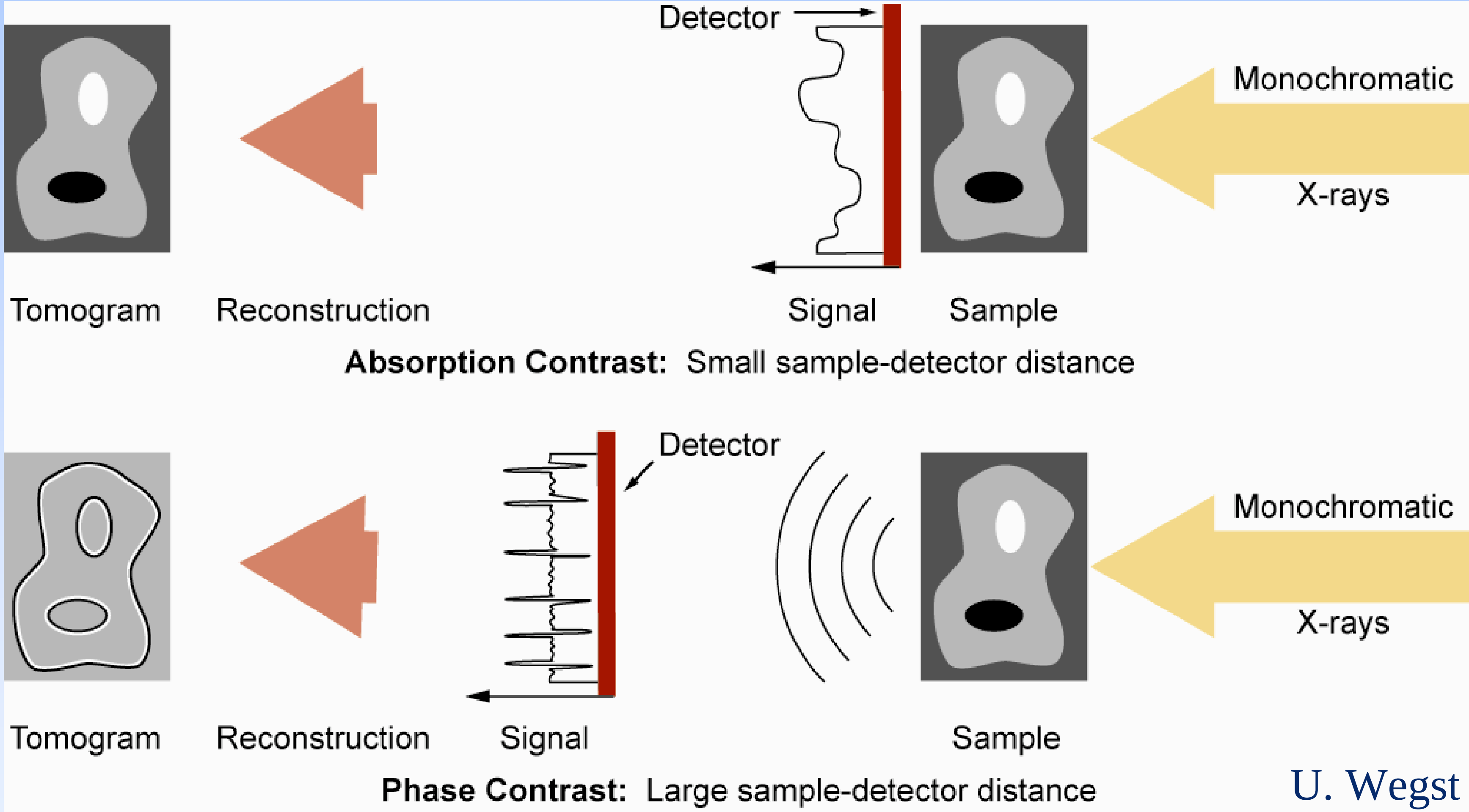
$$I_D(x,y) \approx \underbrace{I_0(x,y)}_{\text{absorption image}} \cdot \left[\underbrace{1 - \frac{\lambda D}{2\pi} \Delta_{xy} \varphi(x,y)}_{\text{phase term, 2D Laplacian phase}} \right]$$

- Tomography (3D)

$$o(x,y,z) \approx \underbrace{\mu(x,y,z)}_{\text{absorption term}} - \underbrace{D \, \Delta_{xyz} \delta(x,y,z)}_{\text{phase term, Laplacian refractive index}}$$

