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# *Prospects for hard X-ray phase contrast imaging*

Ian Robinson

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*University of Illinois, Urbana, USA*

[Franz Pfeiffer](#), Timm Weitkamp, Oliver Bunk, Christian David

*Swiss Light Source, Paul Scherrer Institut, Switzerland*

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# *Outline*

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Phase Contrast X-ray Imaging

New methods: DEI and Shearing Interferometer

Coherent X-ray Diffraction

How to Solve the **Phase** Problem for Nanocrystal Shapes

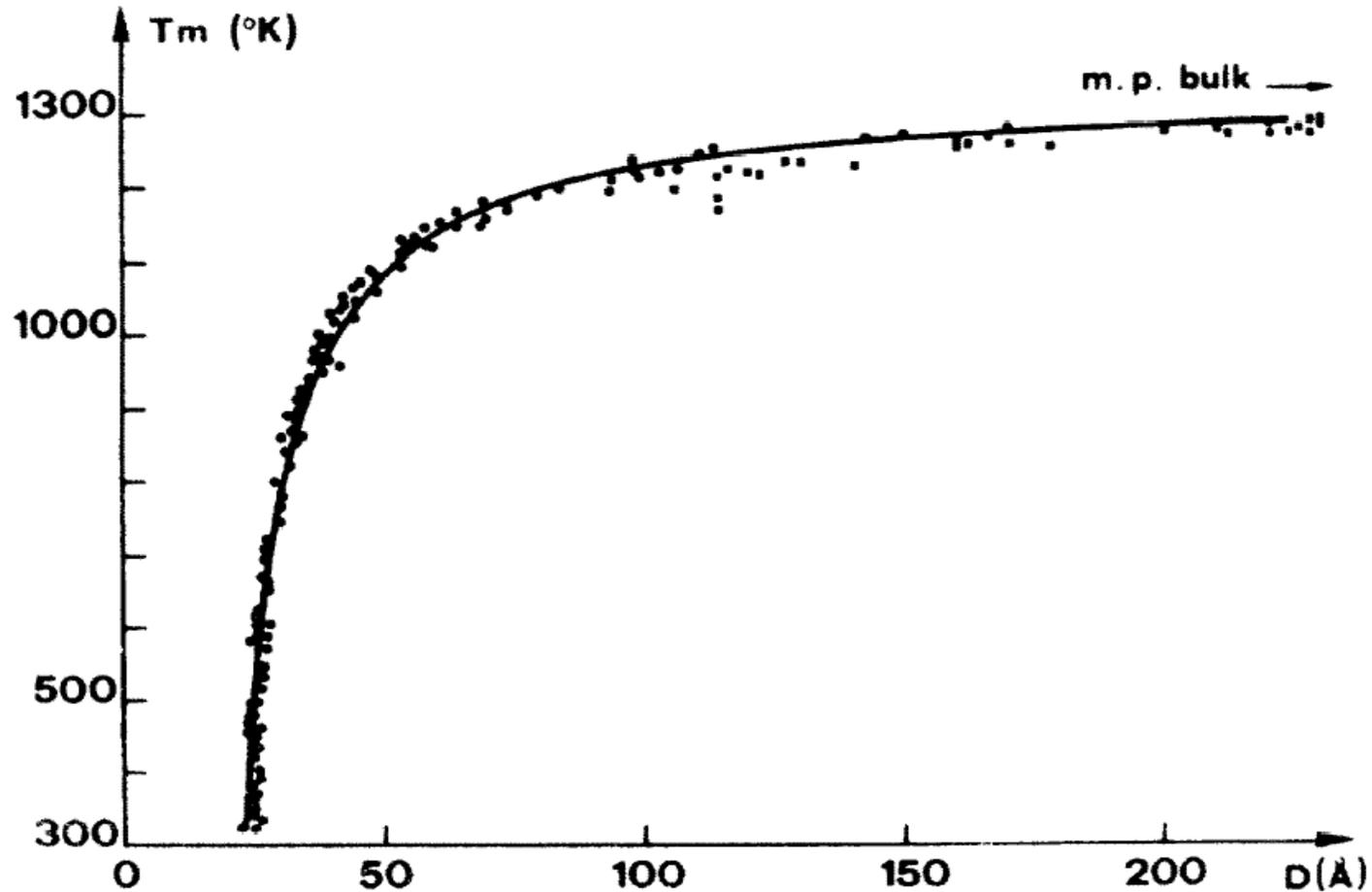
Extension to **Phase** Objects

Opportunities at UCL and FELs

# *Size-dependent Melting of Au Particles*

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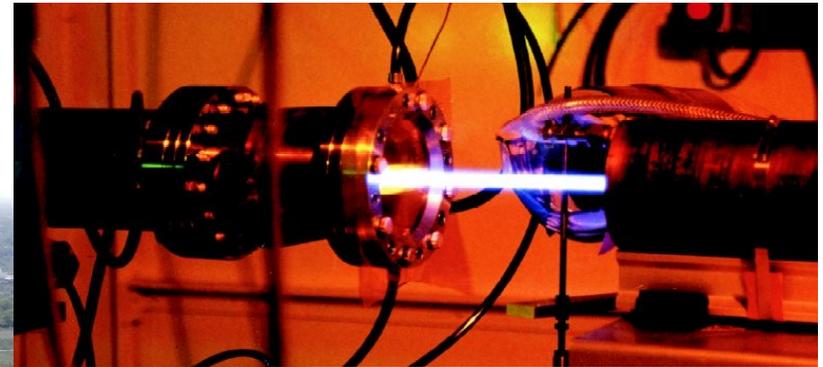
*P. Buffat and J-P. Borel, Phys. Rev. A 2287-97 (1975)*



# *Synchrotron Radiation*

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Urbana

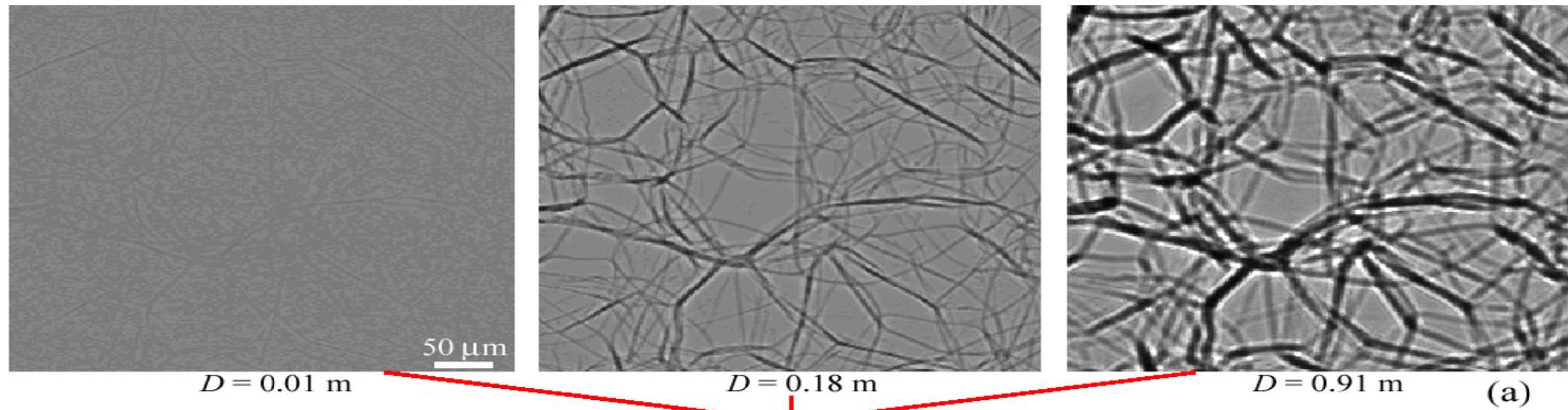


34-ID-C



# *Phase Contrast by Propagation*

*P. Cloetens et al. (1999)*



*Polystyrene foam,  
Propagation images at different distances*

*Far field  
Lensless Imaging,  
Diffraction Microscopy*

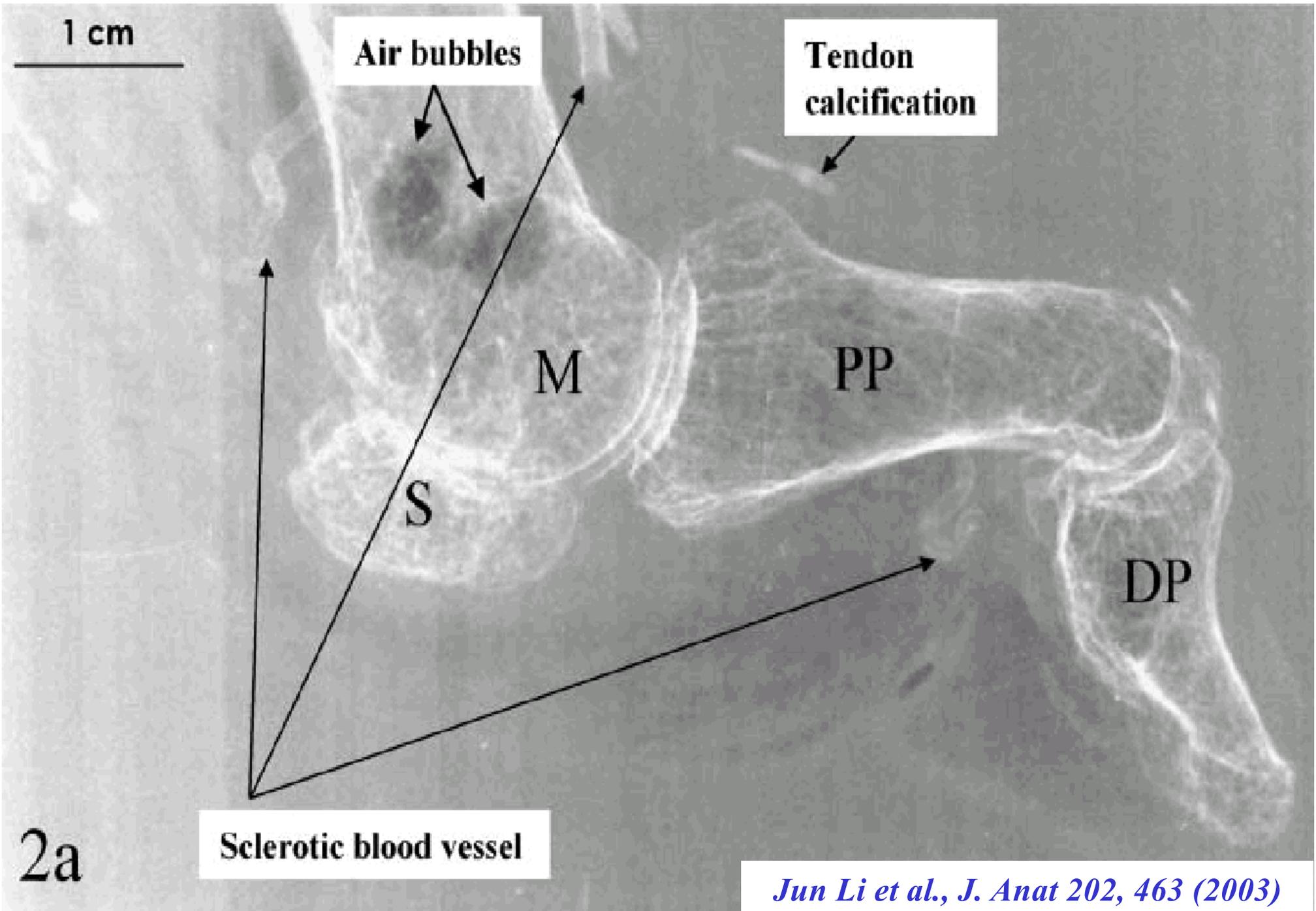
*Near field  
Phase Contrast  
Imaging*

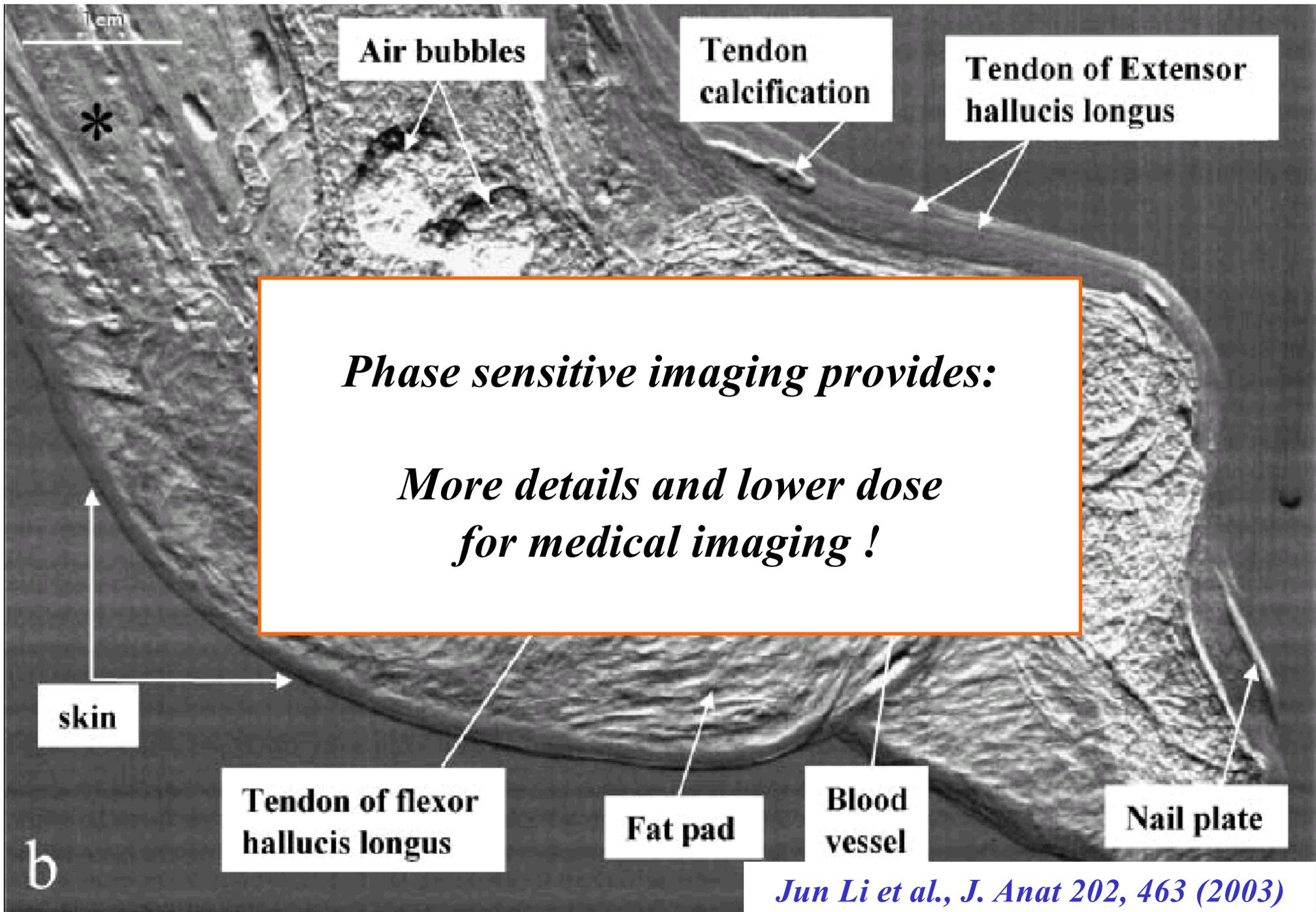
1 nm

1  $\mu$ m

1 mm

1 m

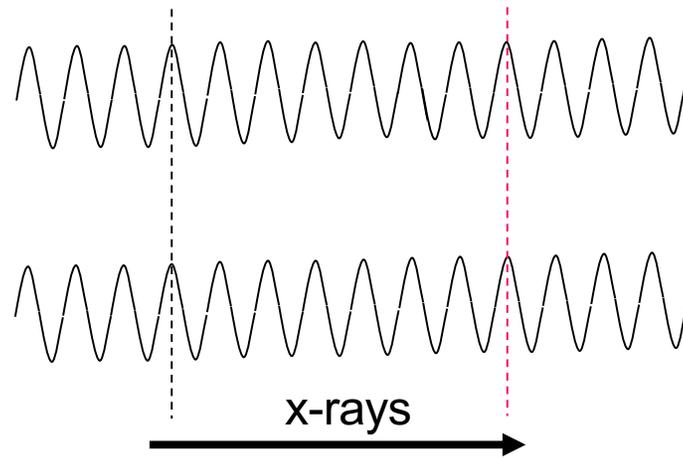




*Jun Li et al., J. Anat 202, 463 (2003)*

# *Phase sensitive x-ray imaging*

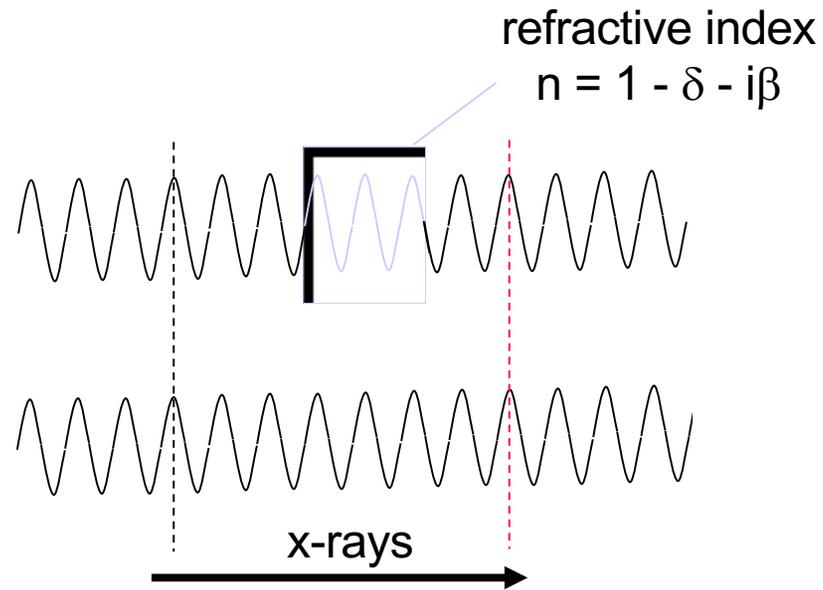
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***Coherent  
Beams***

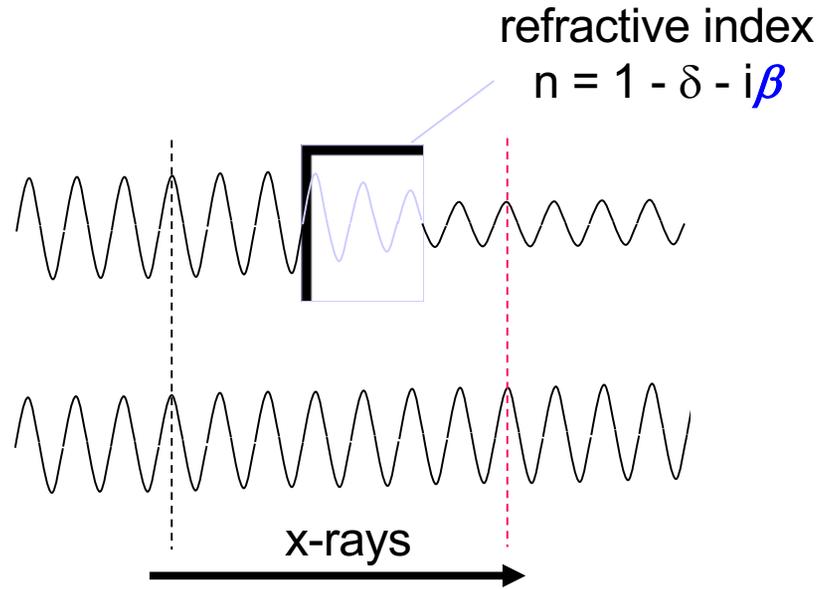
# *Phase sensitive x-ray imaging*

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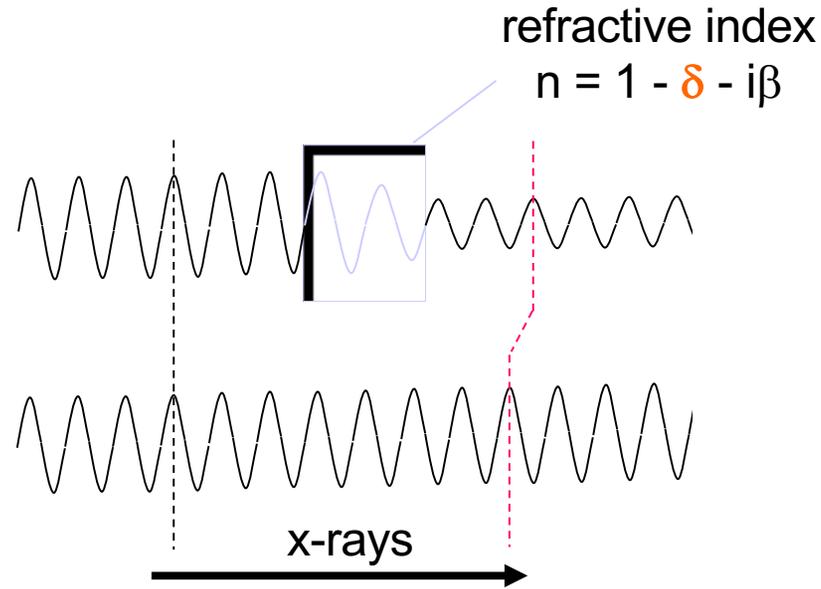
# *Phase sensitive x-ray imaging*