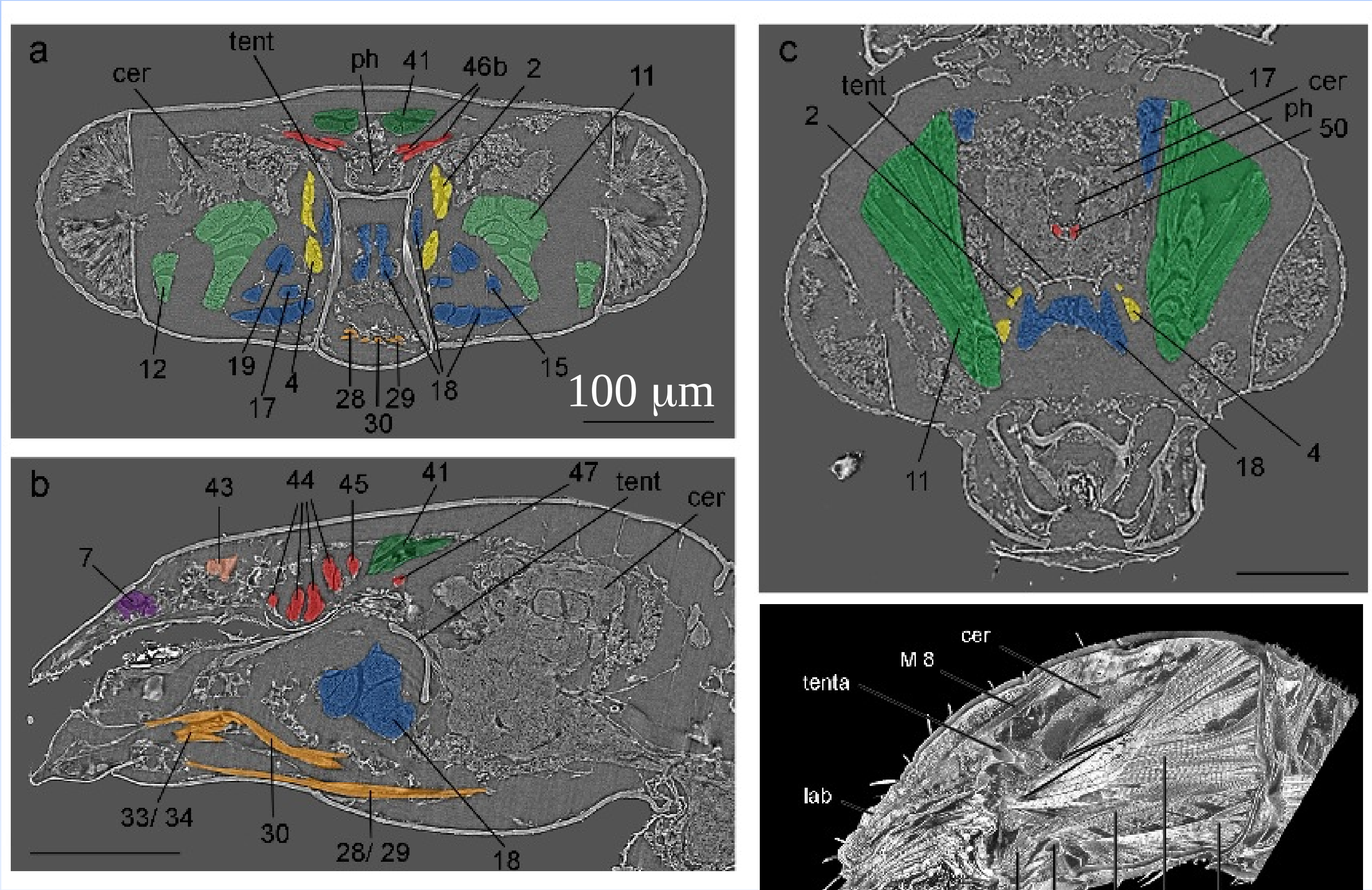
- Detection of
  - cracks
  - holes
  - reinforcing fibres, particles

Edge Detection



U. Wegst

Insect Anatomy



Virtual slices through heads of tiny staphylinid beetles

O. Betz (Zoologisches Institut Tuebingen), U. Wegst (MPI Stuttgart), D. Weide et al, sub. J. Microscopy

Phase Retrieval

- How to retrieve the phase and amplitude in the object plane?
- Phase in image plane is lost

Image(s) $\Rightarrow$ Object ???
Inverse Problem

Australian School: K. Nugent, T. Gureyev, D. Paganin

TIE (transport of intensity)

$$\boxed{\frac{\partial I}{\partial z} = -\frac{\lambda}{2\pi}\Delta_{xy}\varphi}$$

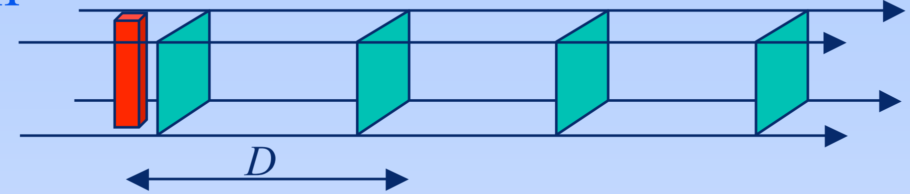
Flemish School: D. Van Dyck, P. Cloetens, JP Guigay

Focus variation method

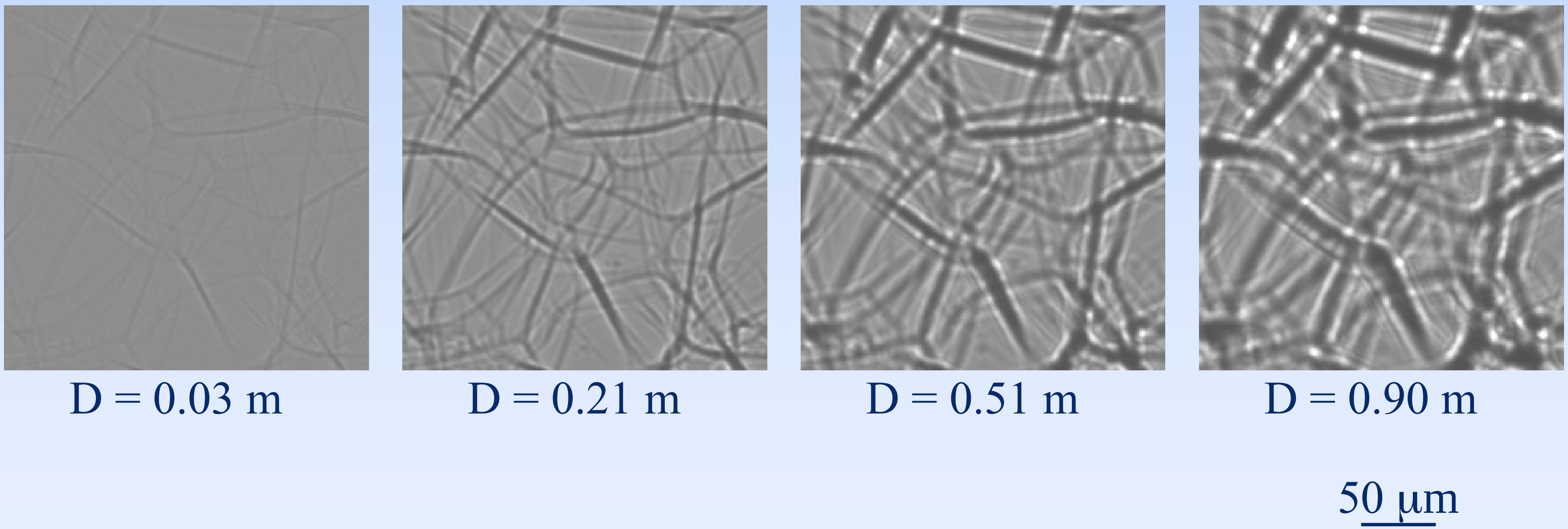
- Series of images recorded at different distances
- Each distance is most sensitive to a specific range of spatial frequencies

Phase Retrieval: Polystyrene Foam

- non-absorbing foam
- 4 images recorded
- E = 18 keV

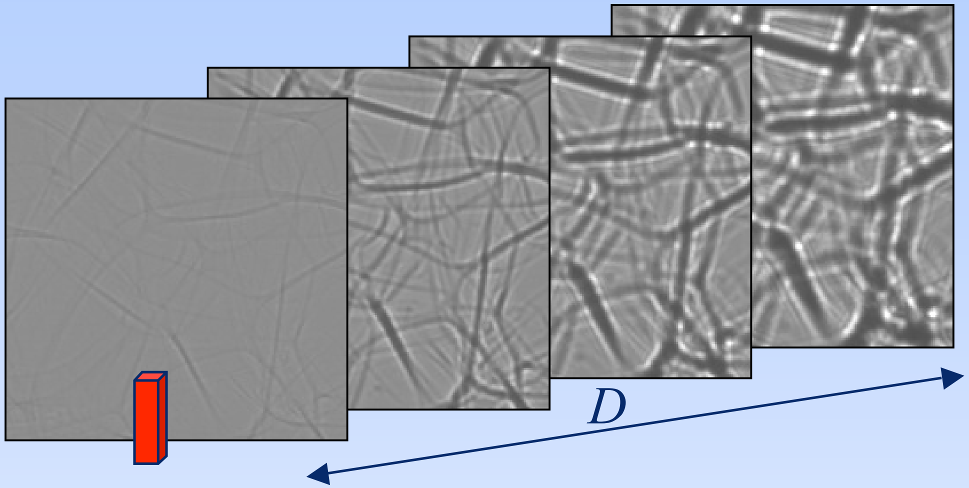


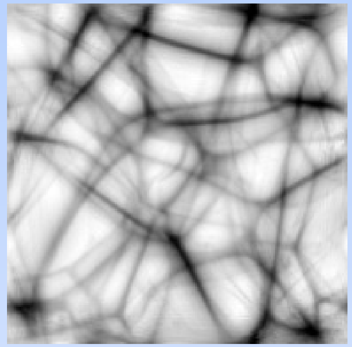
variable $\sqrt{\lambda D}$



Holo-tomography

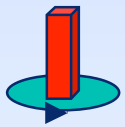
1) phase retrieval with images at different distances

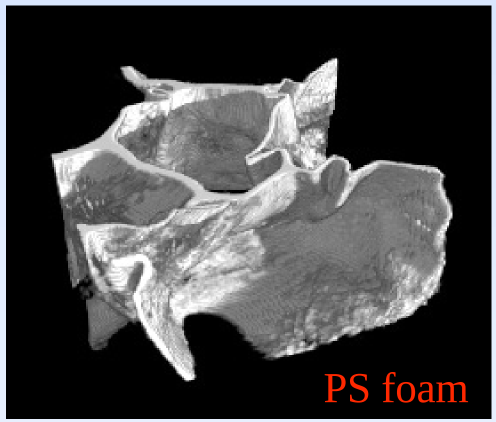




Phase map

2) tomography: repeated for ≈ 1000 angular positions

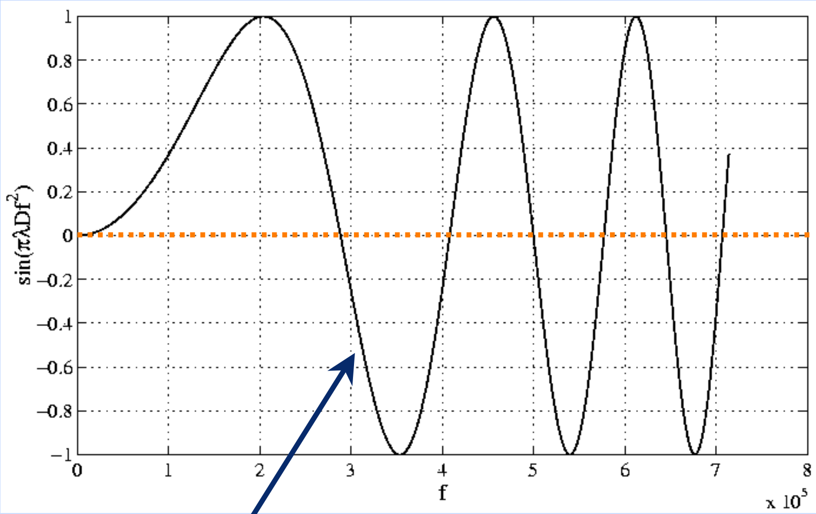




3D distribution of δ or the electron-density
improved resolution
straightforward interpretation
processing

P.Cloetens et al., Appl. Phys. Lett. 75, 2912 (1999)

Phase retrieval



"transfer function"

$\sin(\pi\lambda D f^{2})$

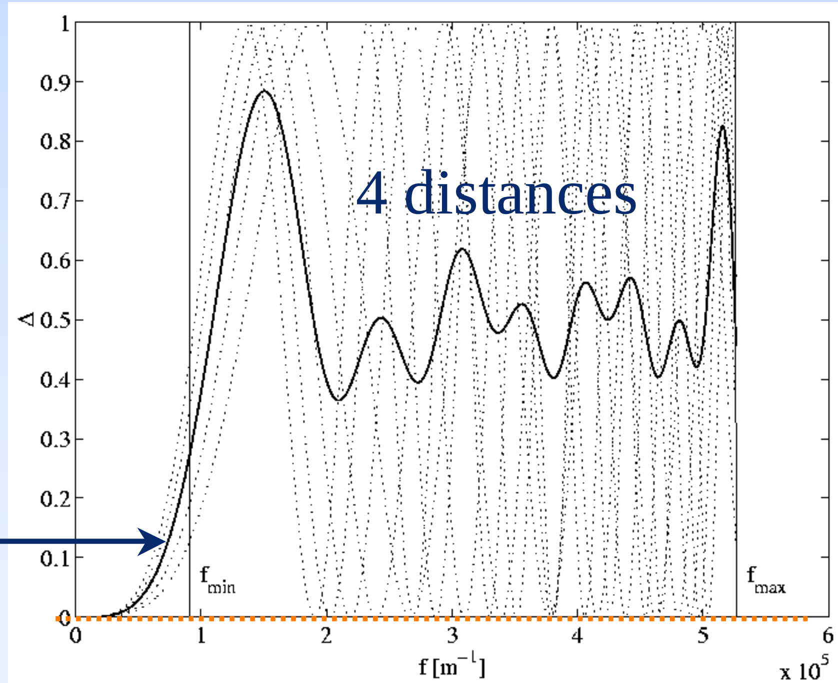
$$\tilde{I}_D(f) = 2\sin(\pi\lambda D f^{2})\cdot\tilde{\varphi}(f)$$