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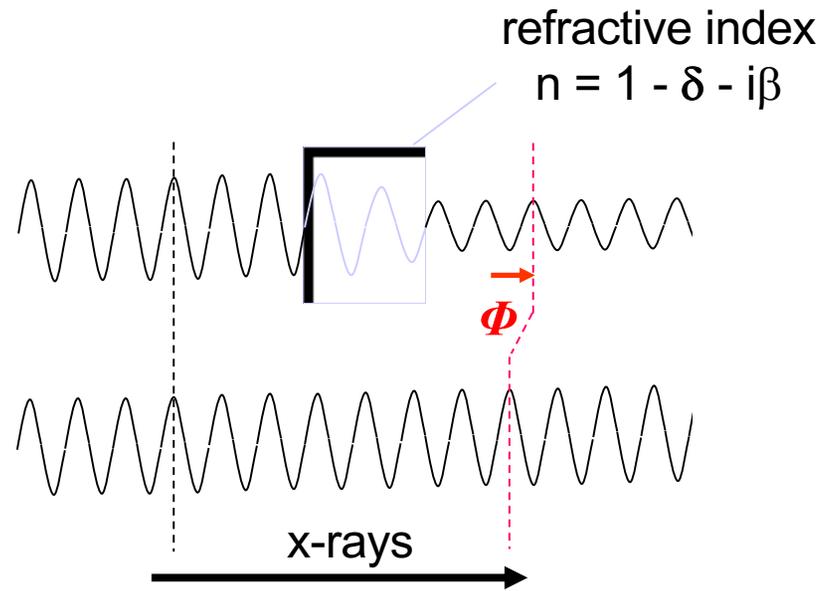
# *Phase sensitive x-ray imaging*

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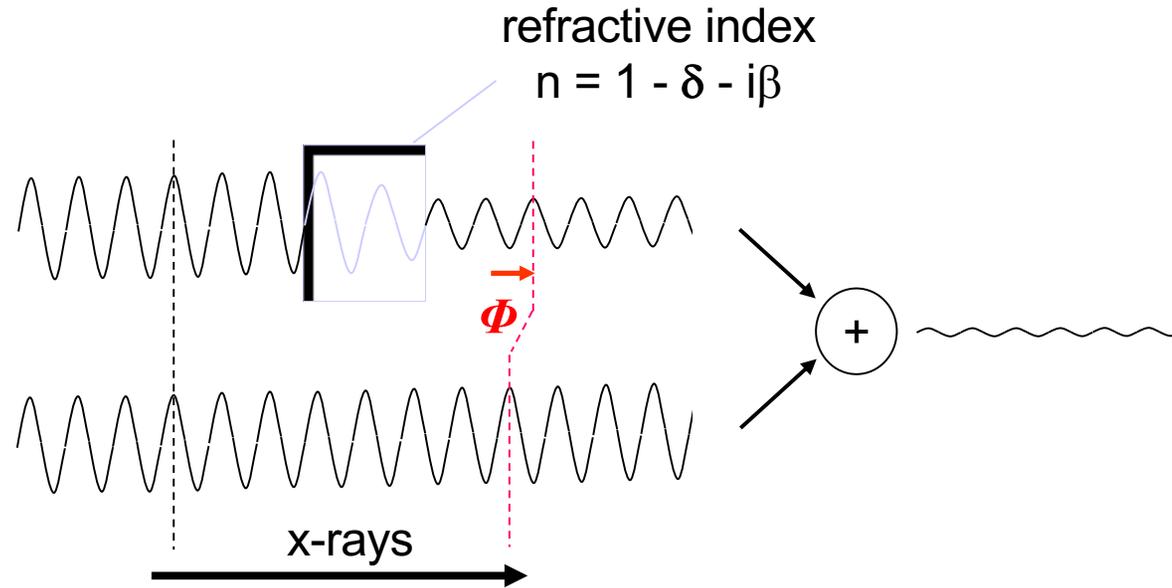
# *Phase sensitive x-ray imaging*

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# *Phase sensitive x-ray imaging*

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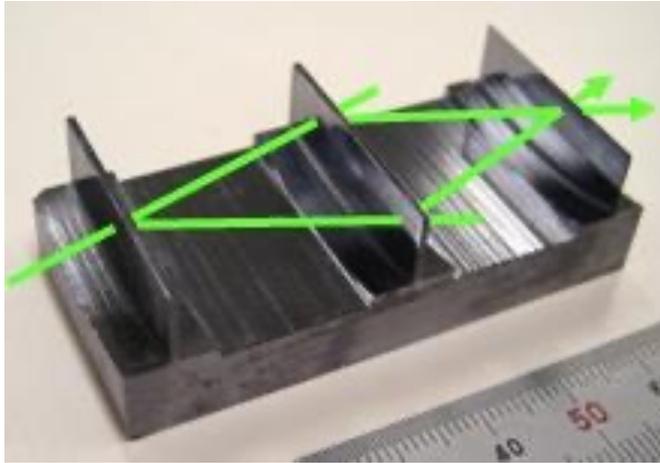
*To obtain phase sensitive images, measure:*

$\Phi$  *with a crystal interferometer (Bonse & Hart 1965)*

# Crystal Interferometers

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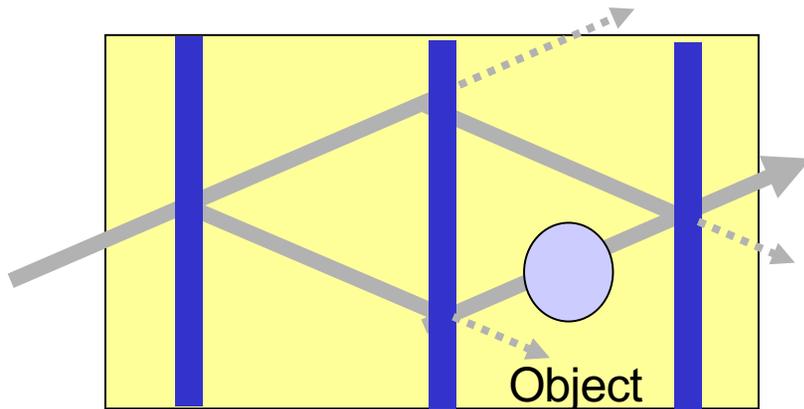
*Bonse & Hart (1965)*



*Momose et al. (2005)*

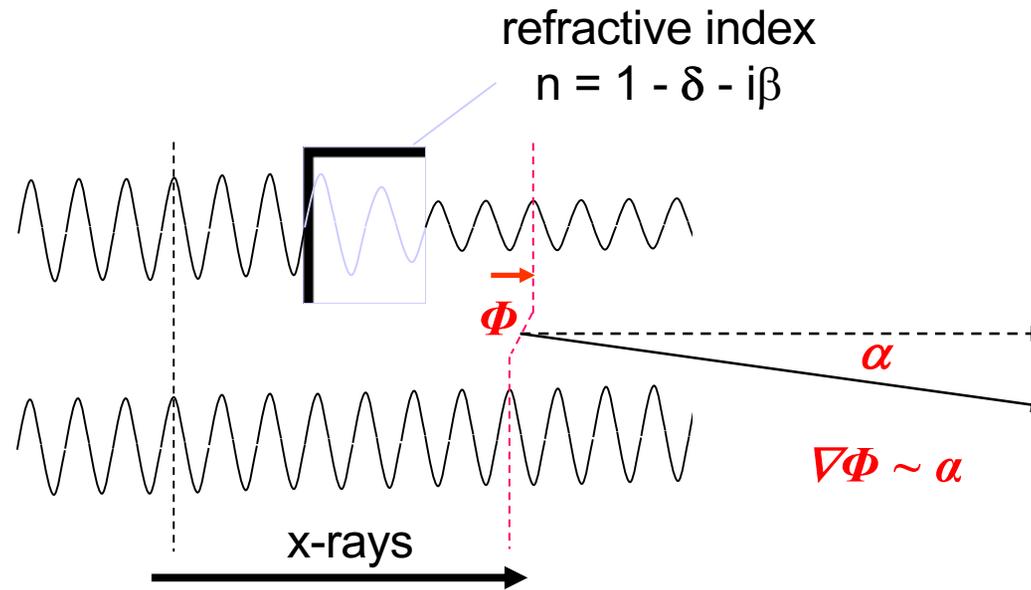


PS/PMMA polymer blend  
Phase tomography



# *Phase sensitive x-ray imaging*

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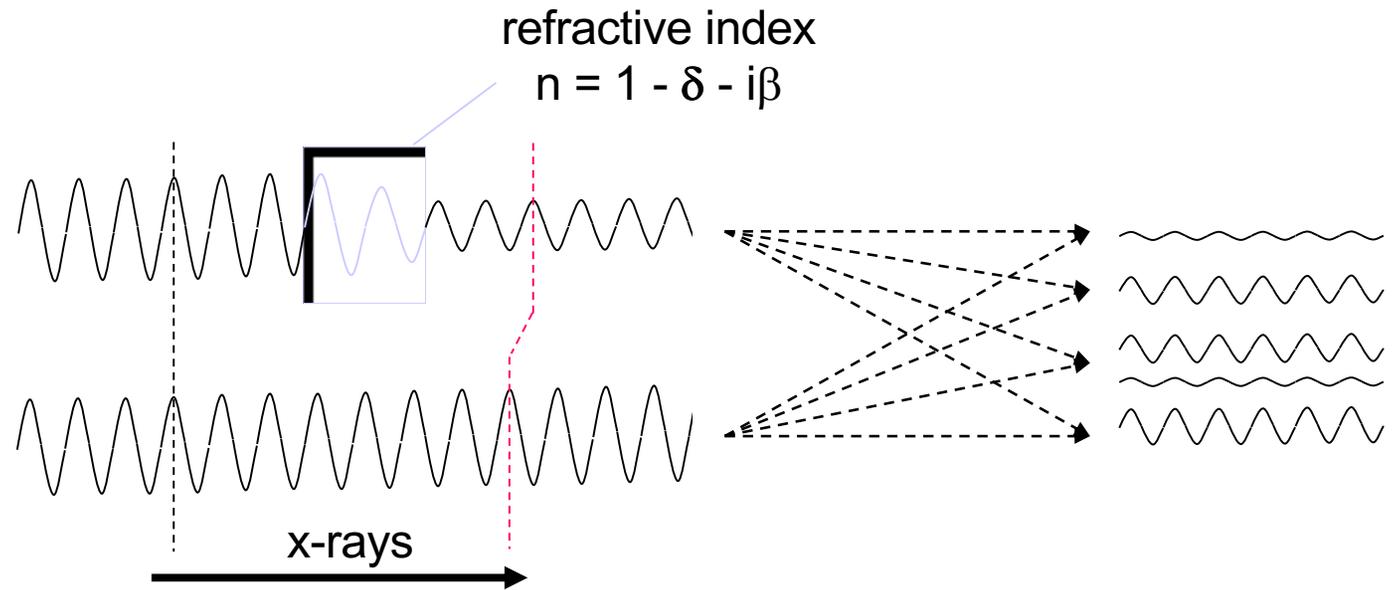


*To obtain phase sensitive images, measure:*

- $\Phi$  with a crystal interferometer (*Bonse & Hart 1965*)
- $\nabla\Phi$  with diffraction enhanced imaging (*Chapman 1997*)

# *Phase sensitive x-ray imaging*

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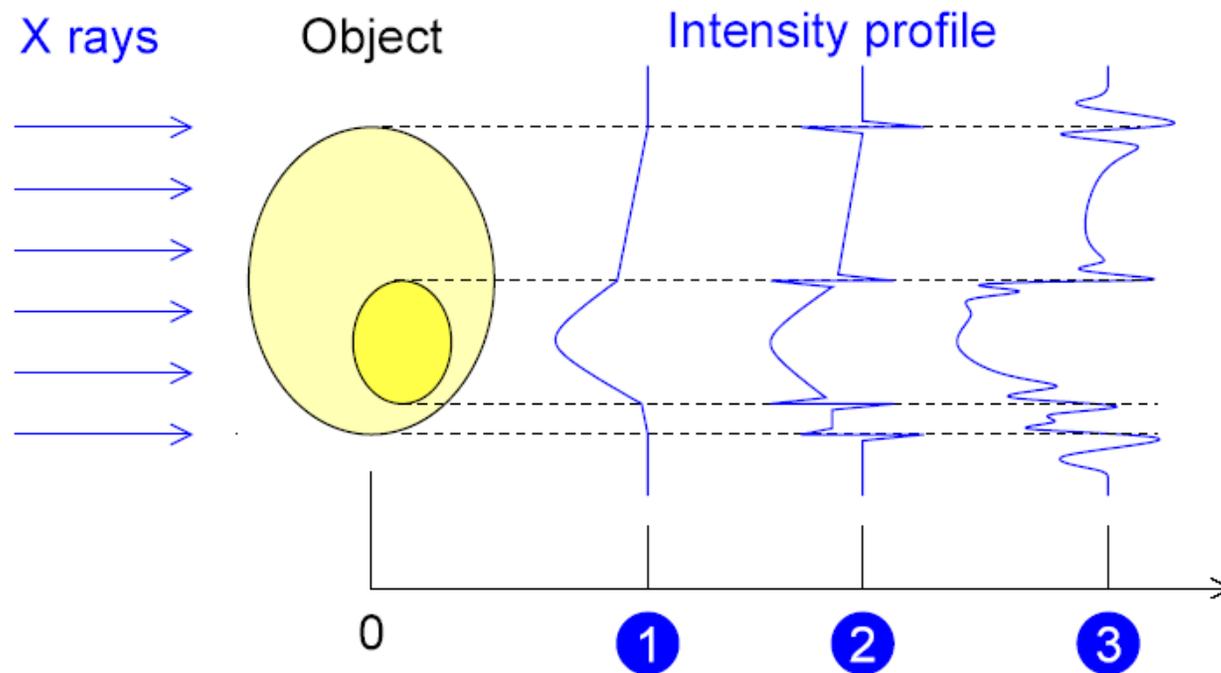
*To obtain phase sensitive images, measure:*

- $\Phi$  with a crystal interferometer (*Bonse & Hart 1965*)
- $\nabla\Phi$  with diffraction enhanced imaging (*Chapman 1997*)
- $\Delta\Phi$  with in-line holography (*Cloetens 1999*)

# *Free Space Propagation*

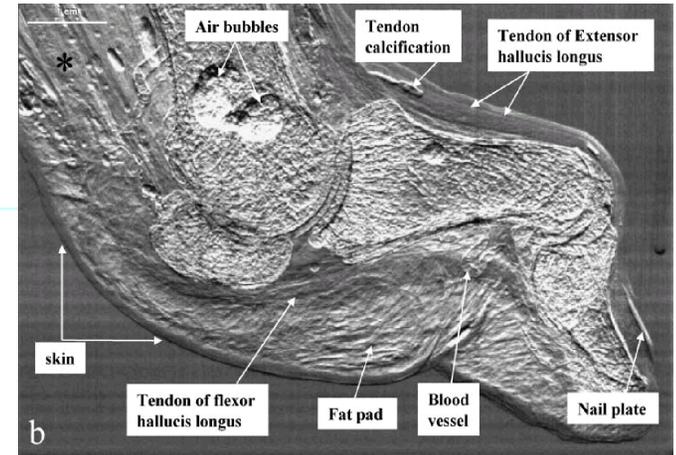
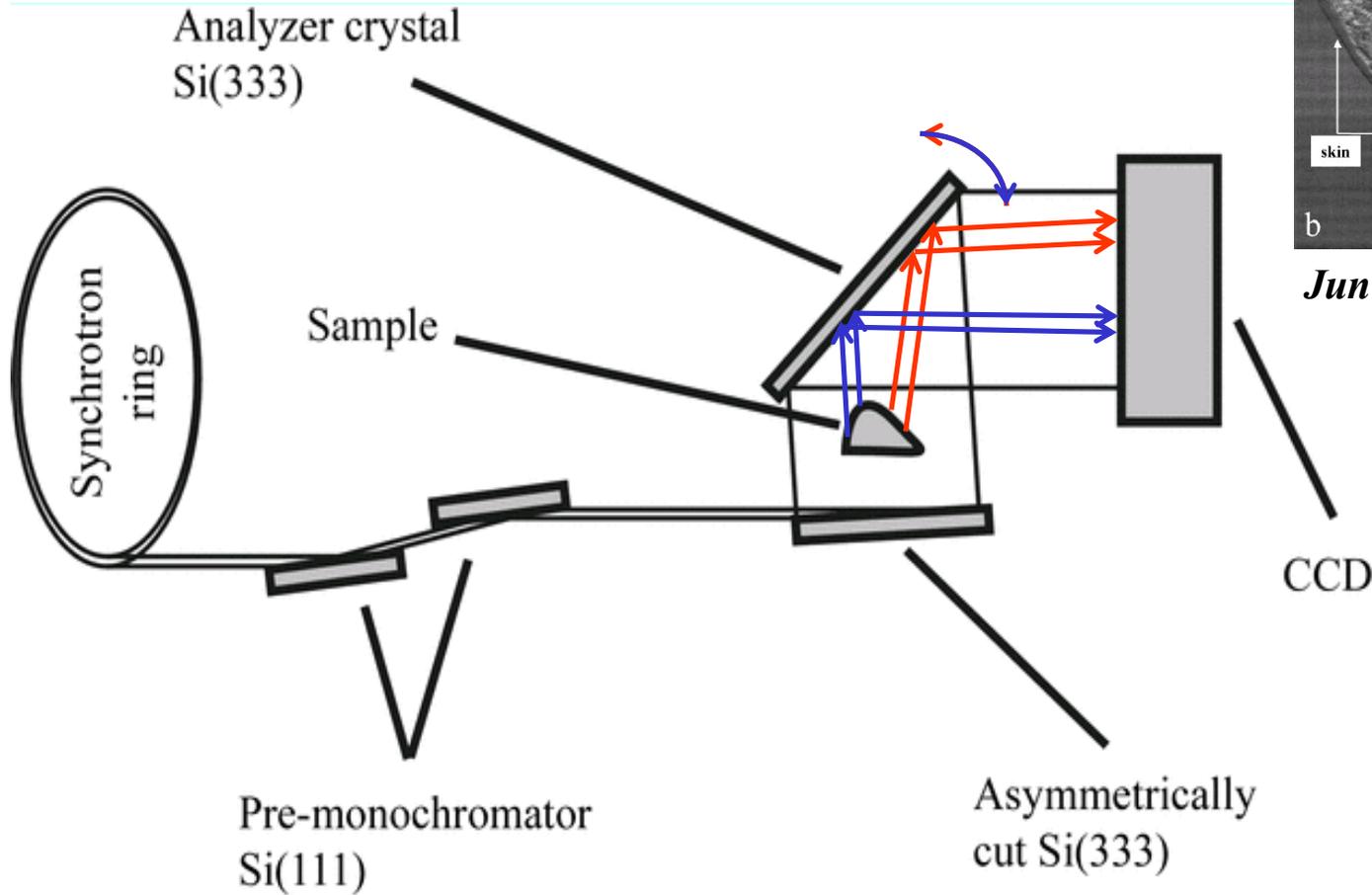
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Image formation with coherent illumination:



# Diffraction Enhanced Imaging (DEI)

*Chapman et al. (1997)*



*Jun Li et al., J. Anat 202, 463 (2003)*

# *Diffraction Enhanced Imaging (DEI)*

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*Good results at  
synchrotron sources*



*Highly monochromatic  
(inefficient)*

*requires parallel beam*

*limited field of view (crystals !)*

*Not suitable for hospital based medical  
imaging systems (e.g. x-ray tubes) !*

# *Free Space Propagation*

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*Simplicity*

*Polychromatic*

*Non-interferometric method  
(no phase-stepping)*



*Limited FOV (high resolution  
detector required)  
or very large distances*

*Low sensitivity at low  
spatial frequencies*

*Requires spatial coherence*

*Not suitable for hospital based medical  
imaging systems (e.g. x-ray tubes) !*

# *Grating Interferometer*

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*Polychromatic*

*Large FOV possible*

*Suitable for spherical waves  
(x-ray tubes)*

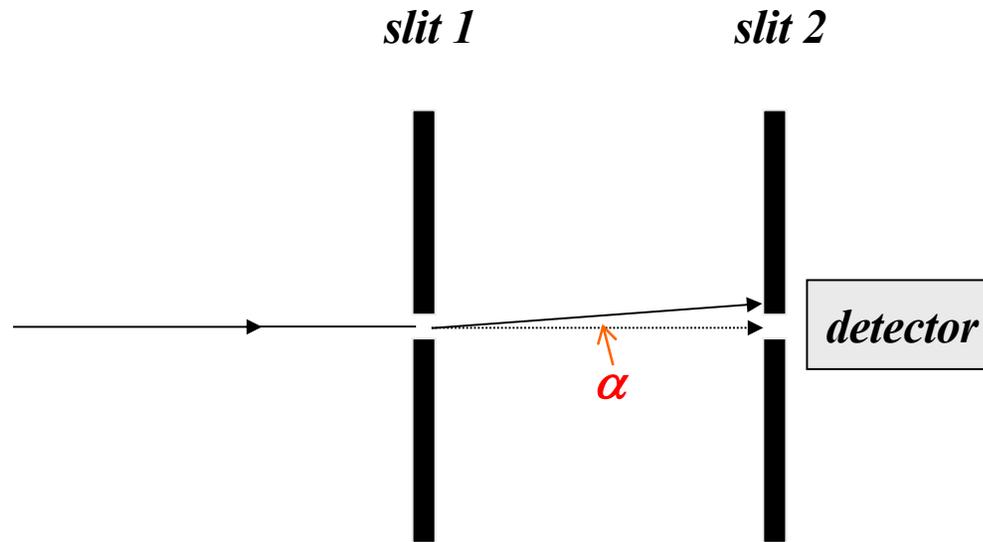


*Requires gratings*

*Suitable for hospital based medical  
imaging systems (e.g. x-ray tubes) !*

# *Grating Interferometer*

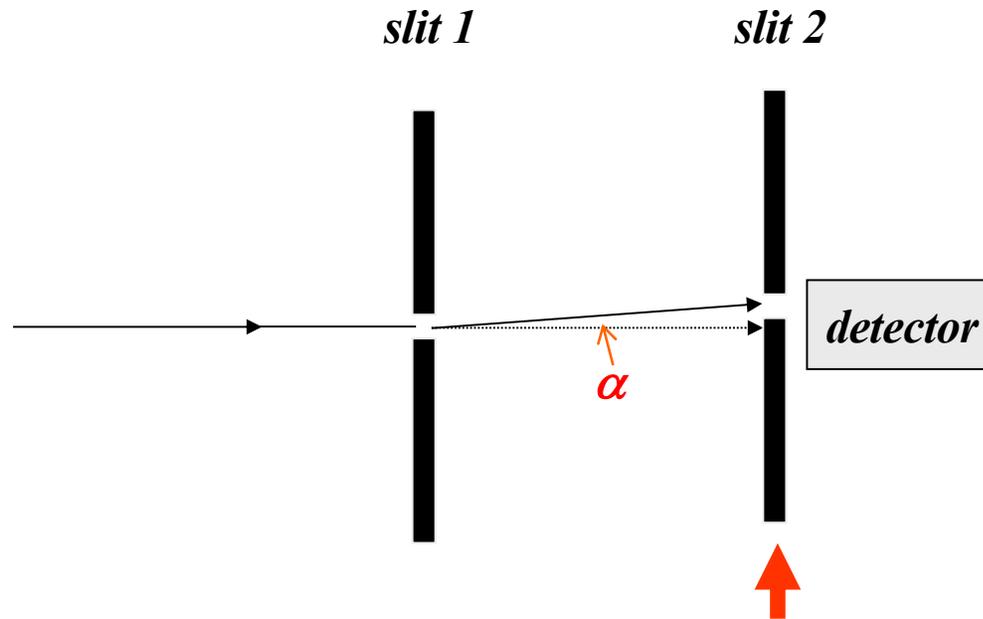
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*Idea: polychromatic detection of angles*