Linear least squares

$$\tilde{\varphi}(f) = \frac{\sum_m \sin(\pi\lambda D_m f^{2})\cdot\tilde{I}_m(f)}{\sum_m 2\sin^2(\pi\lambda D_m f^{2})}$$

⇒ Optimization
of the choice of distances

$$\frac{1}{N}\sum_{m=1}^{N} 2\sin^2(\pi\lambda D_m f^{2})$$



Non-iterative (fast!)

Phase Tomography of Arabidopsis seeds

3D structure of Arabidopsis seeds in their **native state**

- wet sample, no preparation
- no staining, no fixation, no cutting, no cryo-cooling

Holotomographic approach

Contrast proportional to the electron density

4 distances, 800 angles

$E = 21$ keV

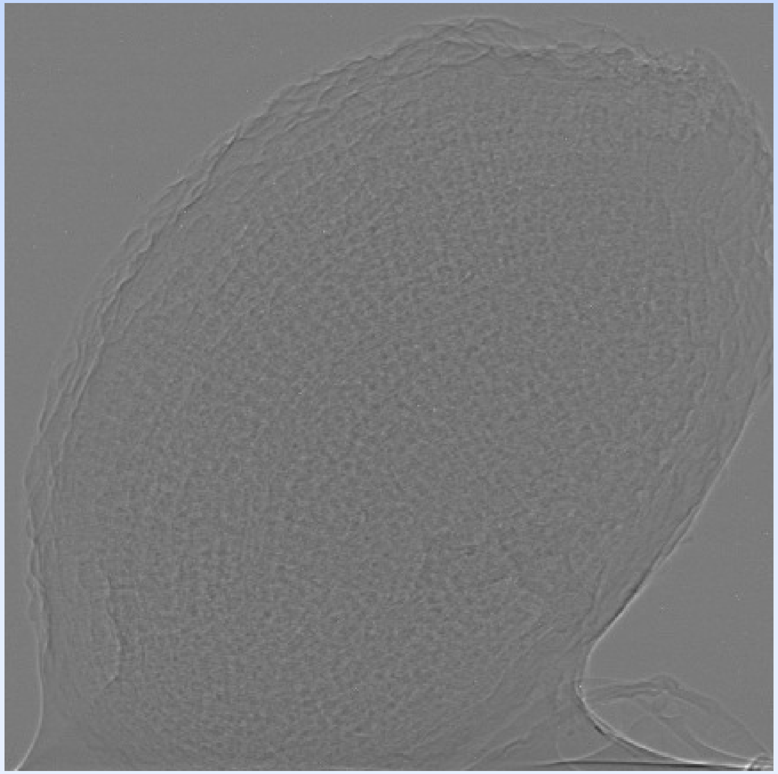
P Cloetens, R Mache, M Schlenker, S Lerbs-Mache, *PNAS* (2006) 103, 14626