# *Grating Interferometer*

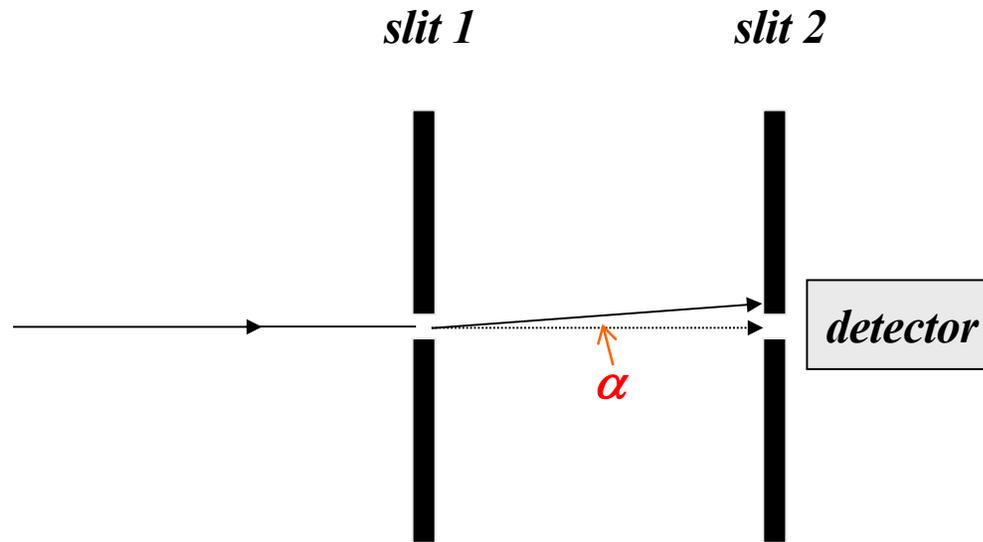
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*Idea: polychromatic detection of angles*

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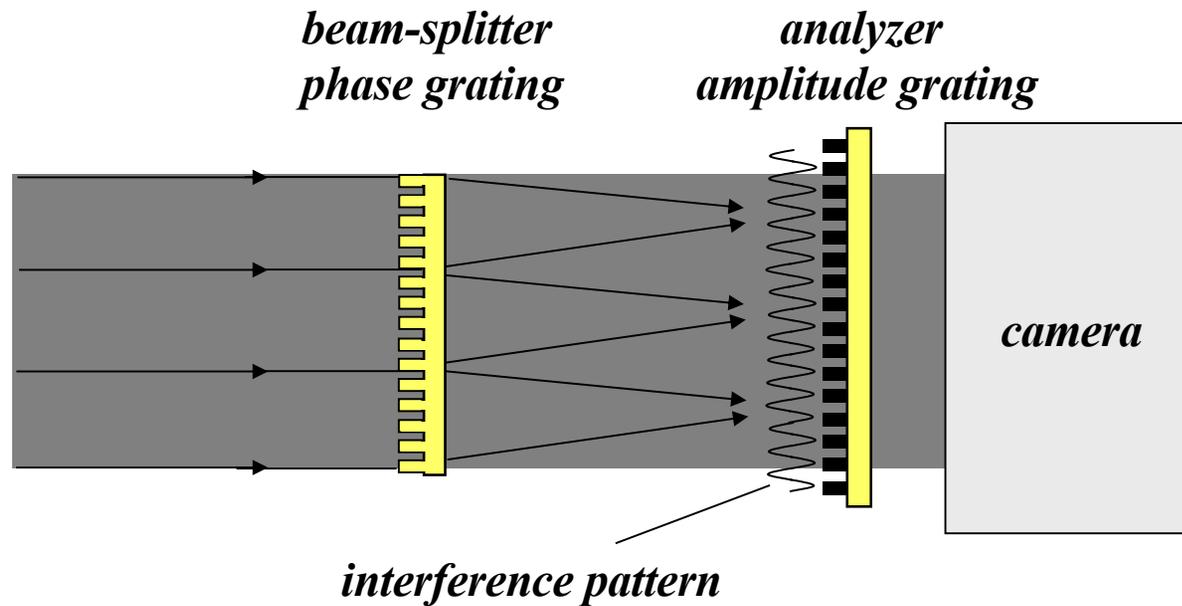
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*Idea: polychromatic detection of angles*

# Grating Interferometer

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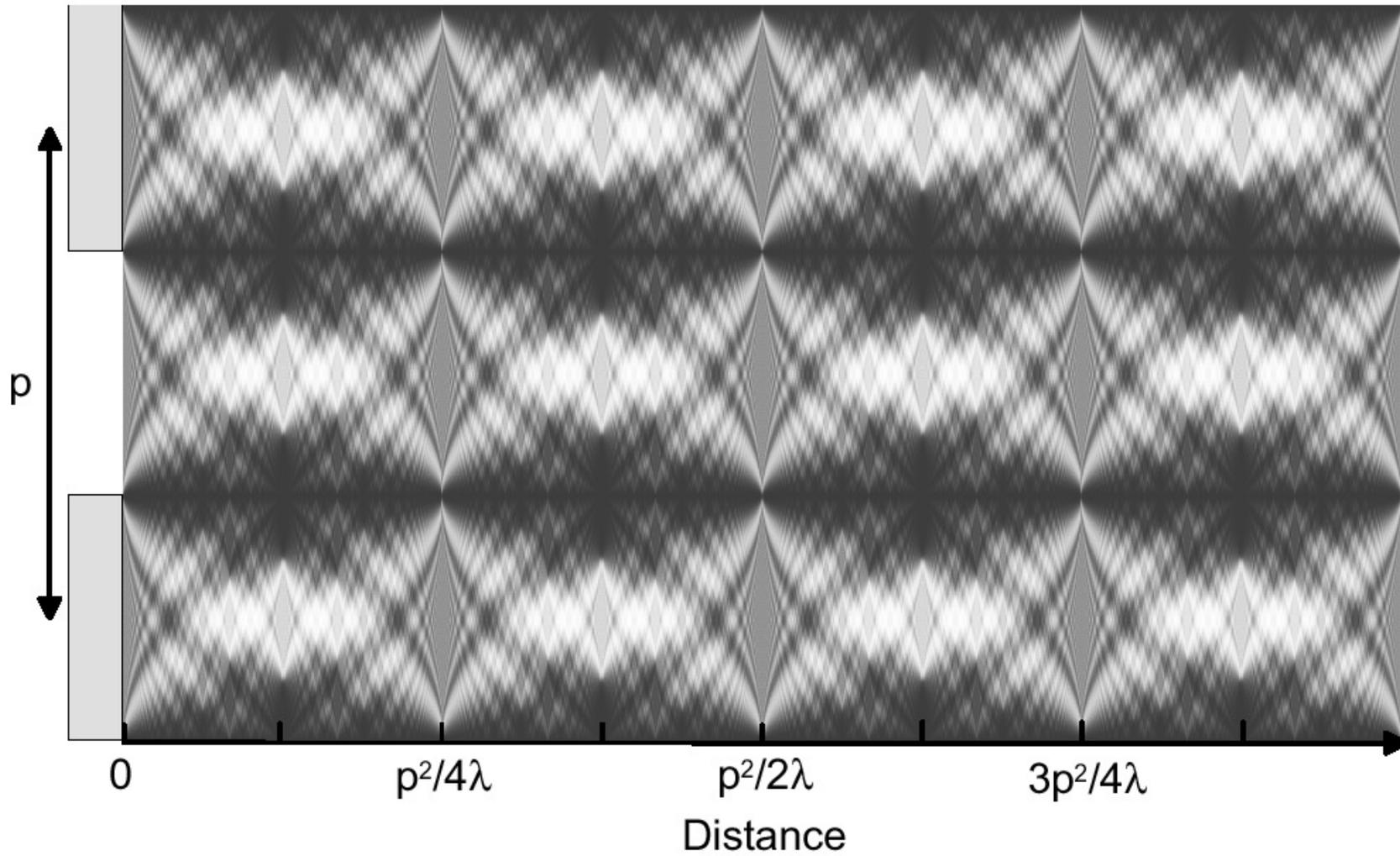


- *phase grating as beam splitter*
- *absorption grating as transmission mask*
- *x-ray wavelength  $\lambda \sim 0.1 \text{ nm}$ , grating periods  $\sim 2\text{-}4 \mu\text{m}$*

*Patent pending, # 05 012 121.9 (2005)*

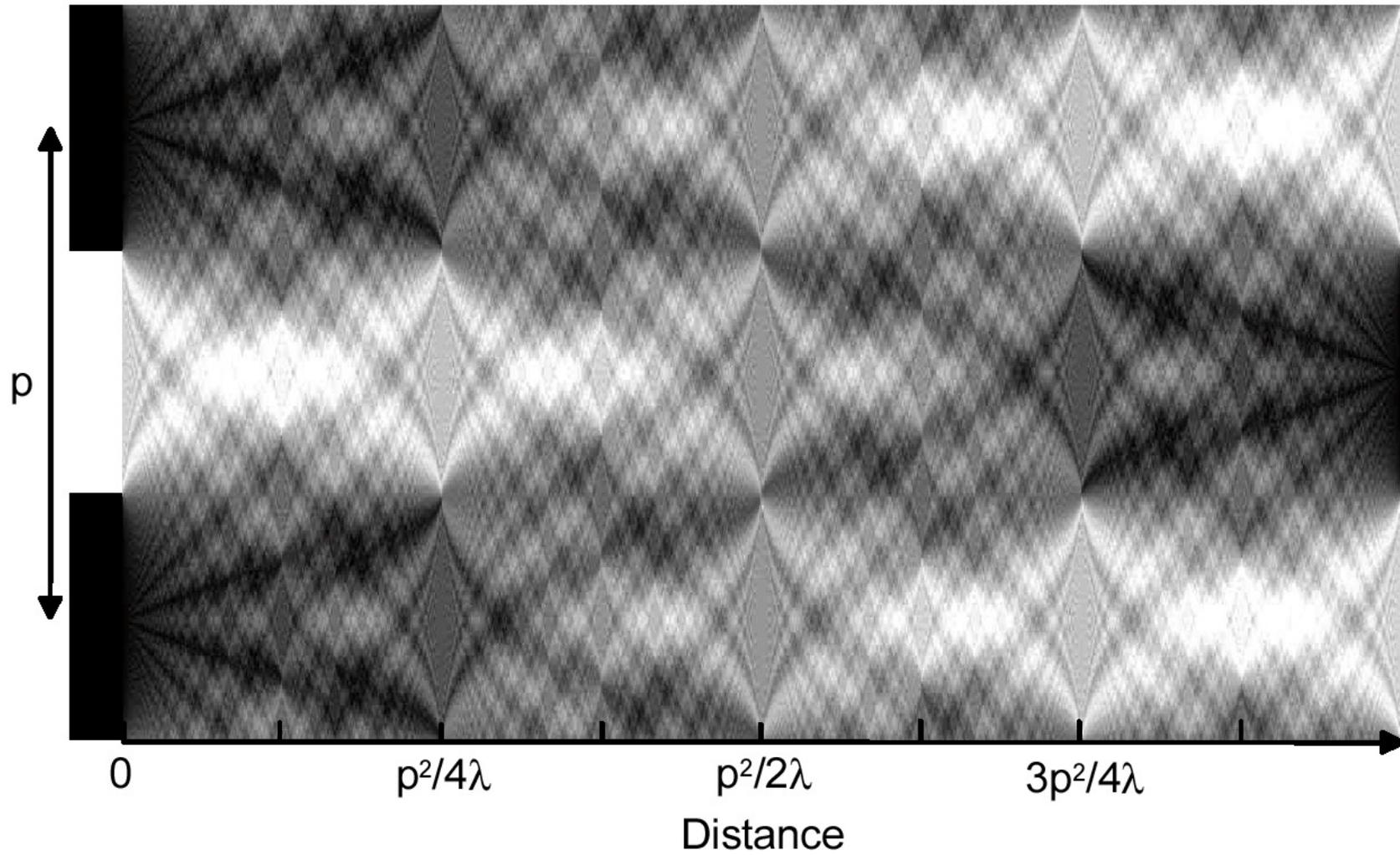
# *The Talbot effect*

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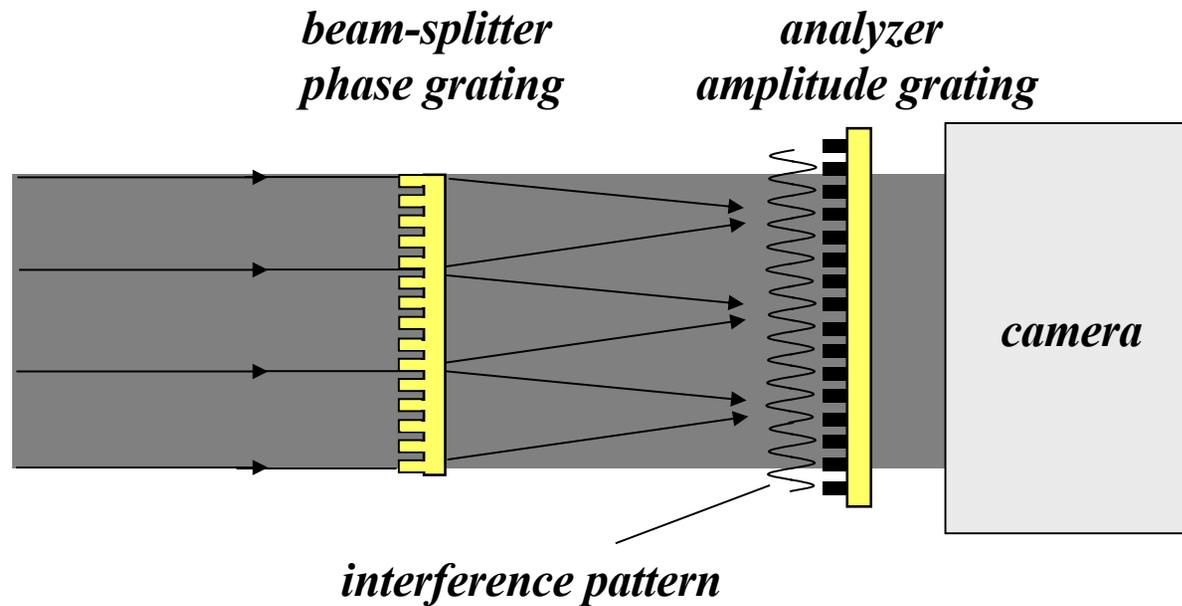
# *The Talbot effect*

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# Grating Interferometer

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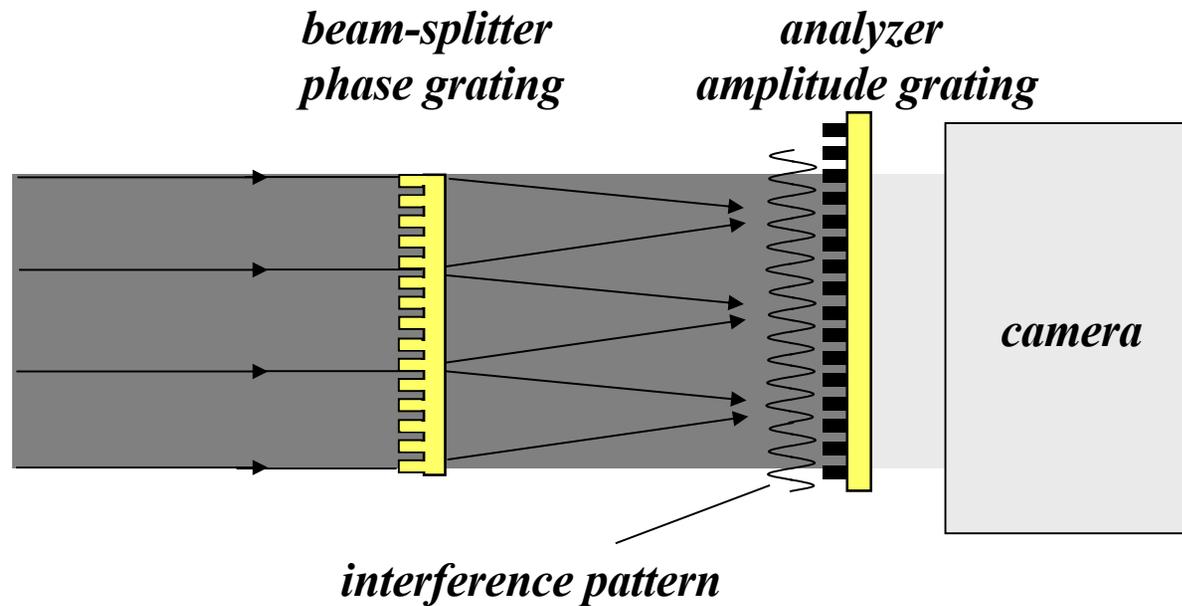


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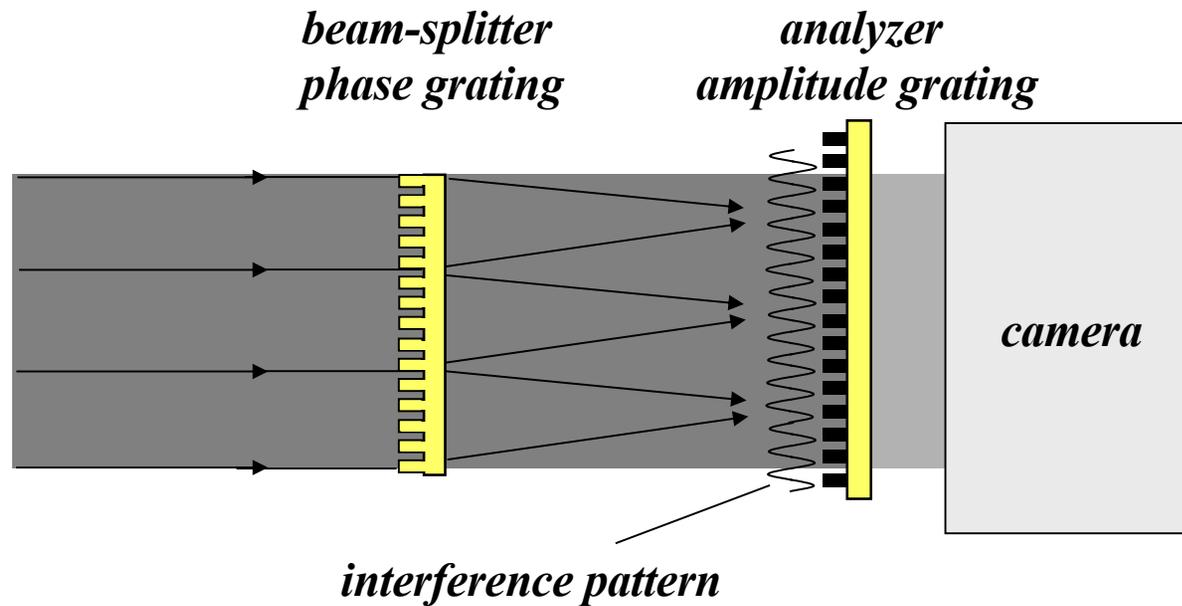


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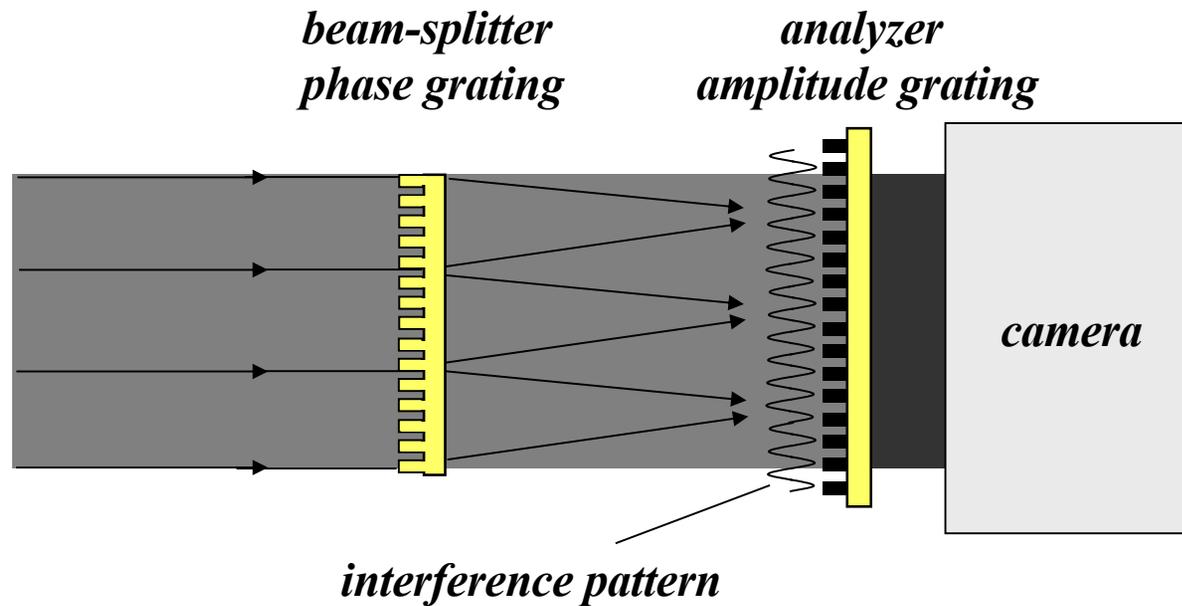


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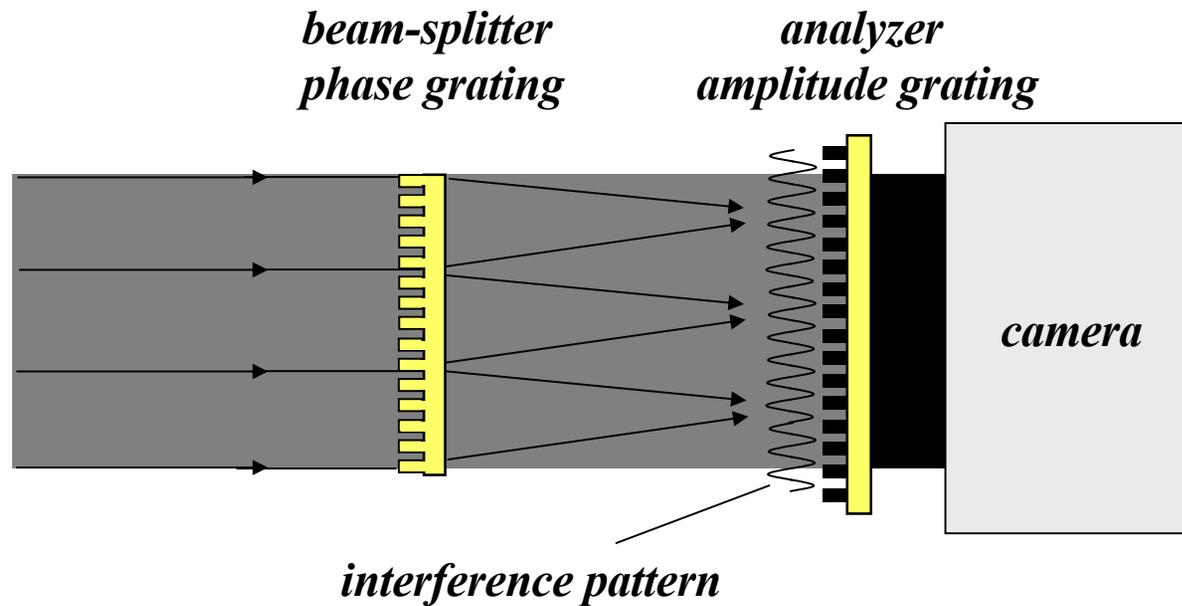


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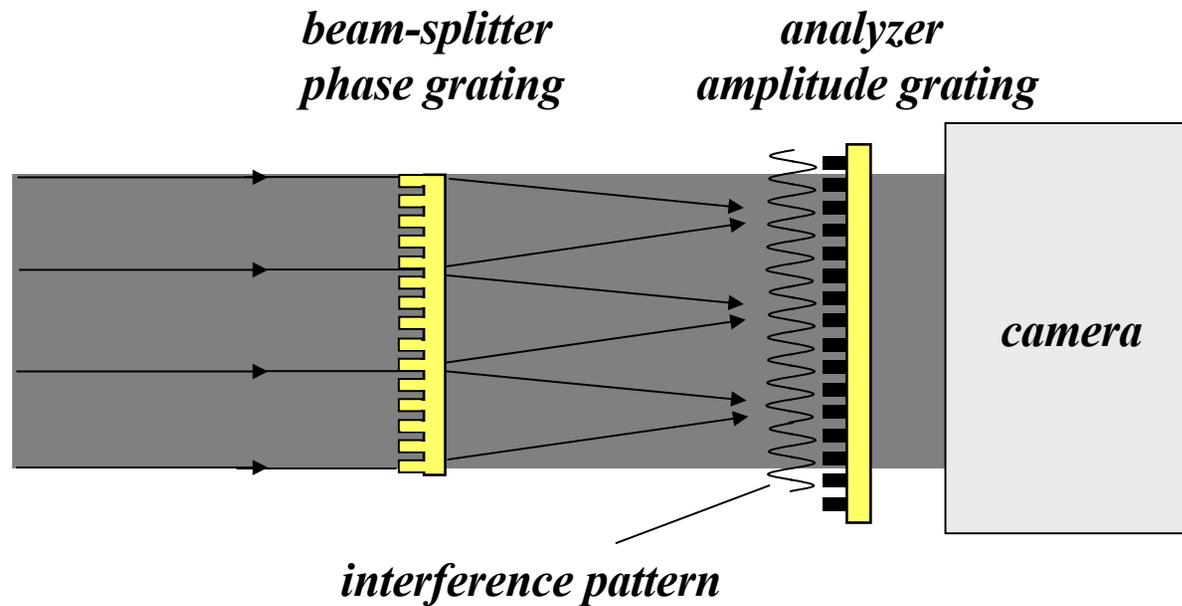


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*Patent pending, # 05 012 121.9 (2005)*

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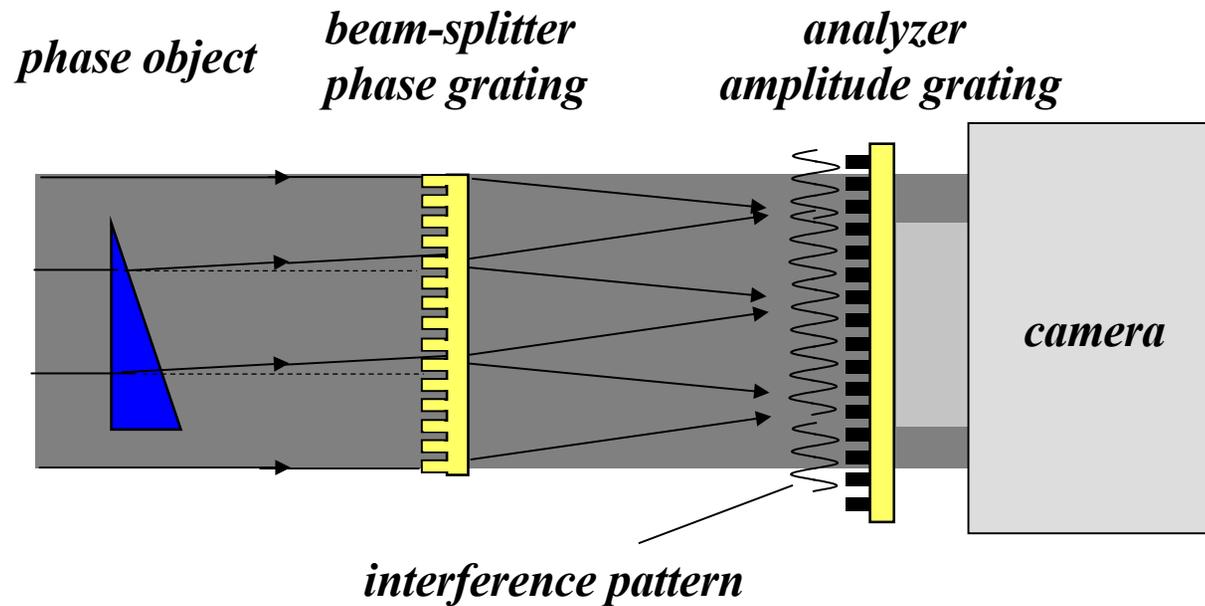
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*Patent pending, # 05 012 121.9 (2005)*

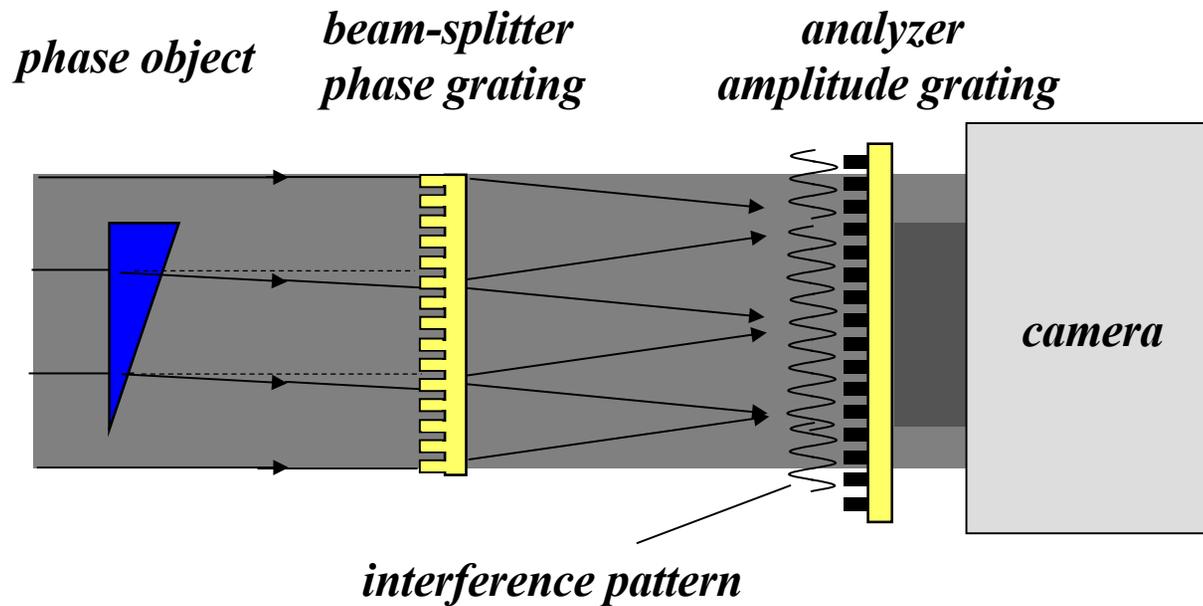
# Grating Interferometer



- *phase grating as beam splitter*
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- *phase object cases intensity to change*

*Patent pending, # 05 012 121.9 (2005)*

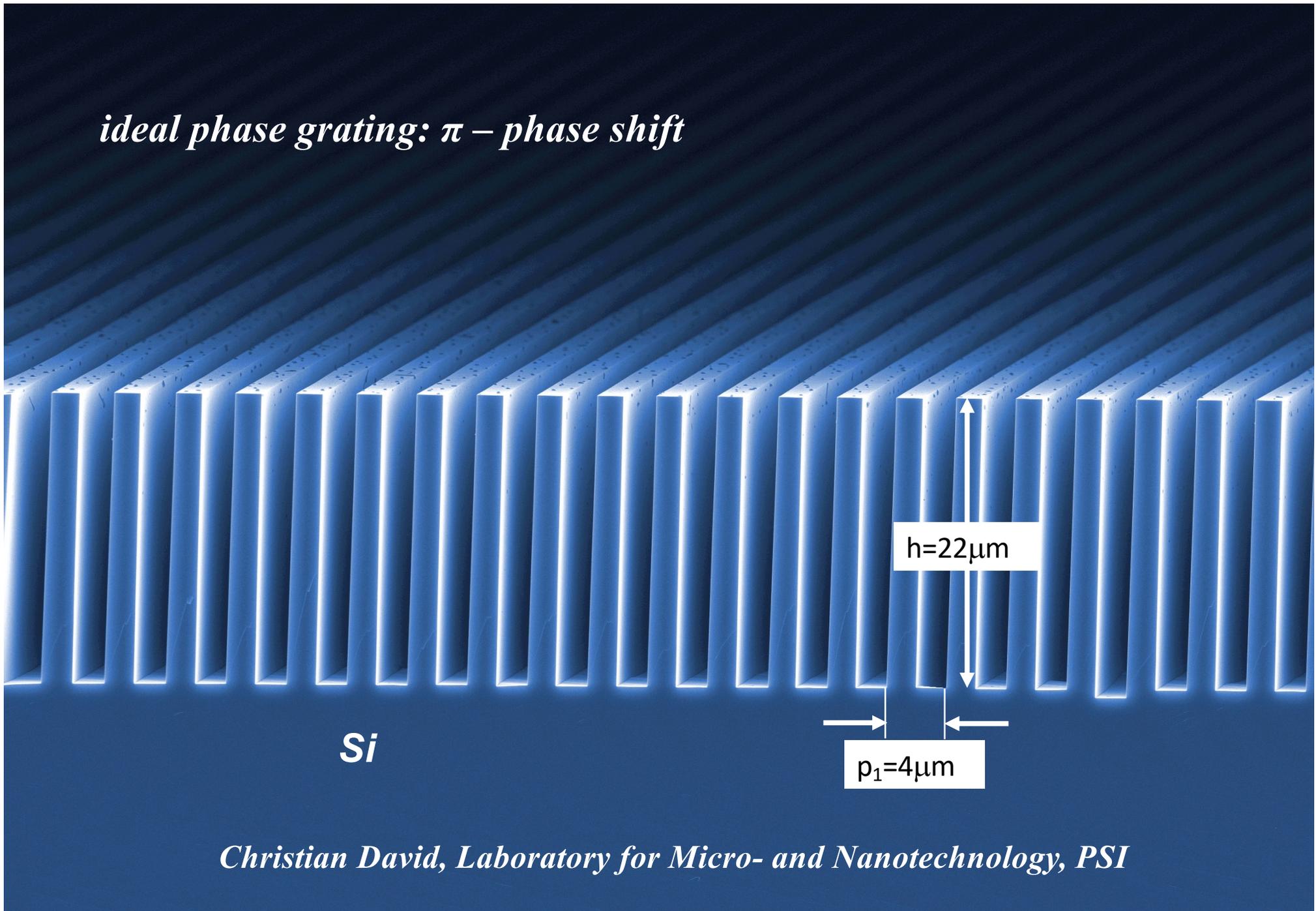
# Grating Interferometer



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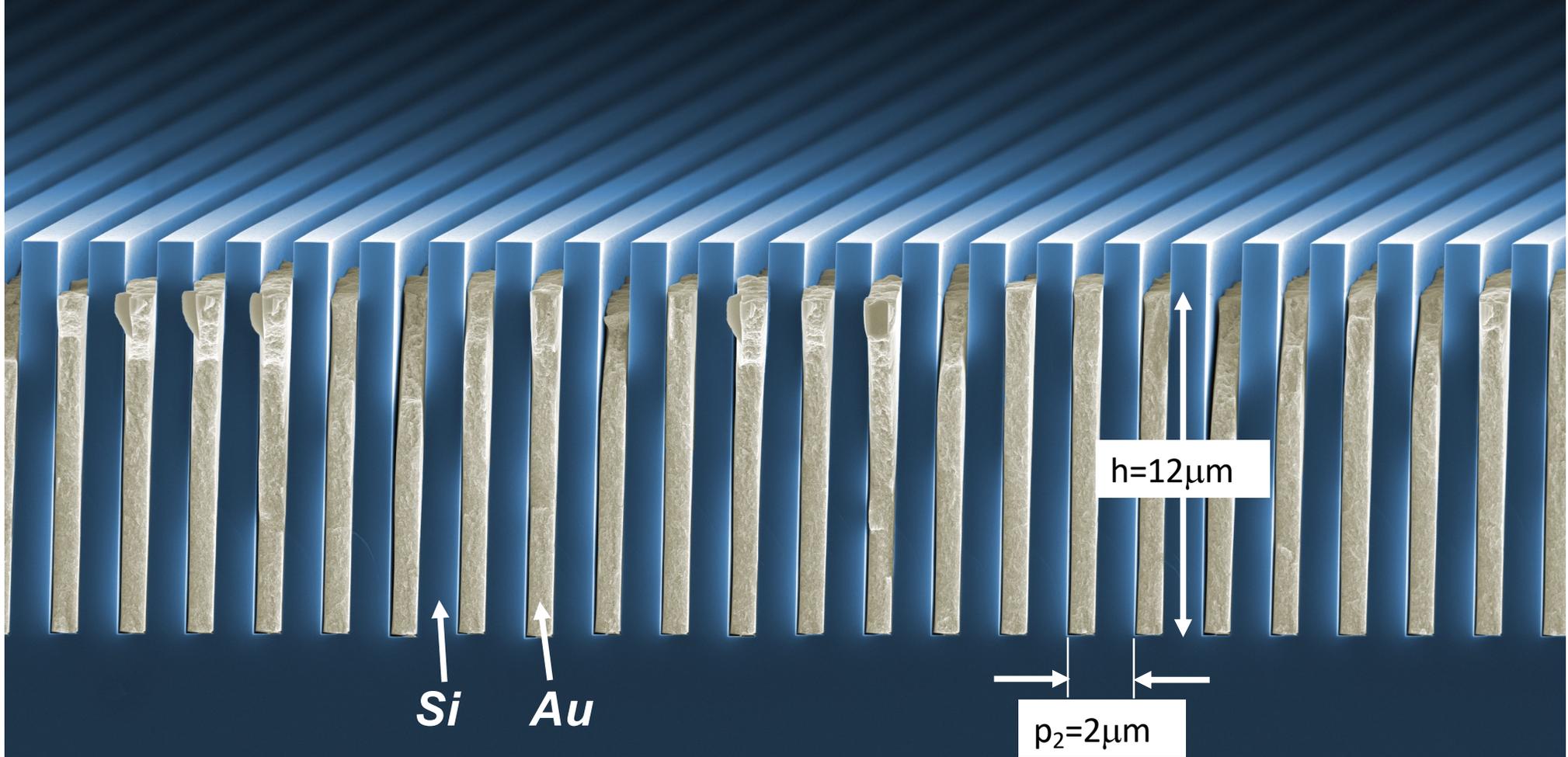
*Patent pending, # 05 012 121.9 (2005)*

*ideal phase grating:  $\pi$  – phase shift*



*Christian David, Laboratory for Micro- and Nanotechnology, PSI*

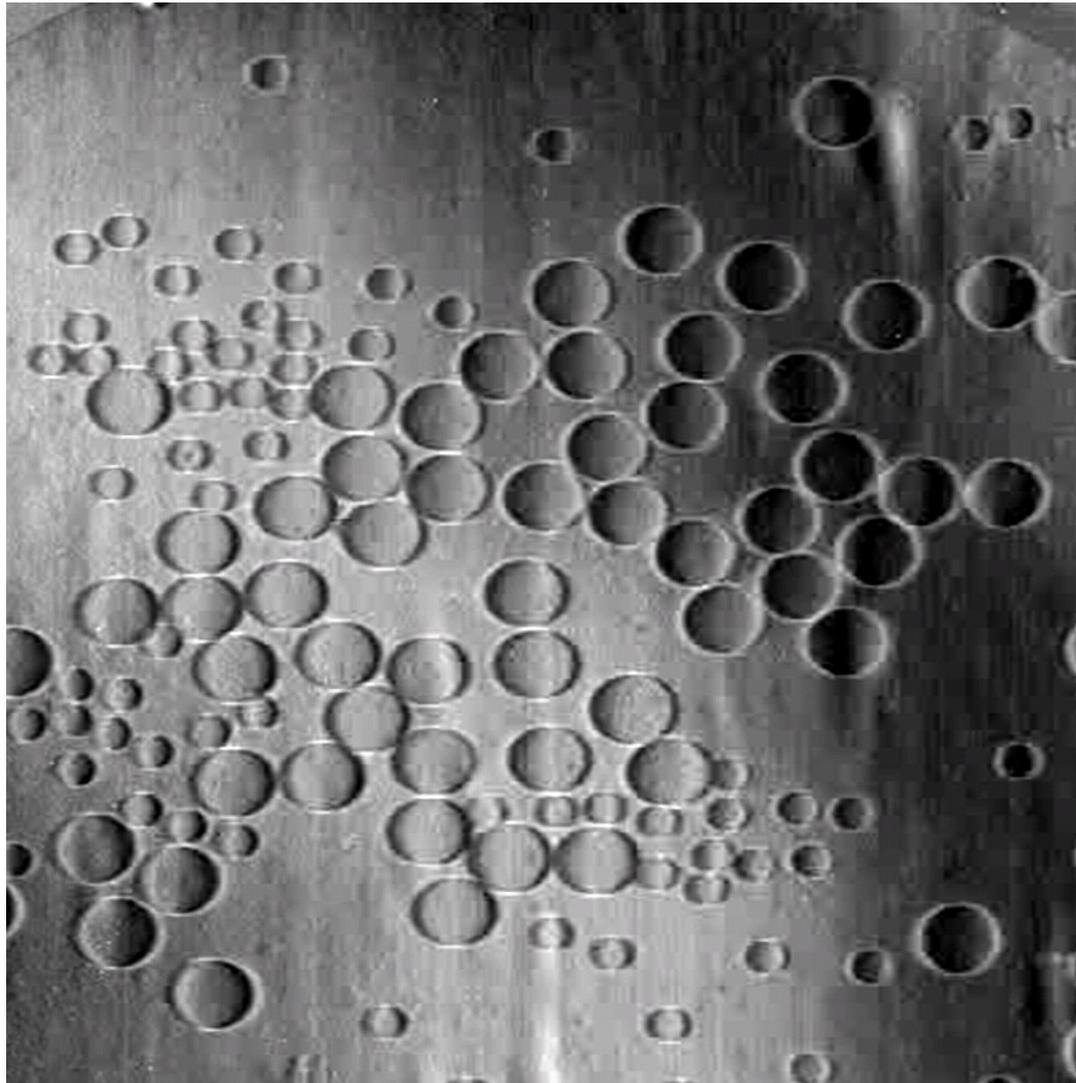
*ideal analyzer grating: strongly absorbing lines*