Phase Tomography of Arabidopsis

In situ 3D imaging of a seed of an Arabidopsis plant

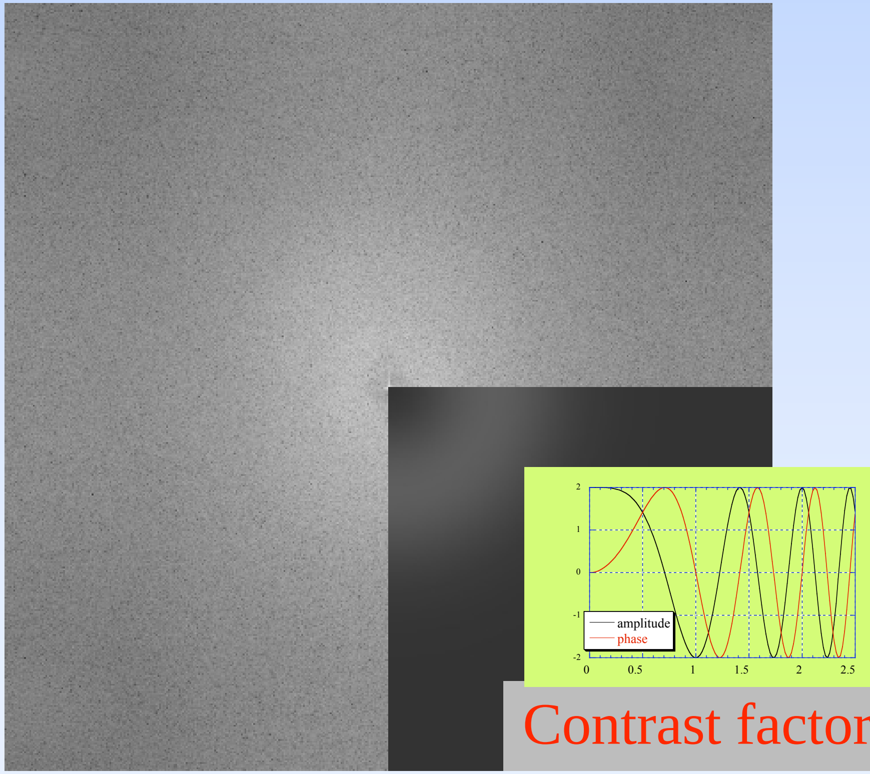
↳ wet sample, no preparation

Radiograph D = 10 mm



50 µm

Spectrum – Fourier transform



Contrast factor

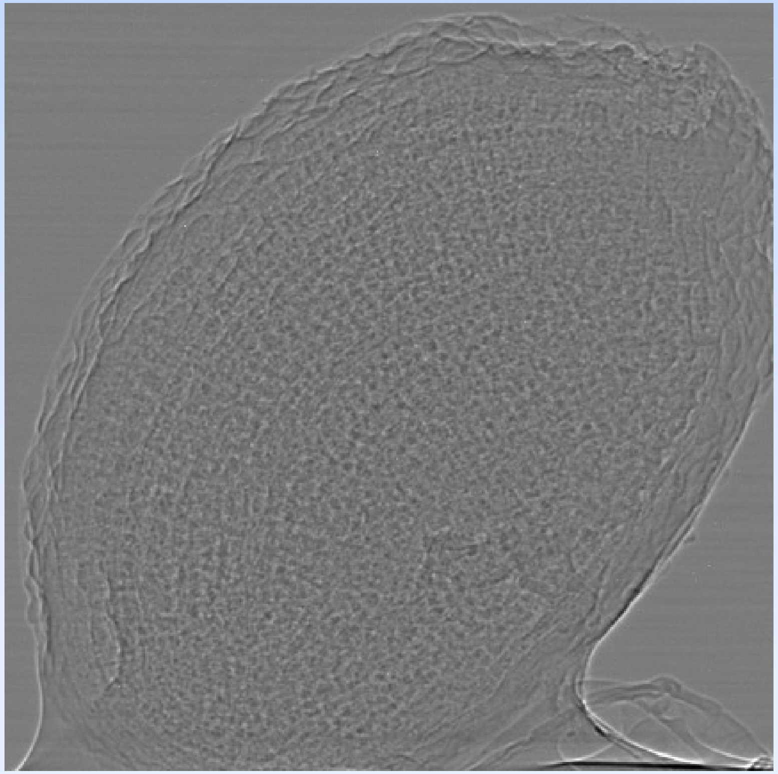
R. Mache (UJF, Grenoble)

Phase Tomography of Arabidopsis

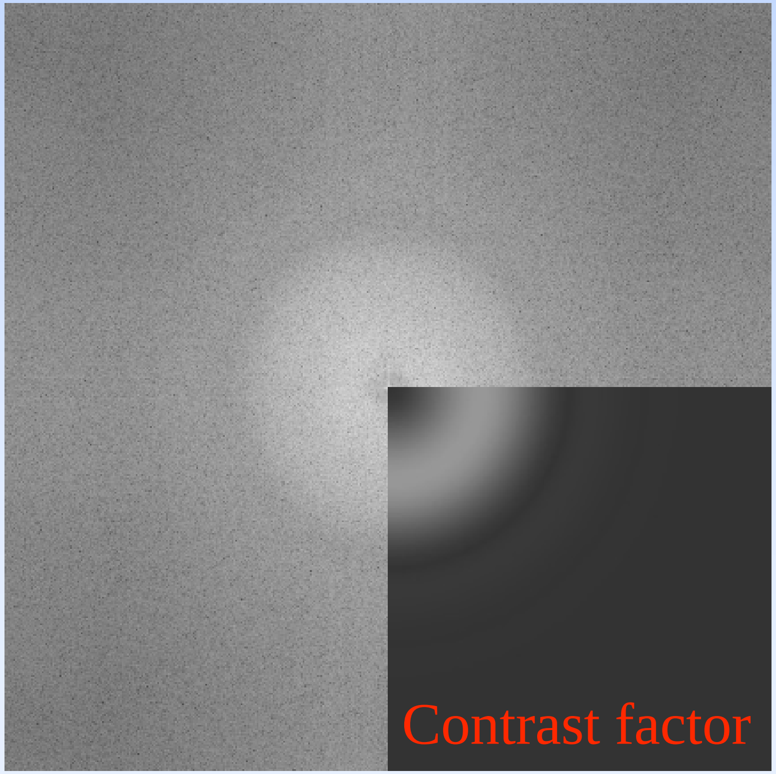
In situ 3D imaging of a seed of an Arabidopsis plant