*Christian David, Laboratory for Micro- and Nanotechnology, PSI*

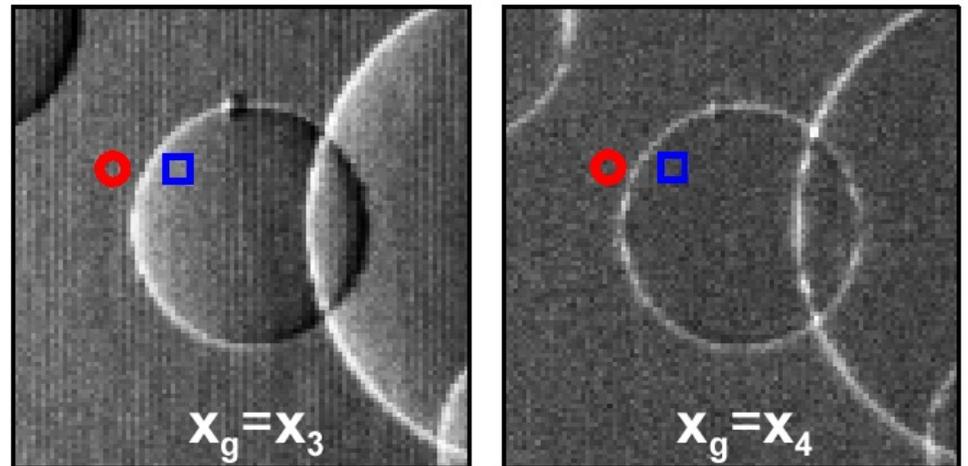
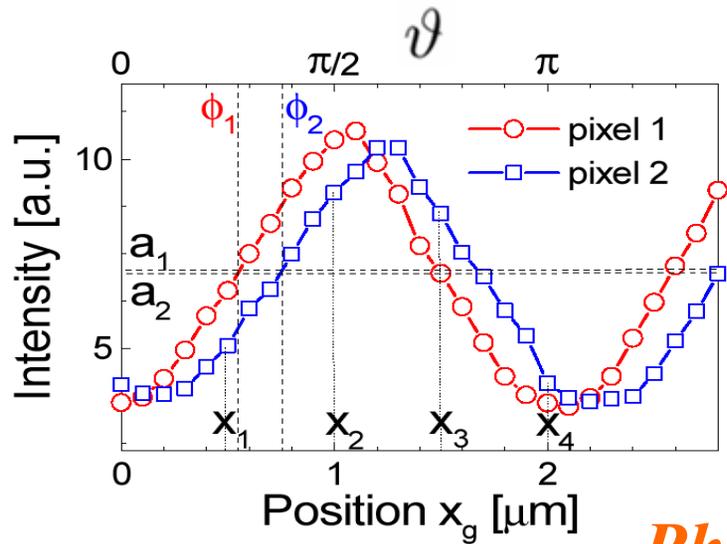
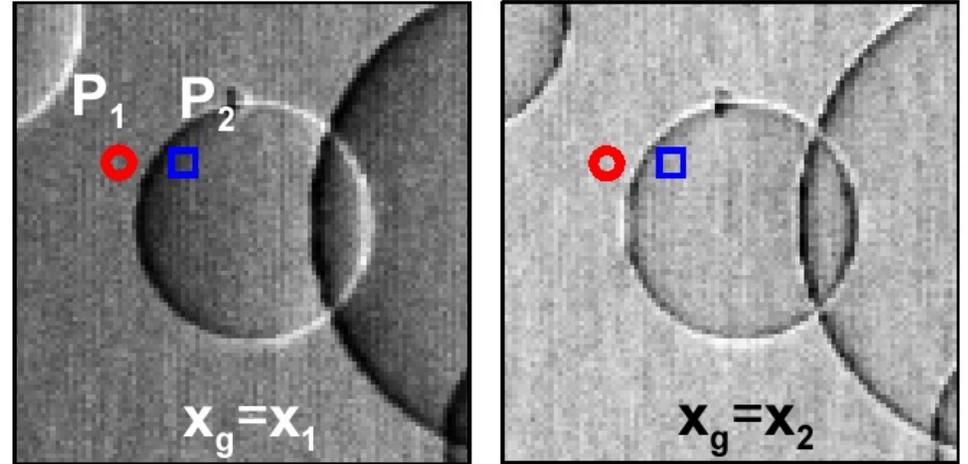
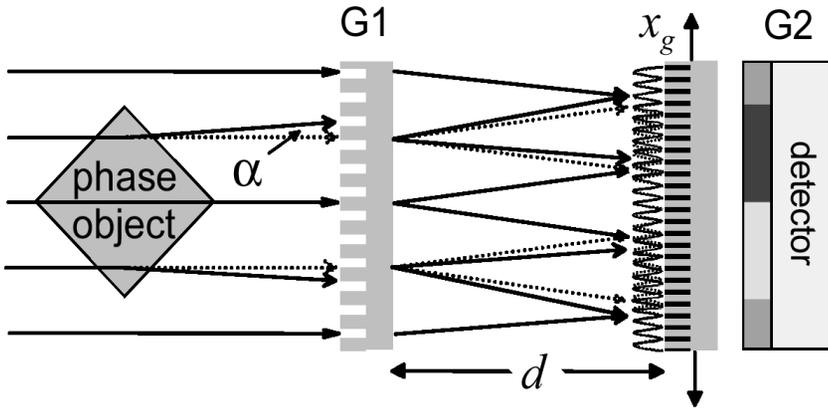
# *Synchrotron results*

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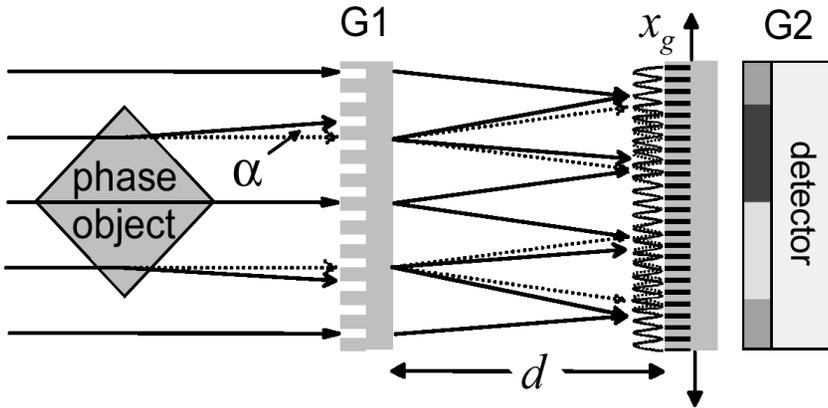
*December 2002,  
polystyrene spheres,  
photon energy: 12.4 keV*

# Separation of phase shift & absorption

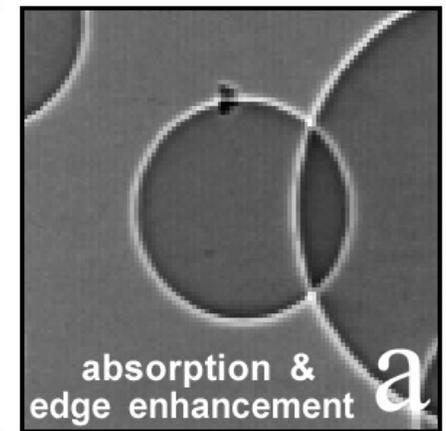
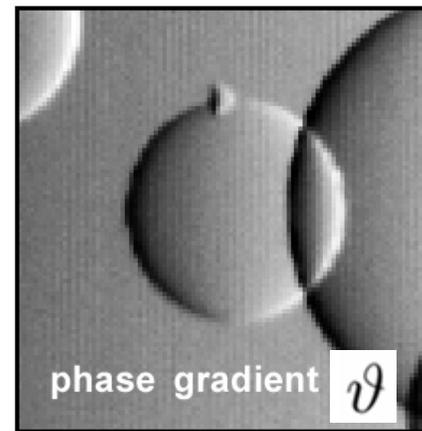
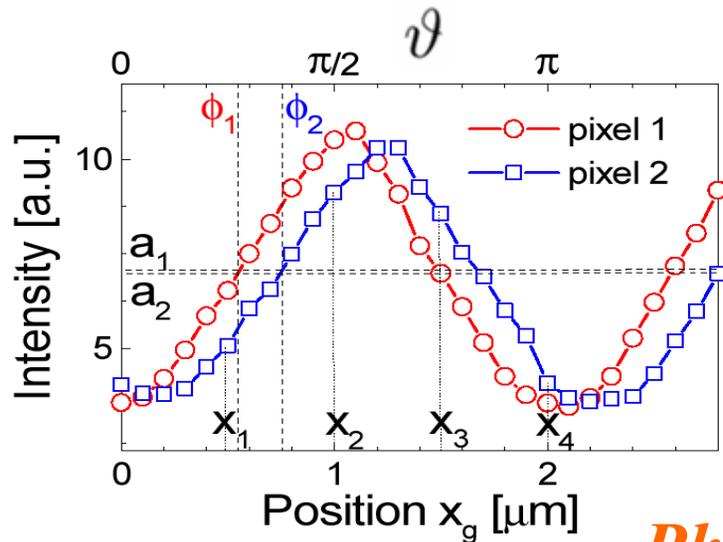
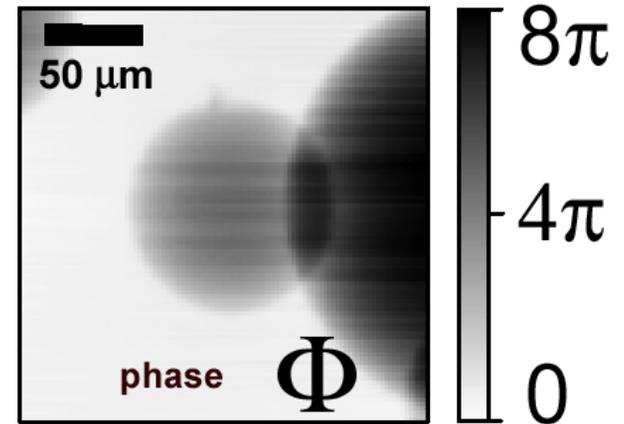


*Phase stepping*

# Separation of phase shift & absorption



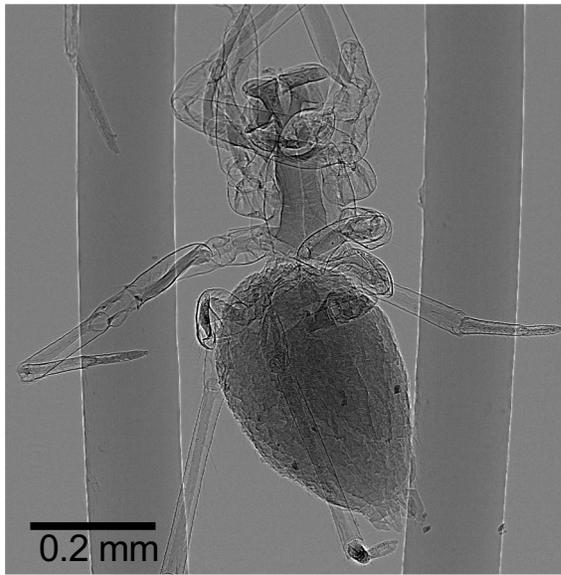
$$\vartheta = \frac{\lambda d}{p_2} \frac{\partial \Phi}{\partial x}$$



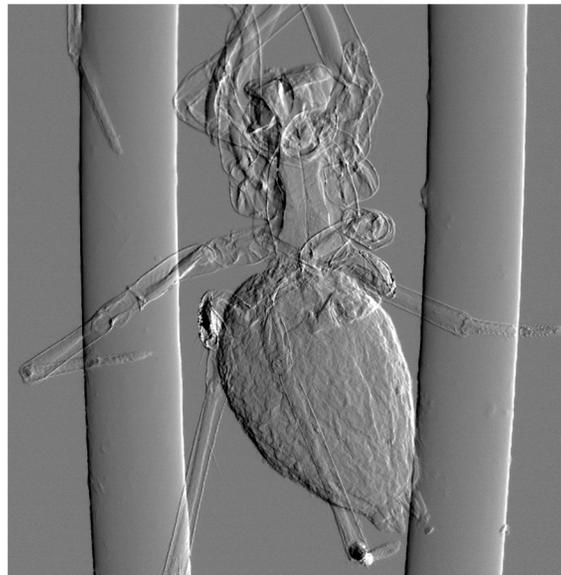
*Phase stepping*

# *Synchrotron results*

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*Transmission*



*Phase gradient*



*Phase*

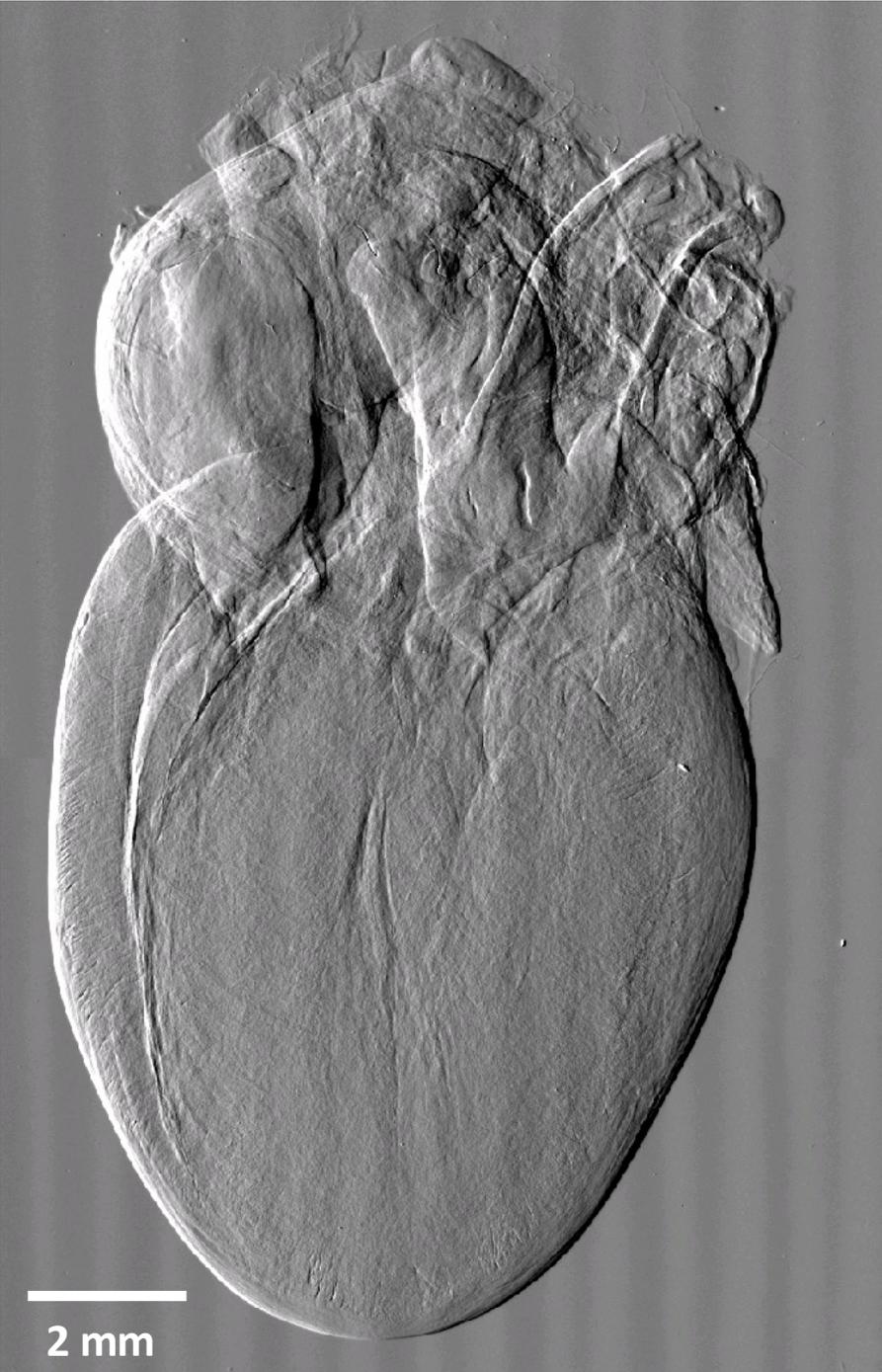
*T. Weitkamp et al., Optics Express 16, 6296 (2004)*

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*Ian Robinson -- Medical Imaging Seminar -- March 2006.*



*T. Weitkamp et al., Optics Express 16, 6296 (2004)*



2 mm

*July 2005,  
Synchrotron results*

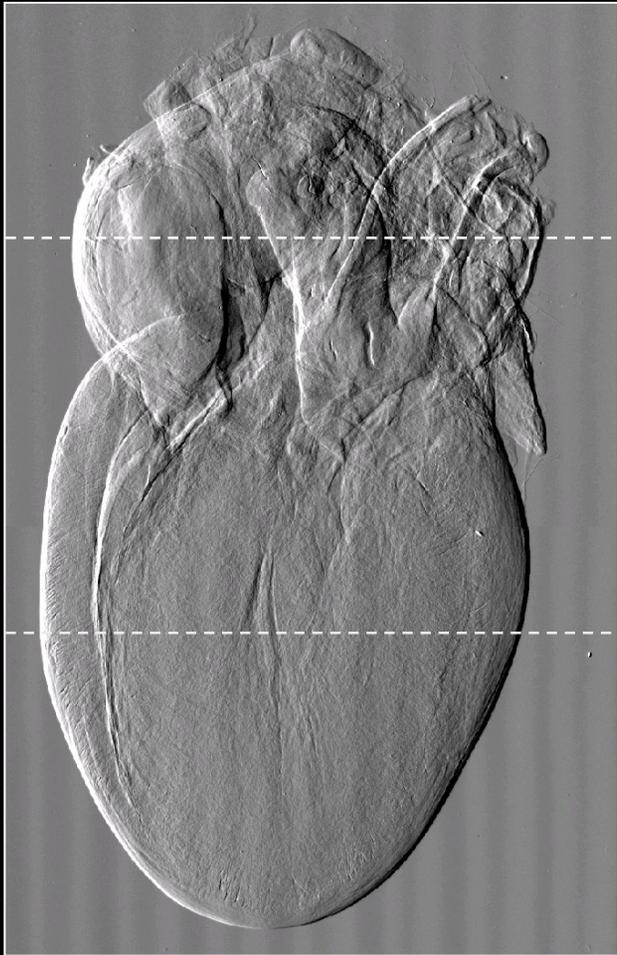


*absorption*

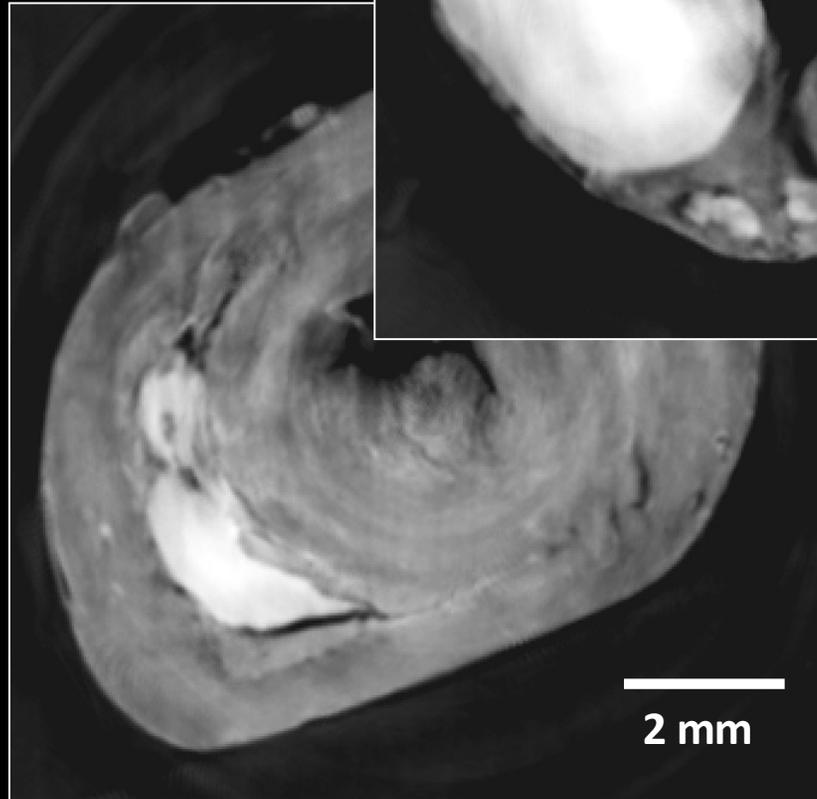
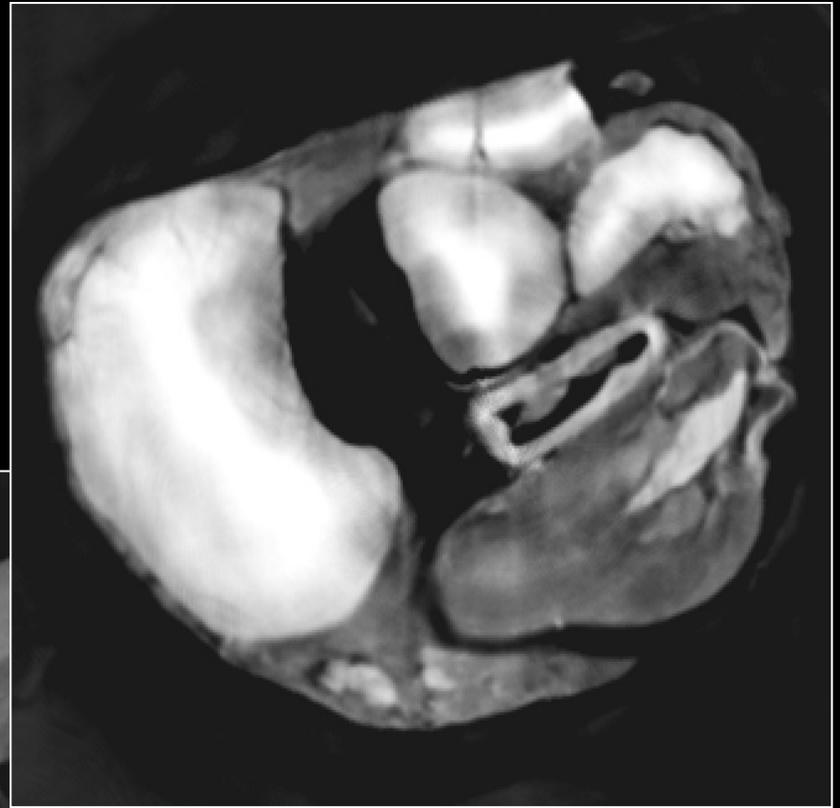