wet sample, no preparation

Radiograph D = 30 mm



Spectrum

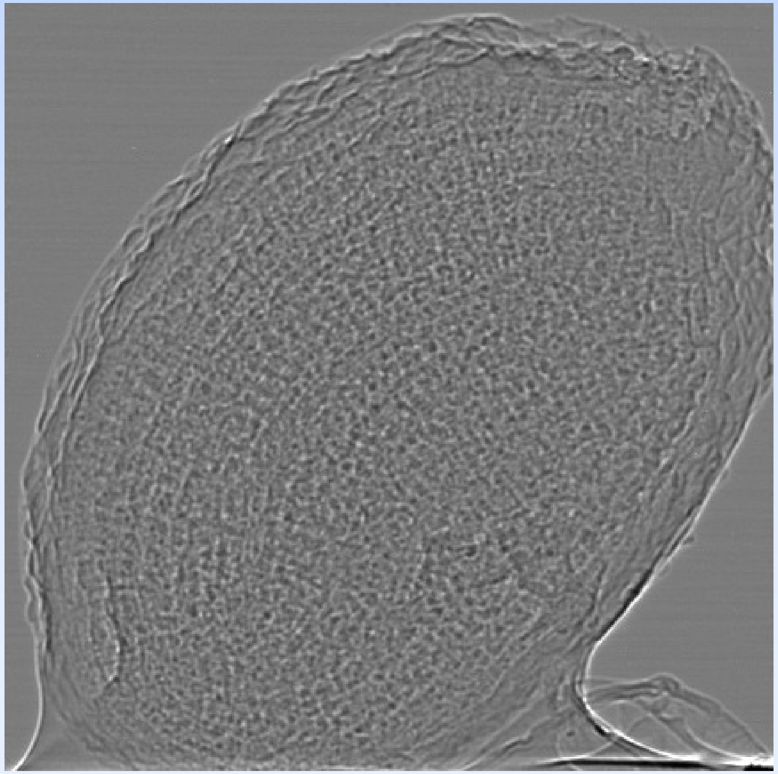


Phase Tomography of Arabidopsis

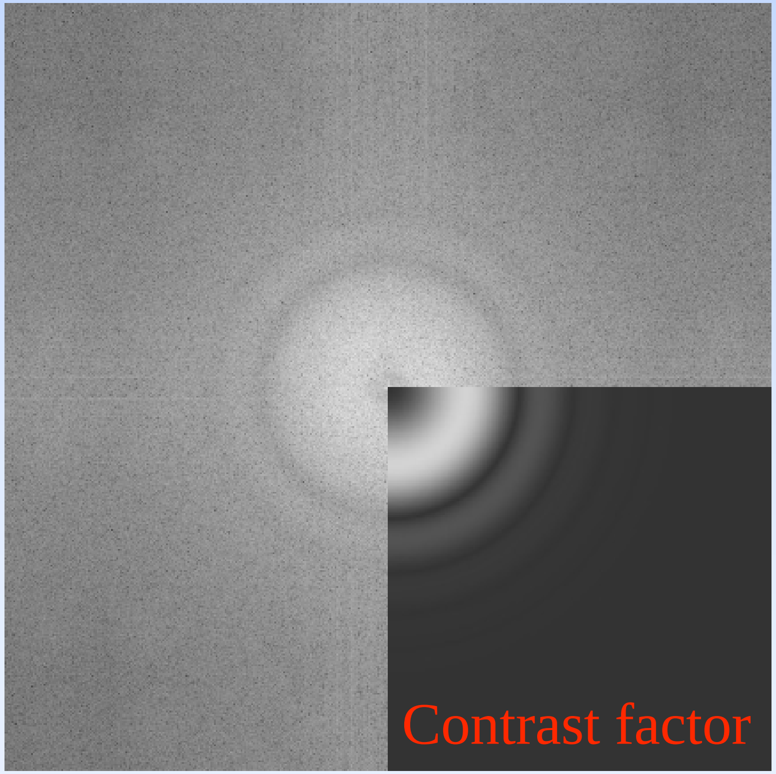
In situ 3D imaging of a seed of an Arabidopsis plant

wet sample, no preparation

Radiograph D = 60 mm



Spectrum

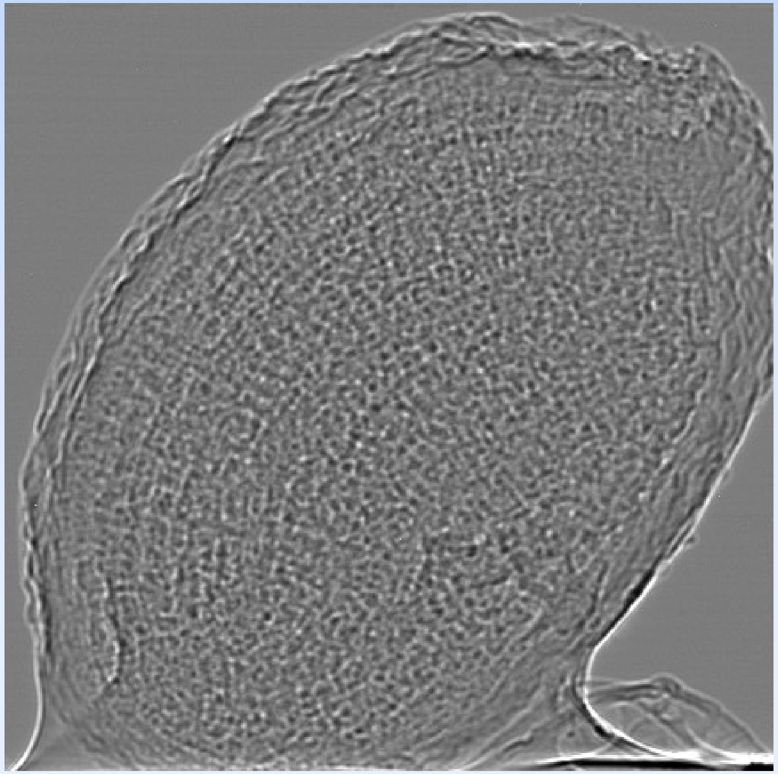


Phase Tomography of Arabidopsis

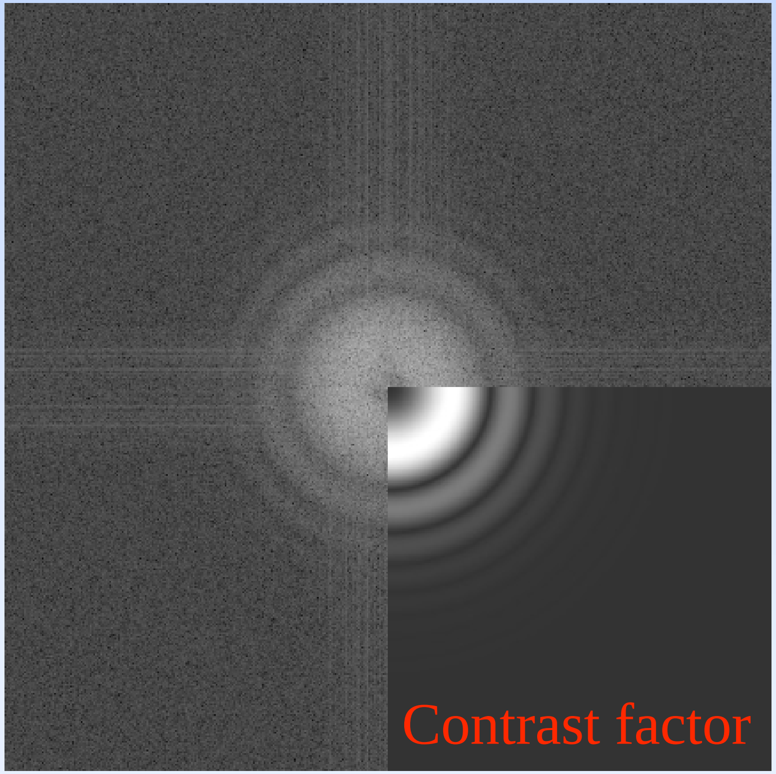
In situ 3D imaging of a seed of an Arabidopsis plant

wet sample, no preparation

Radiograph D = 100 mm



Spectrum



Phase Tomography of Arabidopsis

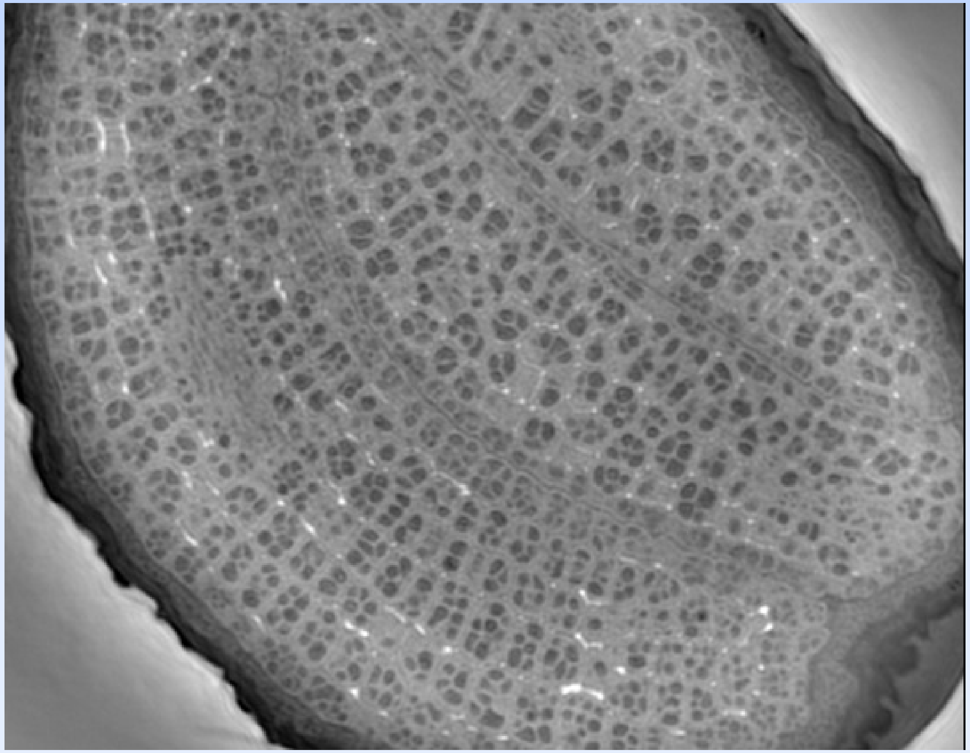
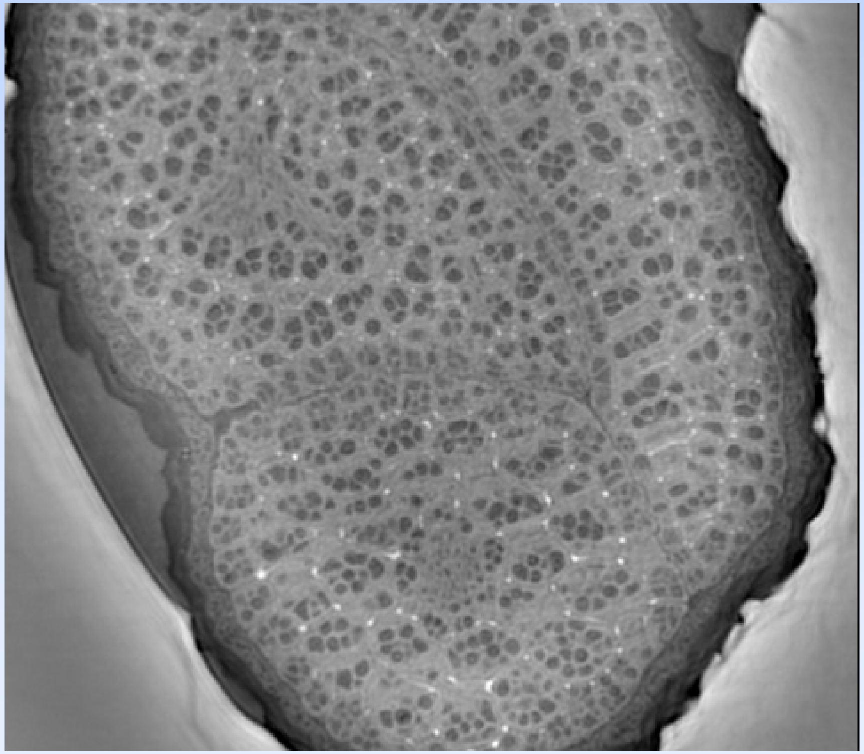
Holotomographic approach