*phase contrast*

*phase contrast  
projections*

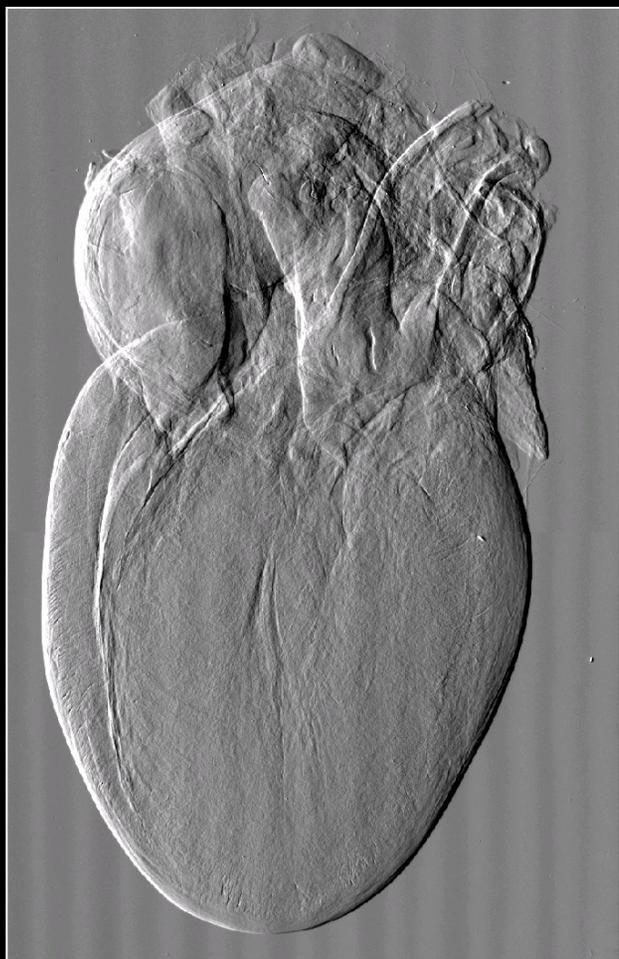


*phase tomograms*



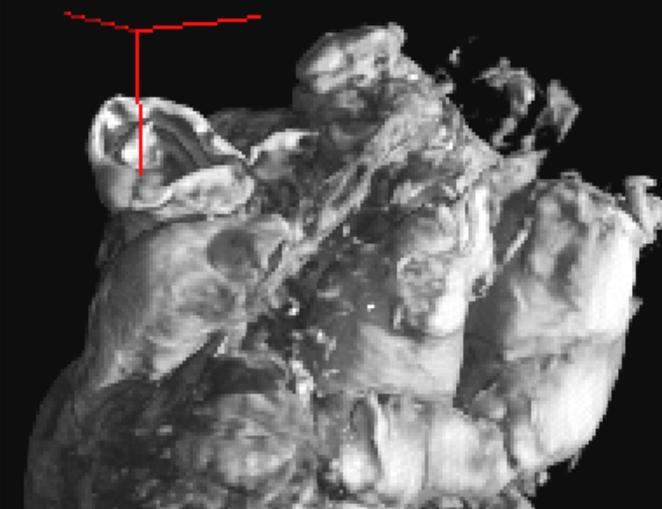
*July 2005,  
Synchrotron results*

*phase contrast  
projections*

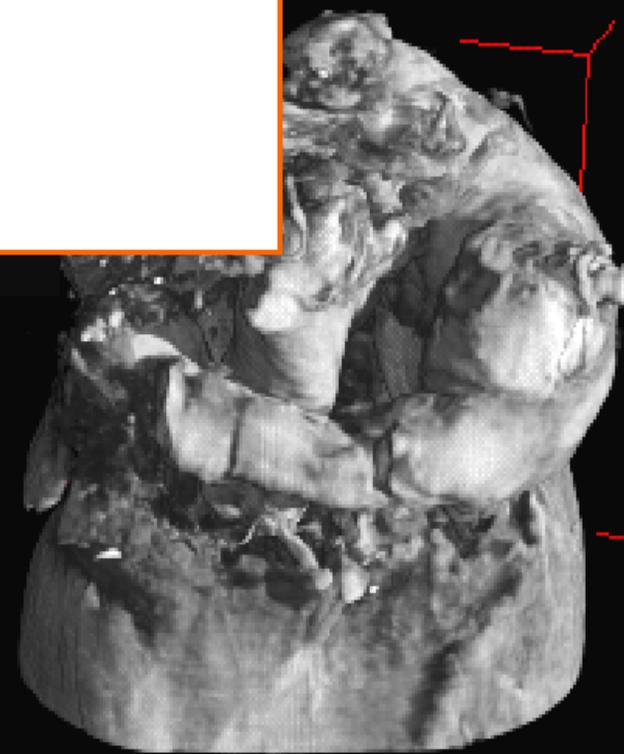


*July 2005,  
Synchrotron results*

*phase contrast  
projections*

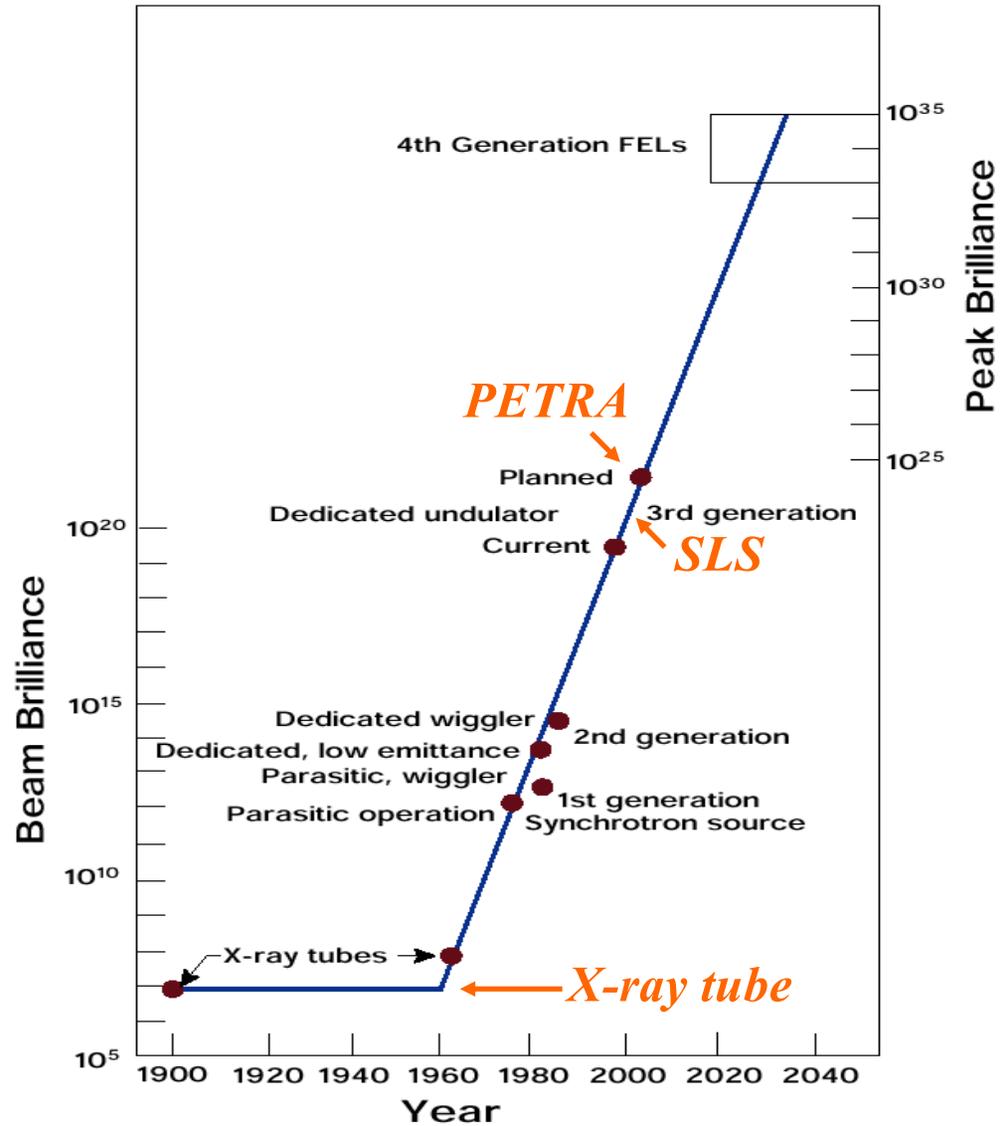


*Into the hospital ?*

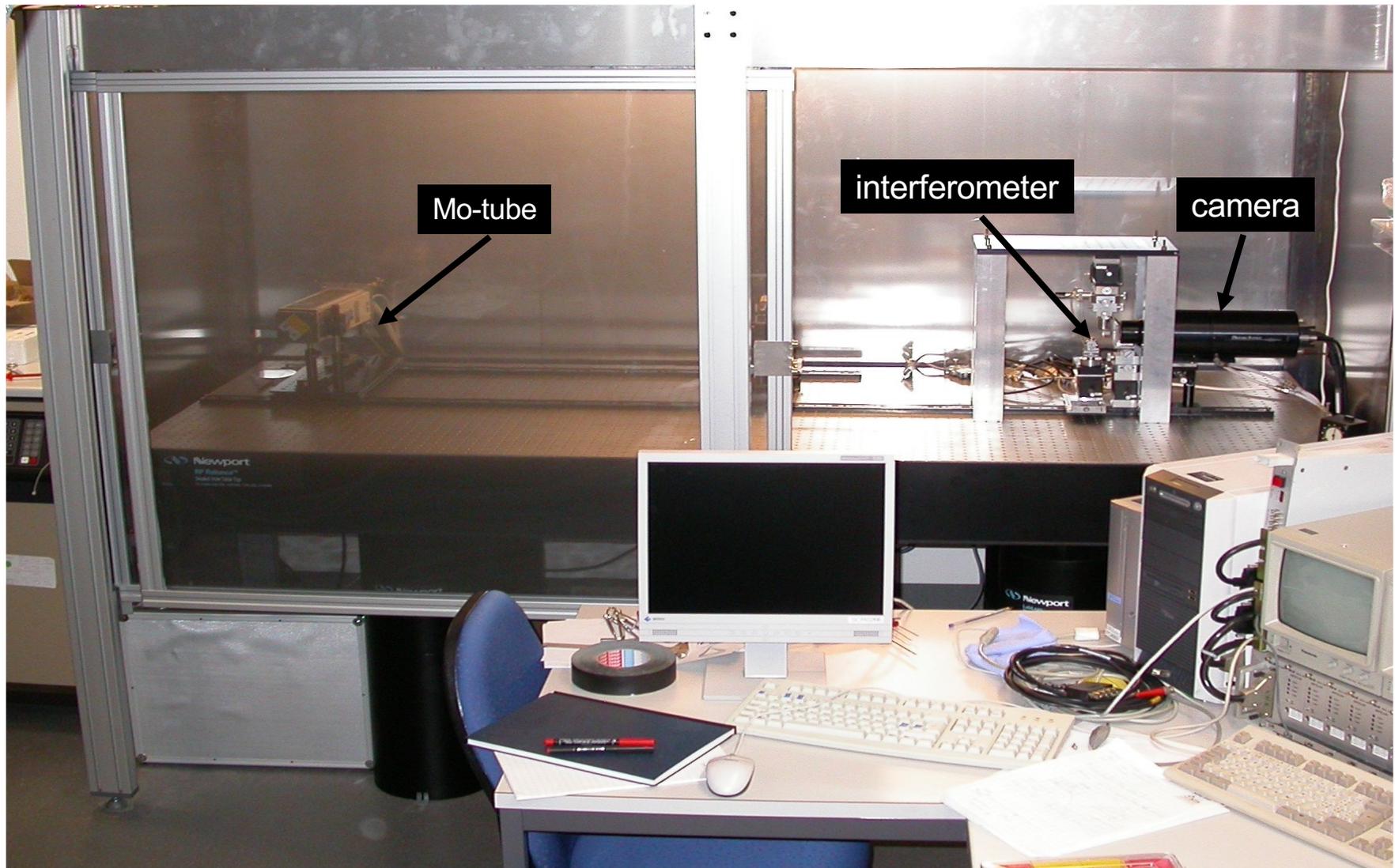


*July 2005,  
Synchrotron results*

# *A step down in brilliance*



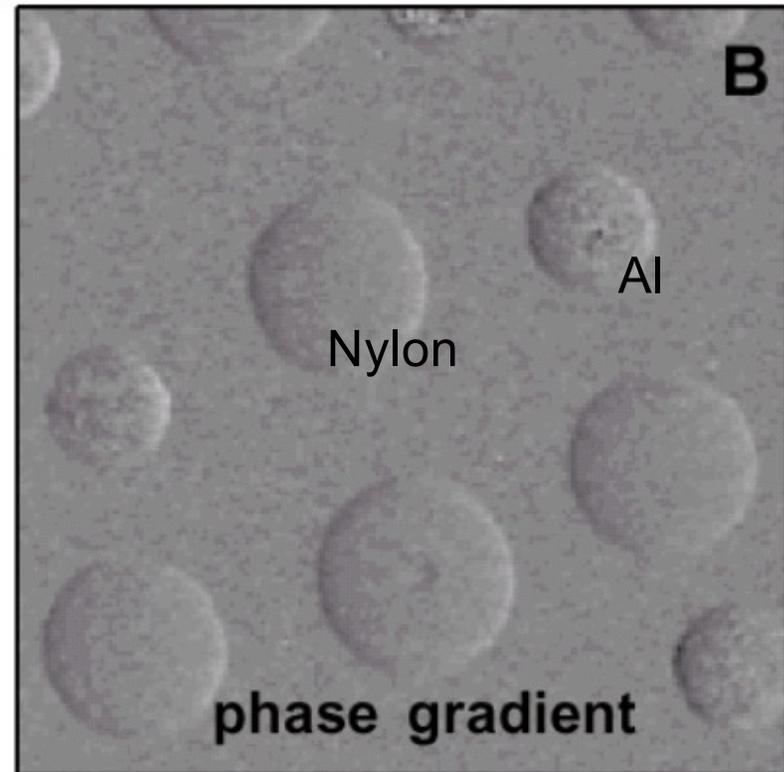
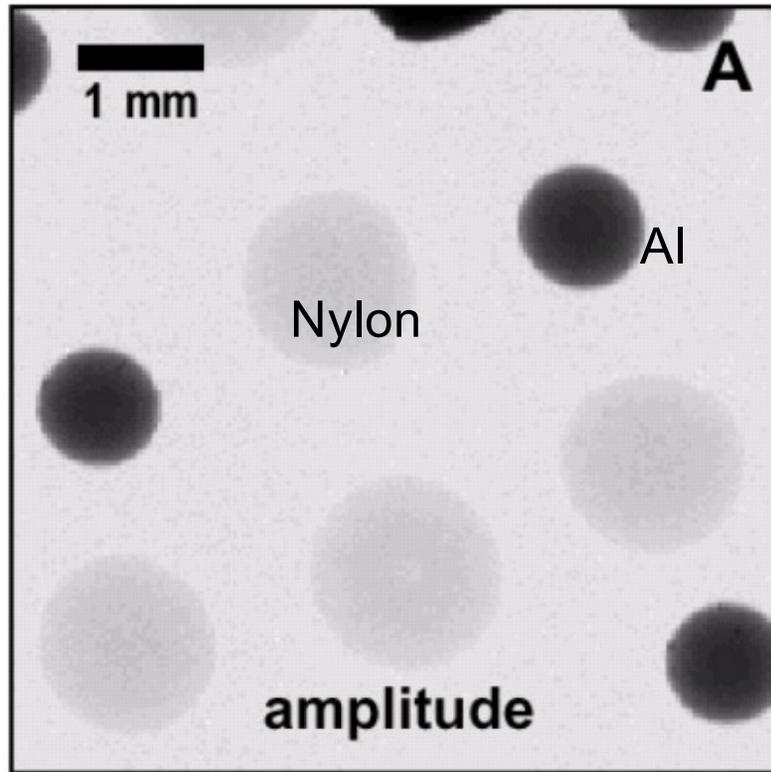
# *X-ray tube test setup*



*Ian Robinson -- Medical Imaging Seminar -- March 2006.*

# *X-ray tube results*

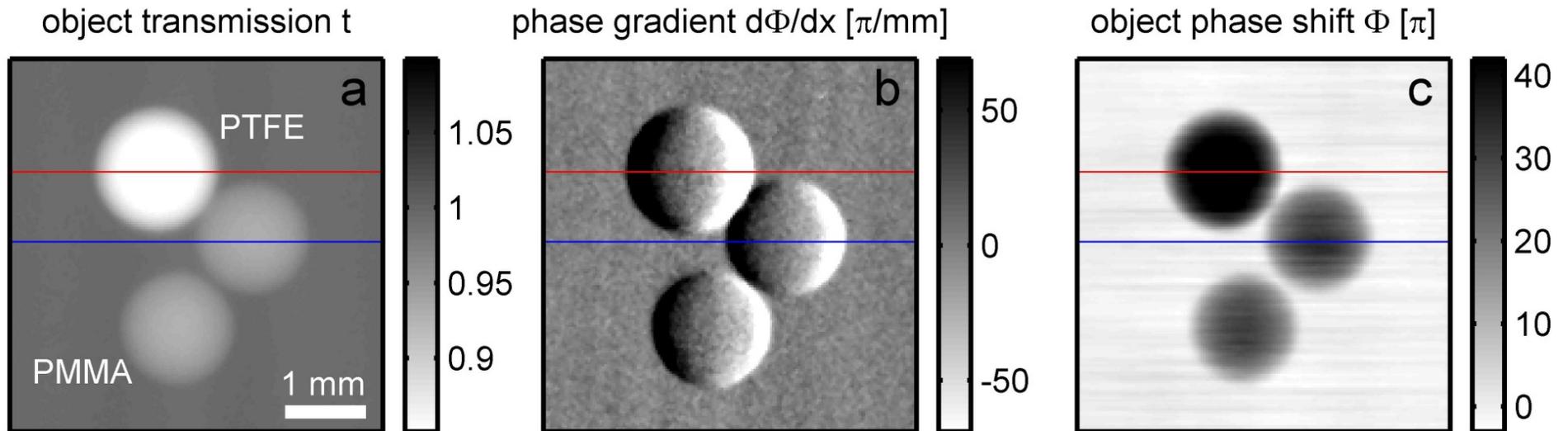
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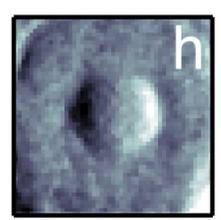
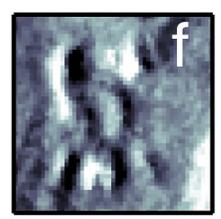
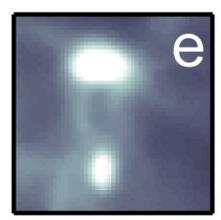
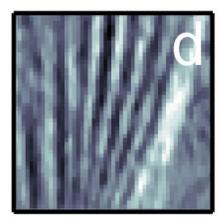
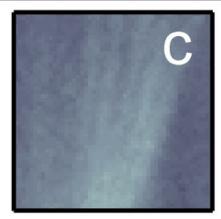
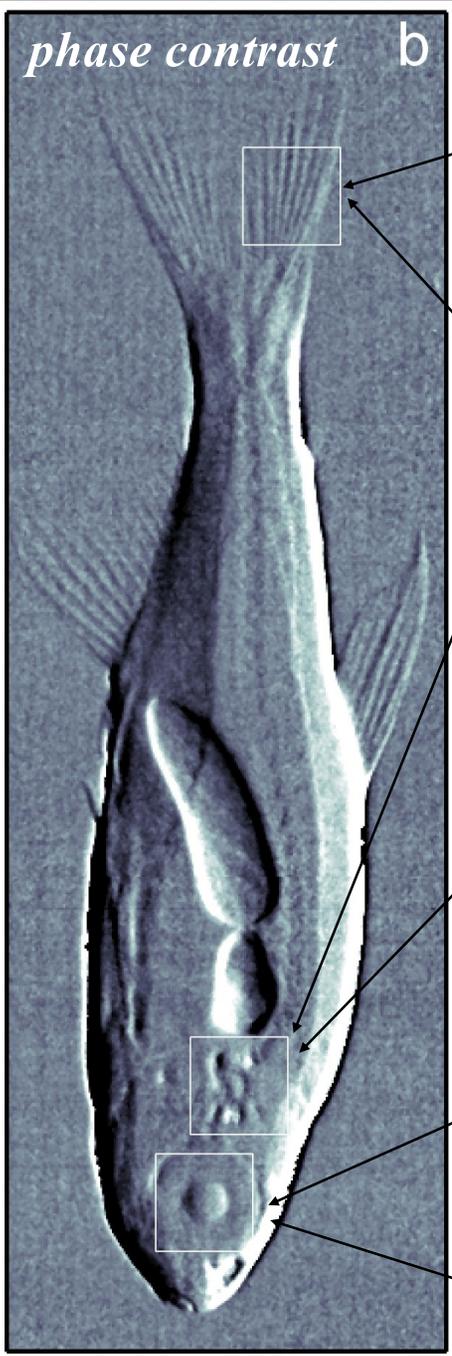
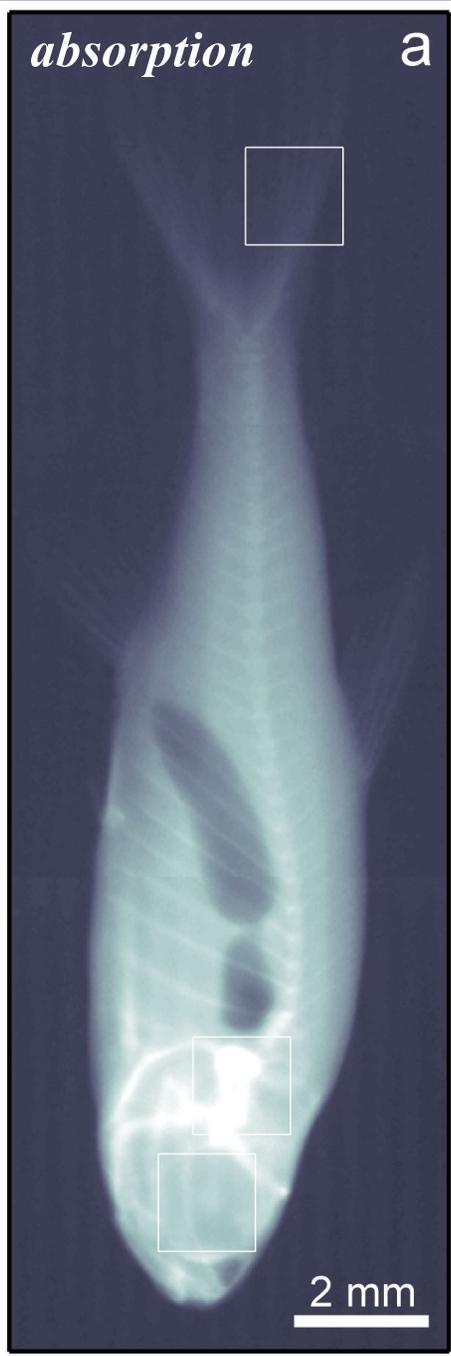
*October 2004, first results !*

# *X-ray tube results*

*standard Seifert X-ray tube source, Mo target 1 kW, point focus: 0.8 x 0.6 mm<sup>2</sup>, distance 1.7 m*



*Pfeiffer et al., submitted (2005)*

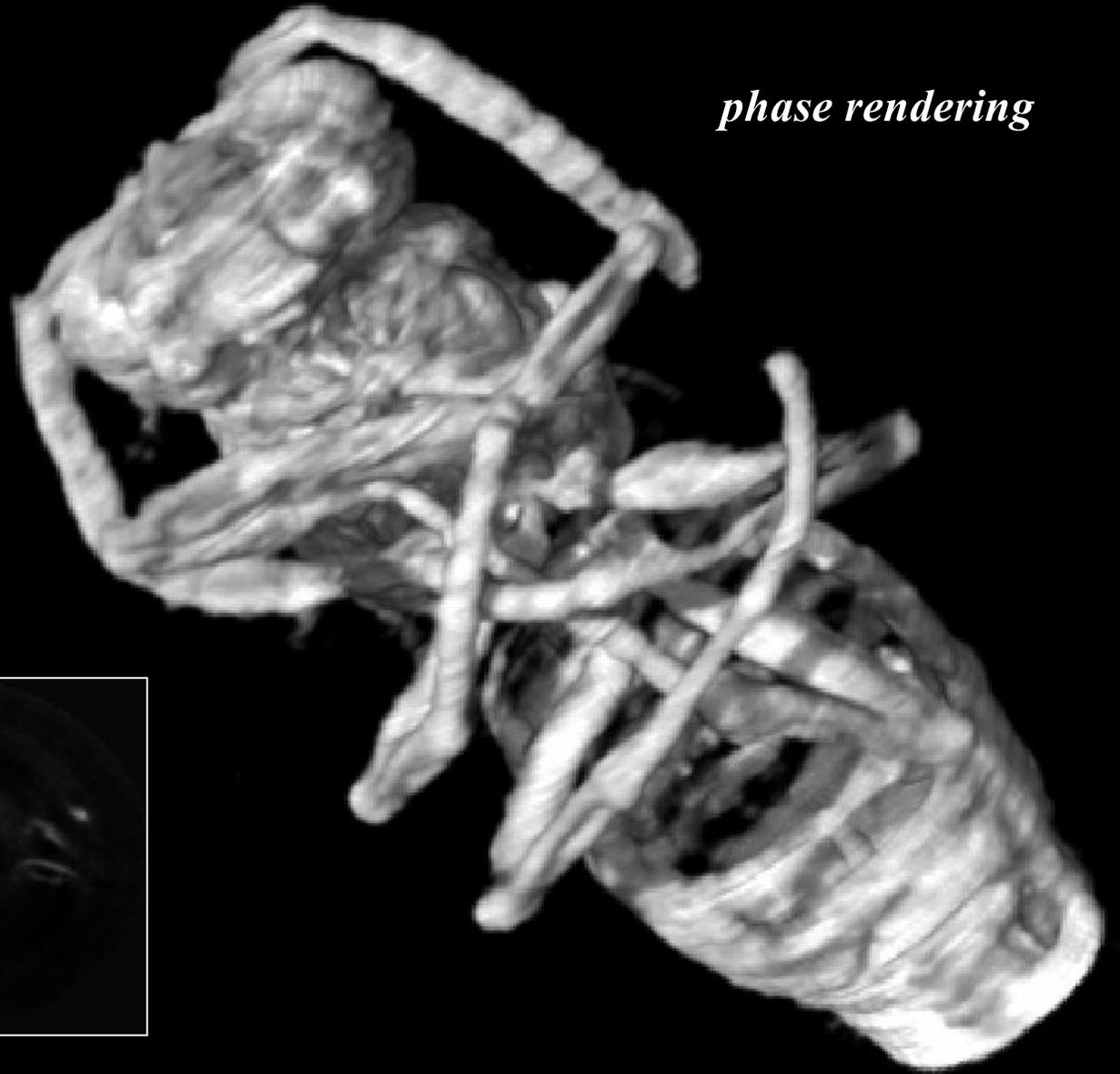


*May 2005, x-ray tube*

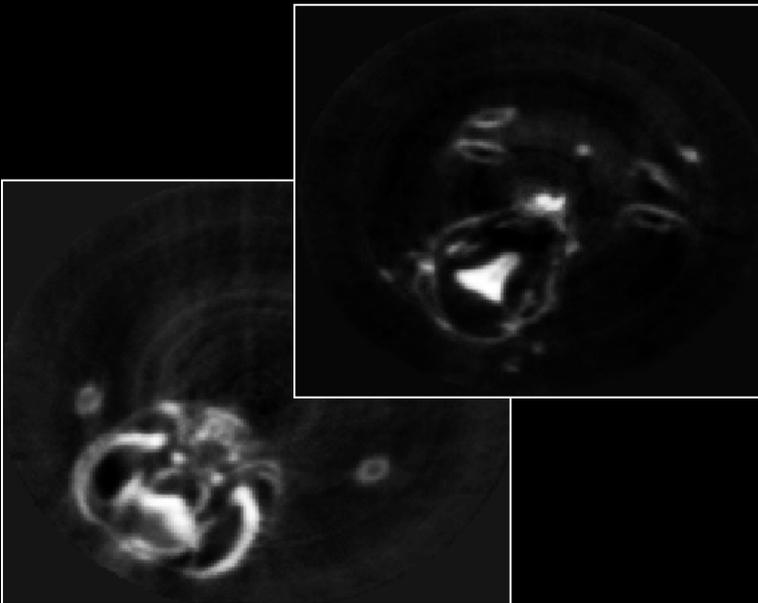
*phase contrast  
projections*



*phase rendering*



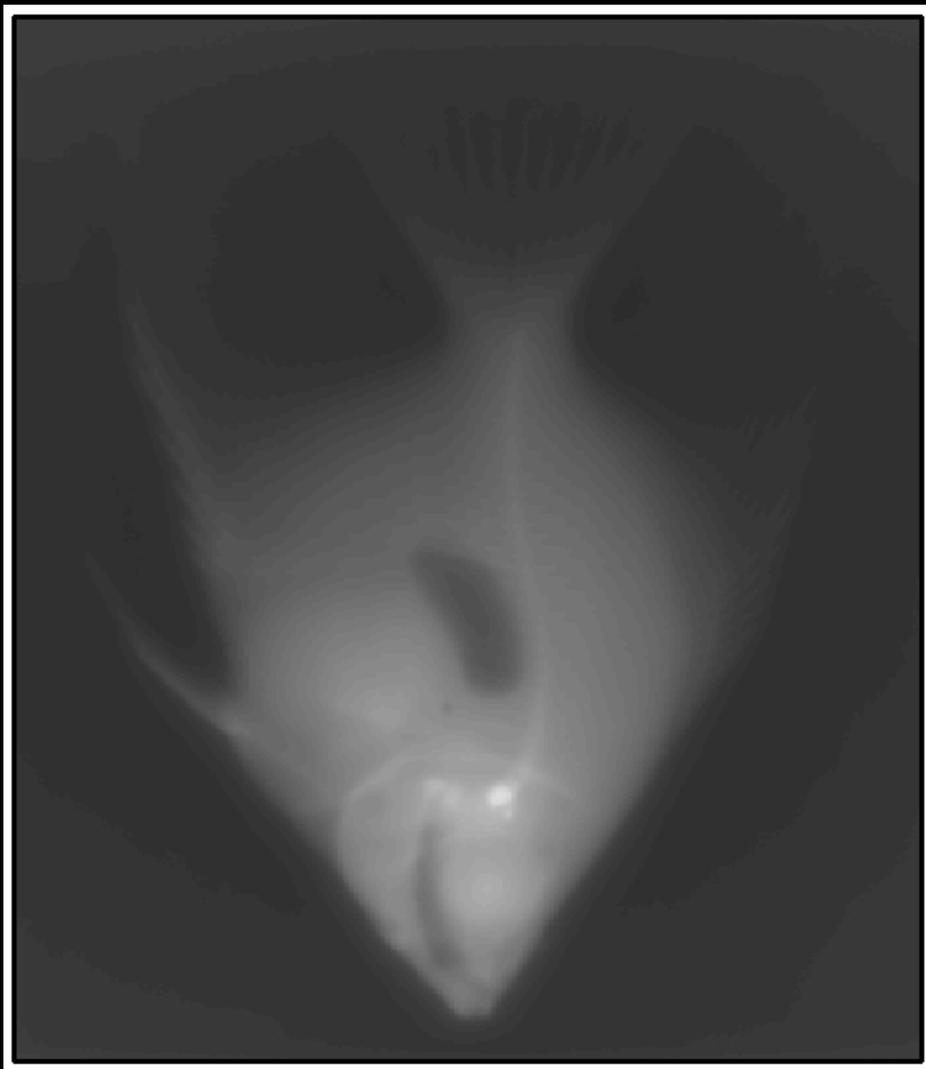
*phase tomograms*



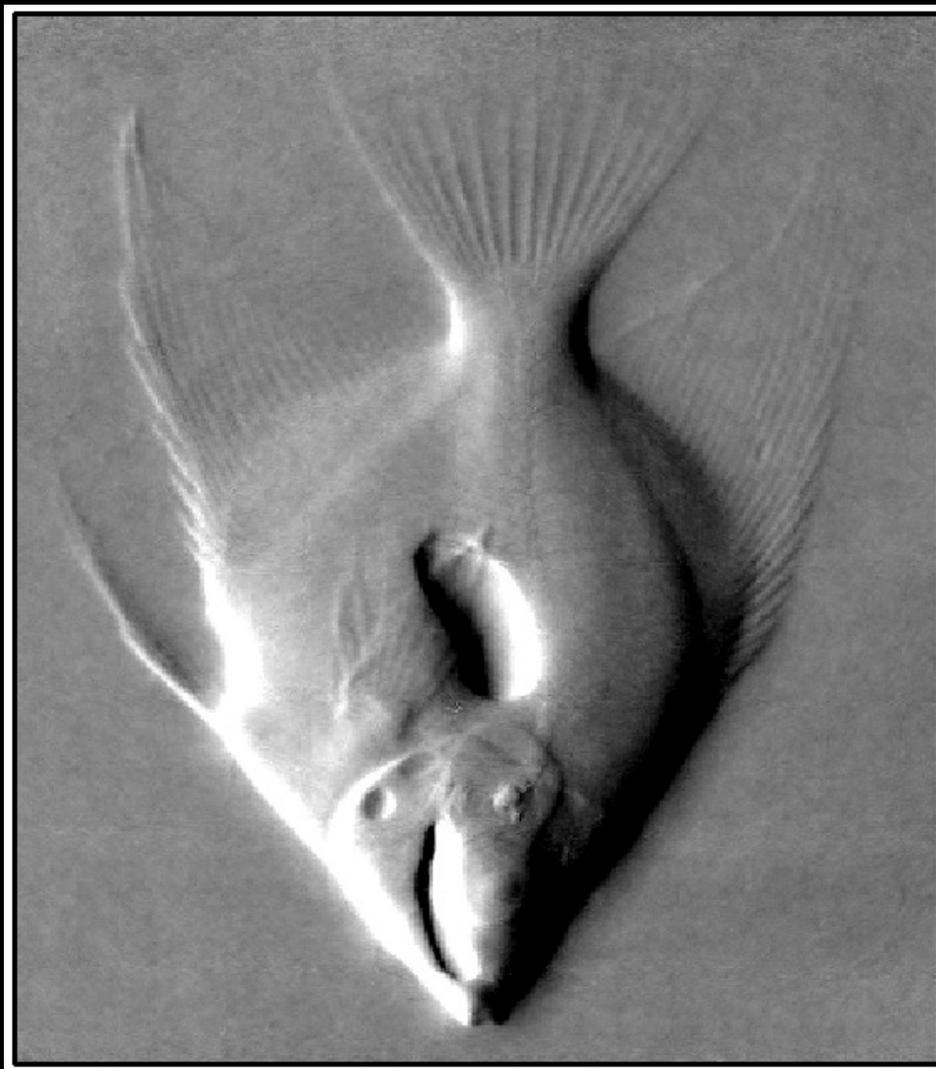
5 mm

*Jan 2006, x-ray tube*

*absorption*



*phase contrast*



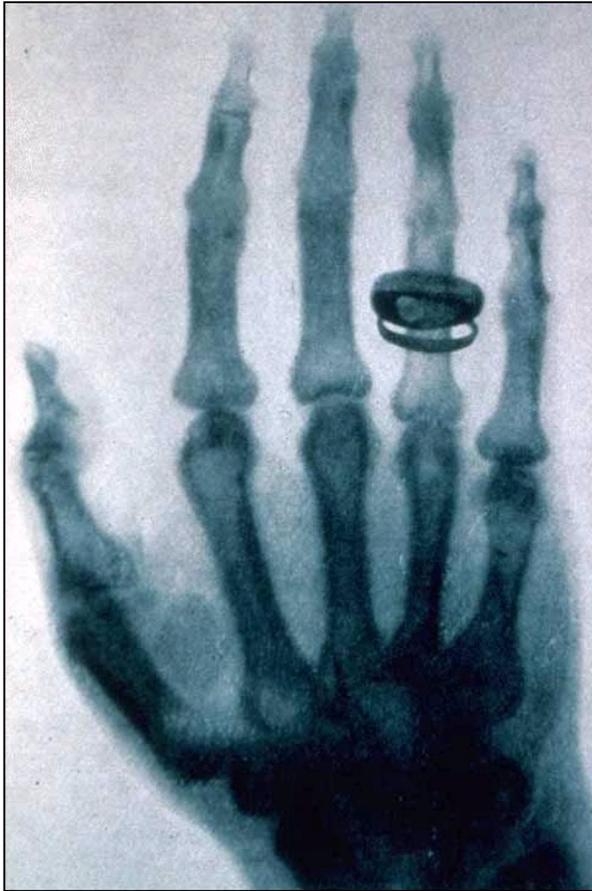
**5 cm !**

*total exposure time: 200 sec*

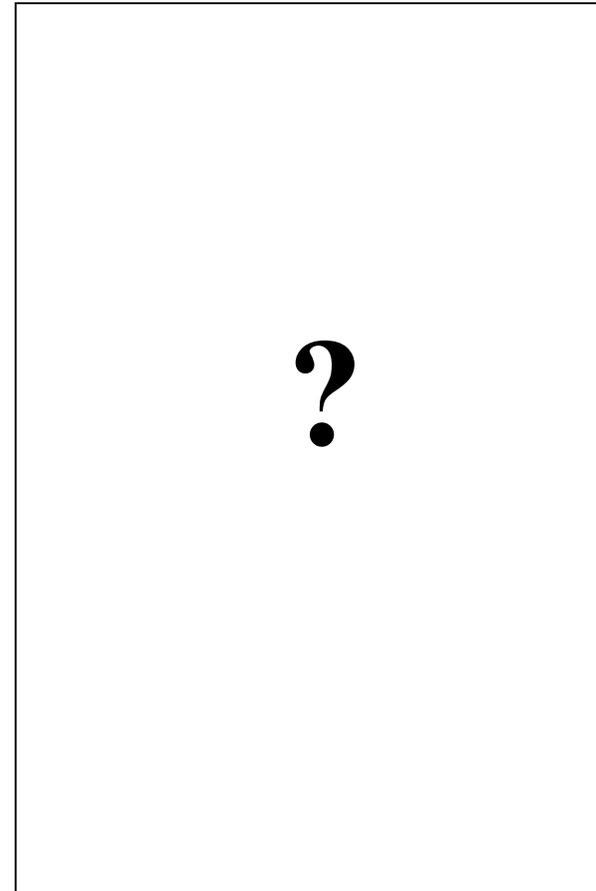
*Jan 2006, x-ray tube*

# *The future ?*

---



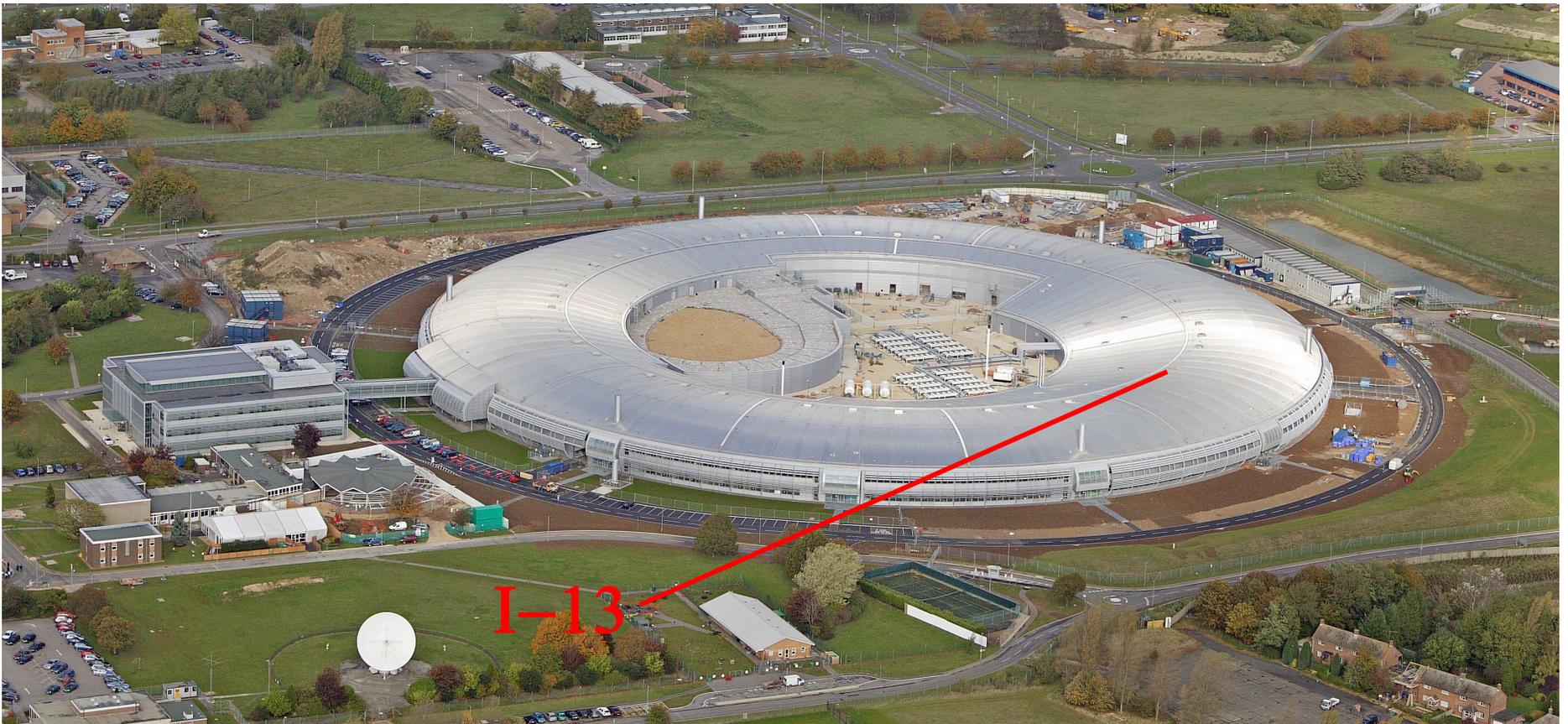
**Absorption Image, 1895**



**Phase Image**

# *Diamond Light Source, Oct 2005*

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*Ian Robinson -- Medical Imaging Seminar -- March 2006.*