Four distances

E = 21 keV

Seed of Arabidopsis

Tomographic Slices

30 µm

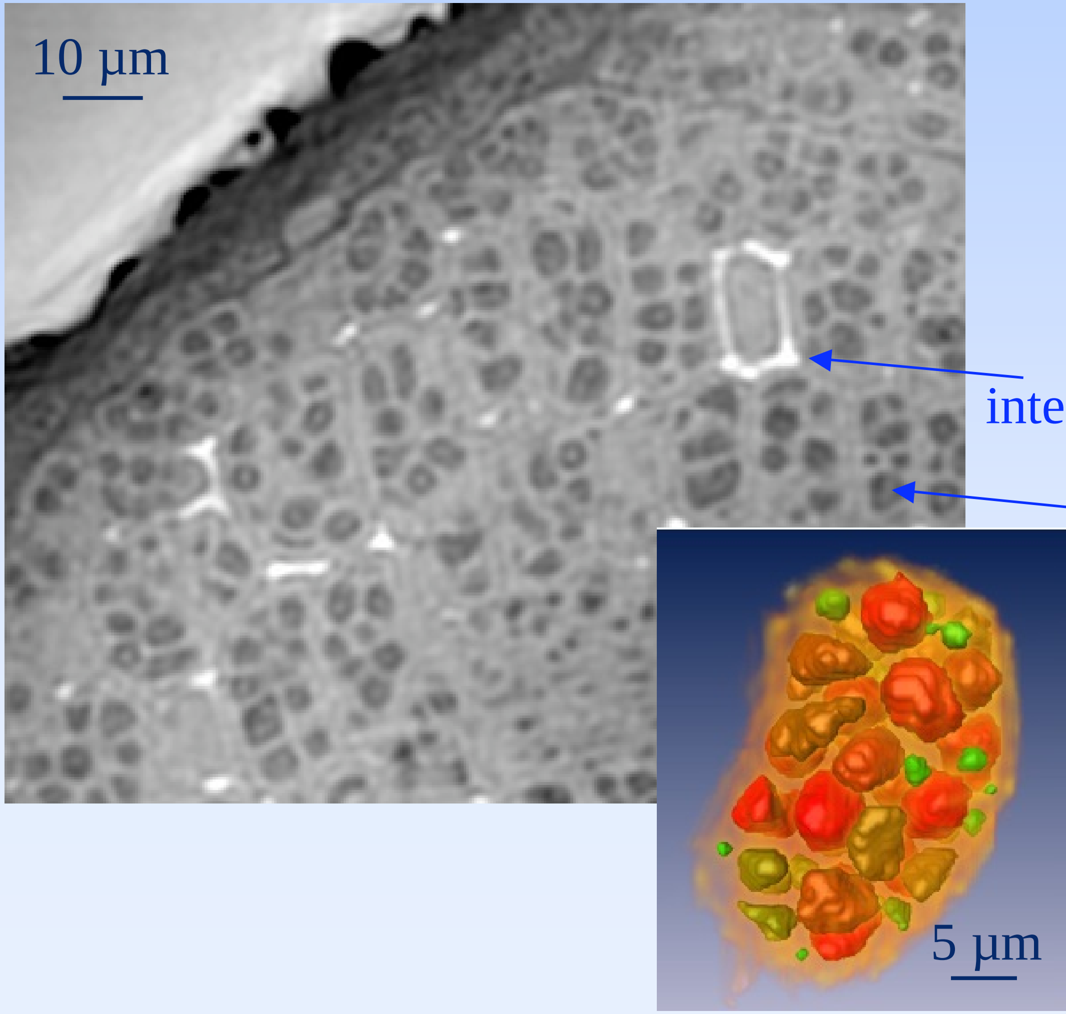
Cotyledon

P Cloetens, R Mache, M Schlenker, S Lerbs-Mache, *PNAS* (2006) 103, 14626

Phase Tomography of Arabidopsis

Seed of Arabidopsis

Tomographic Slice



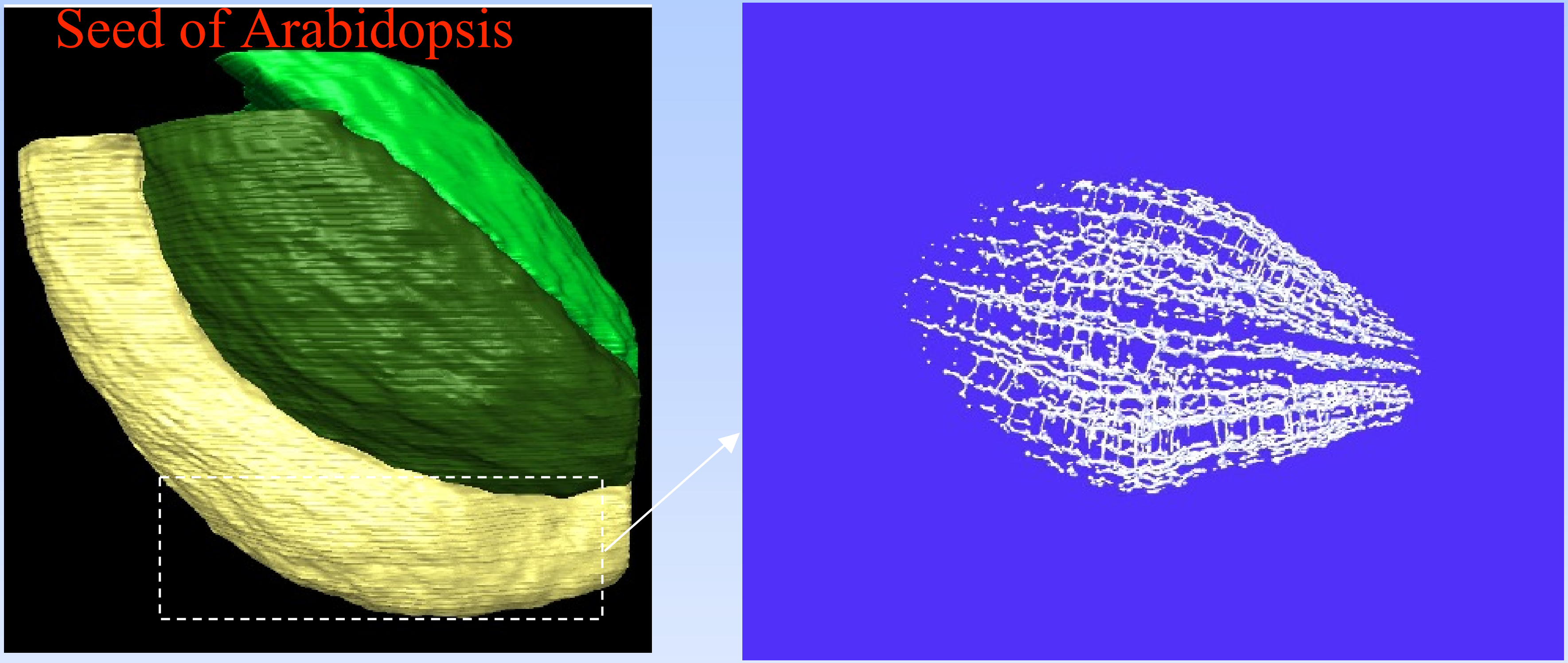
tegumen

protoderm

intercellular spaces

organites
(protein stocks)

Phase Tomography of Arabidopsis



three-dimensional network of intercellular air space

Role? gas exchange during germination and/or rapid water uptake during imbibition

P Cloetens, R Mache, M Schlenker, S Lerbs-Mache, *PNAS* (2006) 103, 14626

Conclusions

- Coherent X-rays allow to perform, *in an easy way*, phase (sensitive) imaging through propagation
- The coherence puts stringent requirements on all beamline optics
- Quantitative mapping of the phase (2D) and density (3D) is possible by combining images at different distances with an adapted numerical algorithm
- New topics in Materials Science and Biology can be investigated

Challenges

- ‘Magnification’ using diffractive or refractive lenses
  projection and a point source
  coherent diffraction imaging
- Phase imaging applied to medical imaging, life sciences
- Phase imaging with neutrons, lab sources (polychromatic)

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