# *I16 Materials and Magnetism Beamline*

---



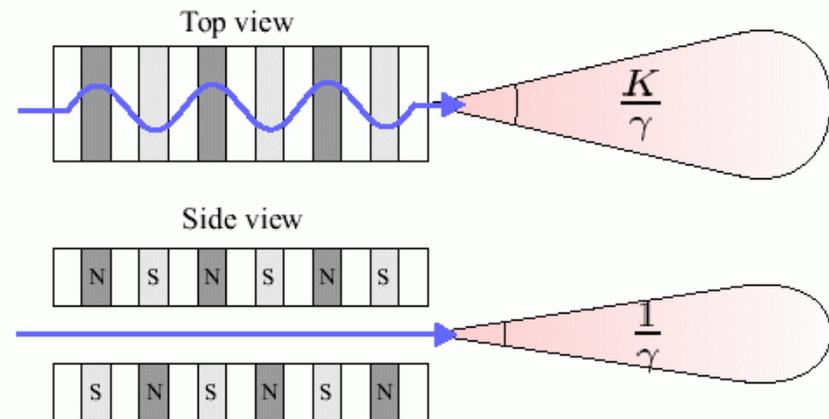
---

*Ian Robinson -- Medical Imaging Seminar -- March 2006.*

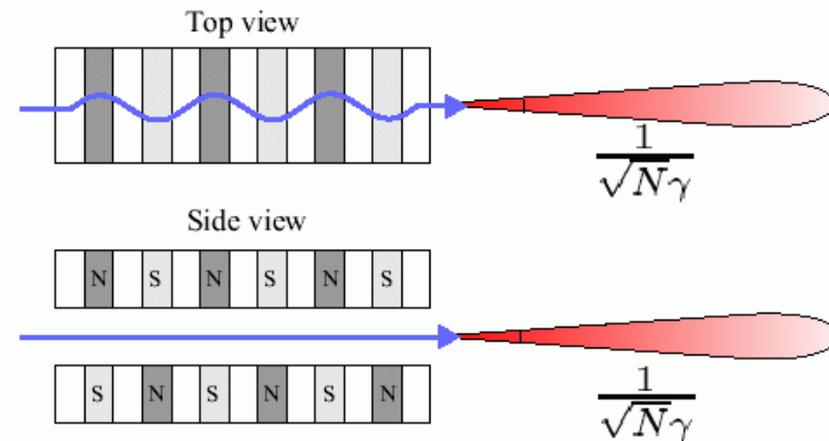
# Undulator Radiation Source



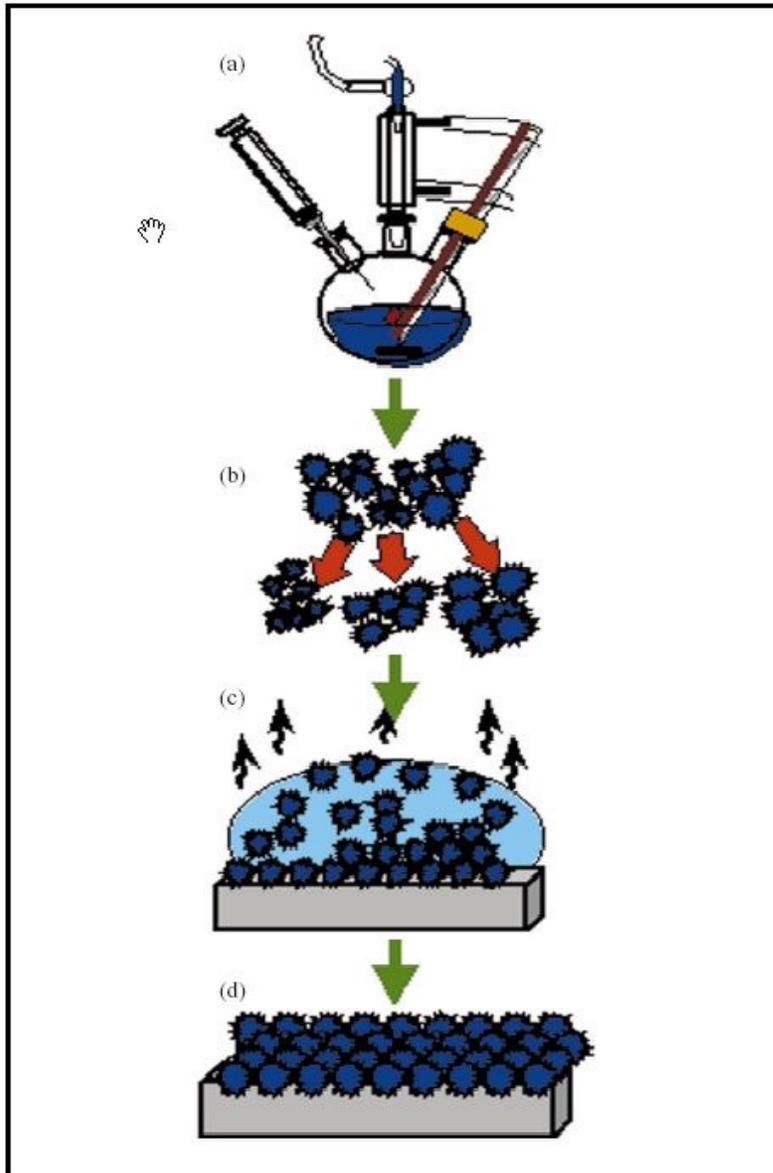
(a) Wiggler



(b) Undulator

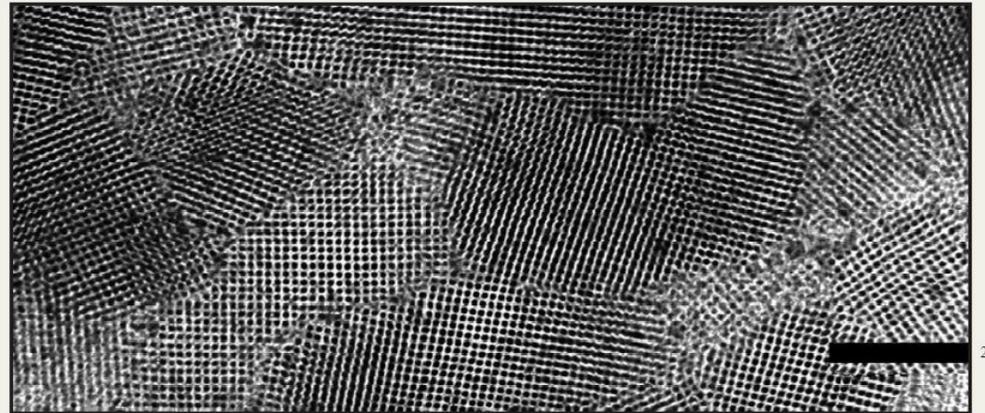


# *Chemical Synthesis of Nanocrystals*



- Reactants introduced rapidly
- High temperature solvent
- Surfactant/organic capping agent
- Square superlattice (200nm scale)

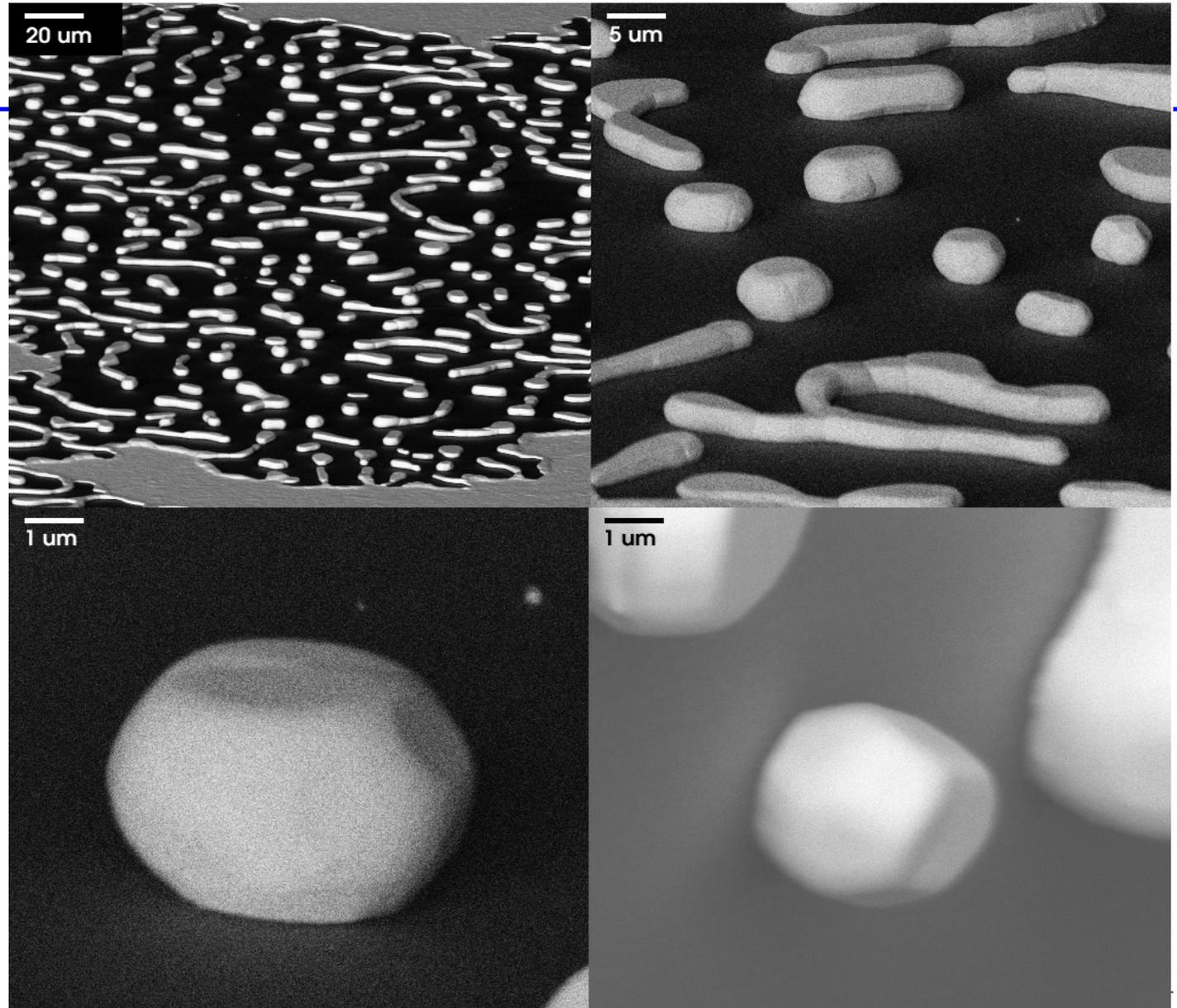
C. B. Murray, IBM J. Res. & Dev. **45** 47 (2001)



# *SEMS*

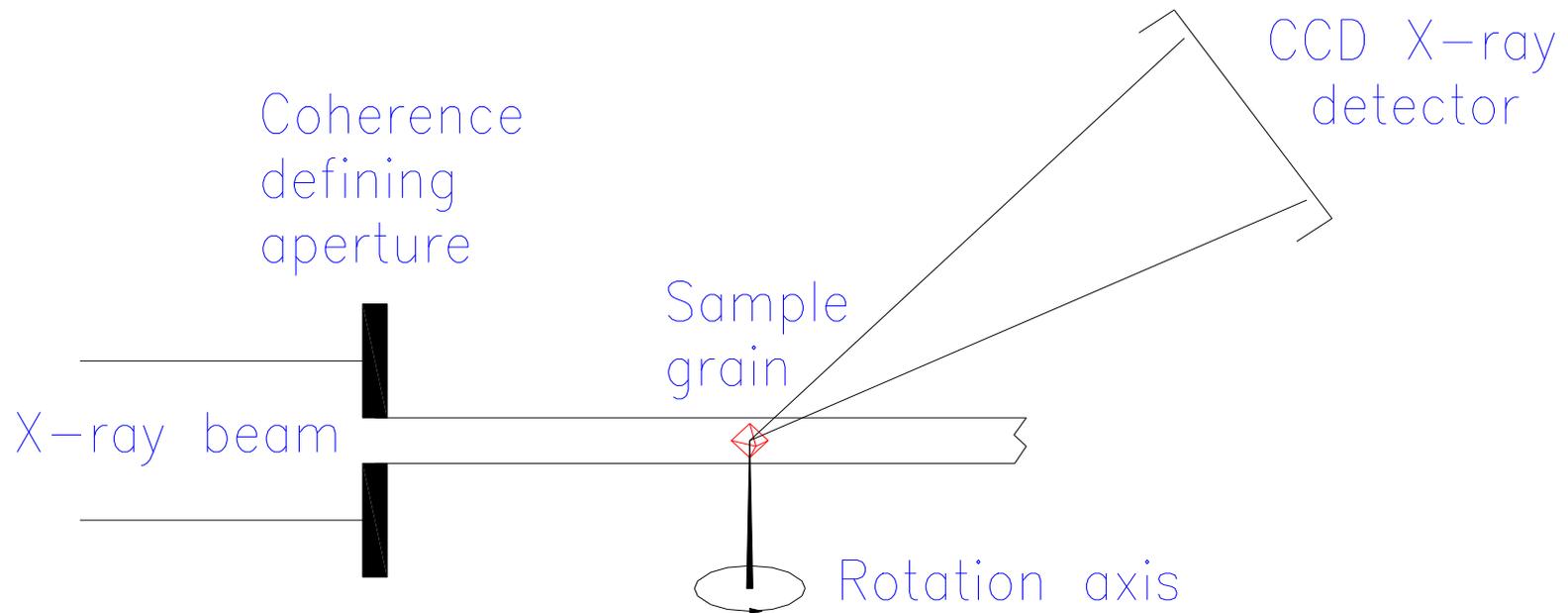
---

Sample preparation:  
Au blanket film  
Quartz substrate  
Annealed at 950°C  
for 70 hrs.



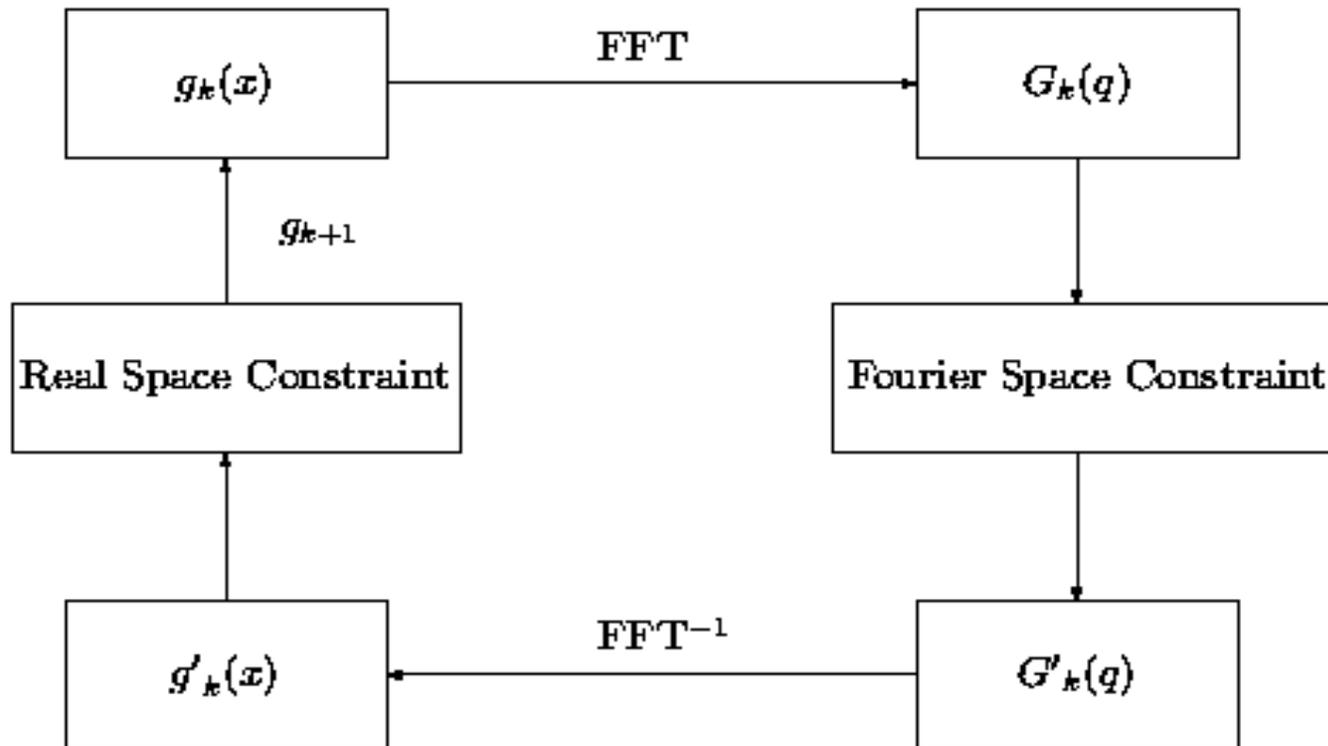
# *Lensless X-ray Microscope*

---



# Generic “Error Reduction” method

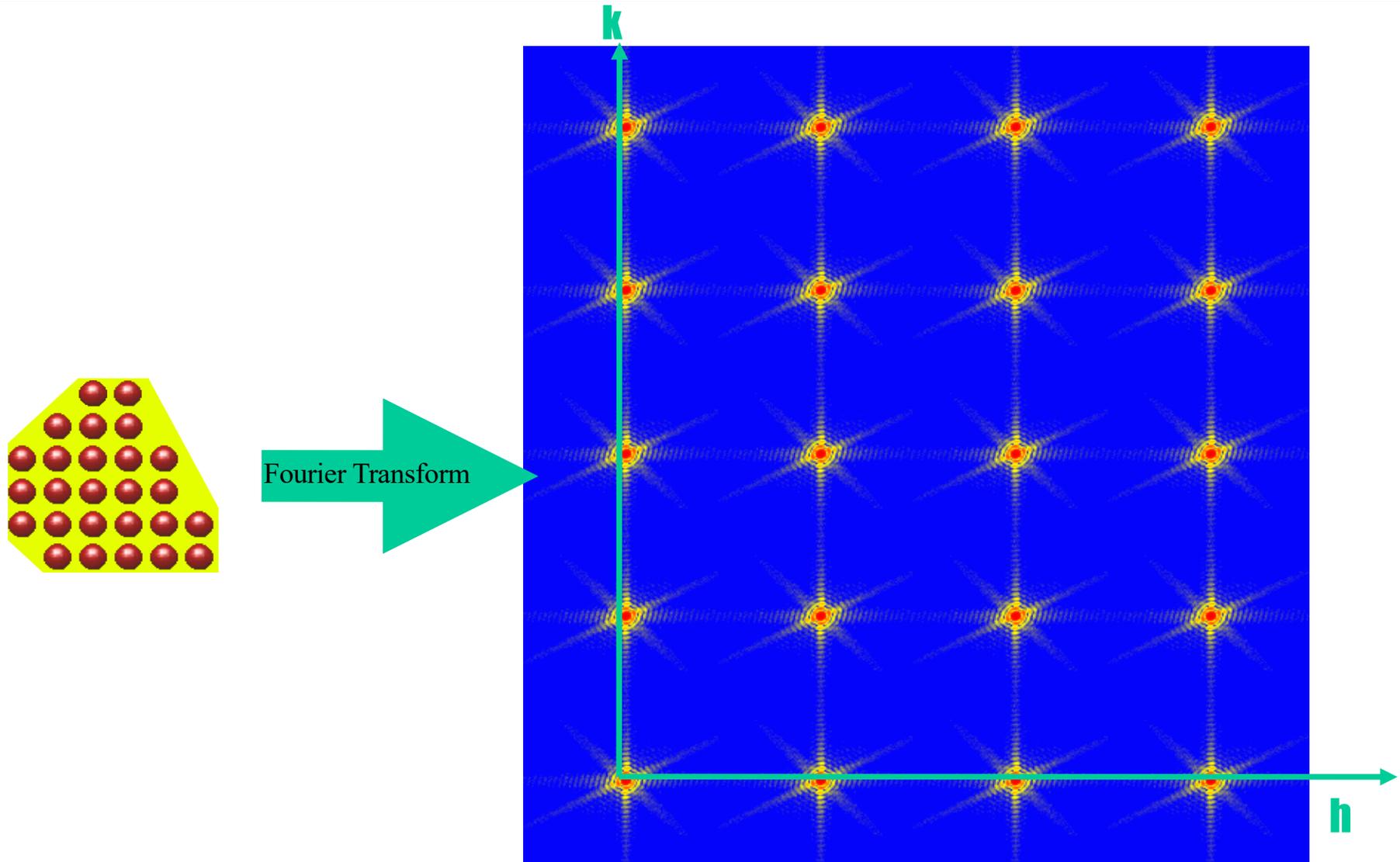
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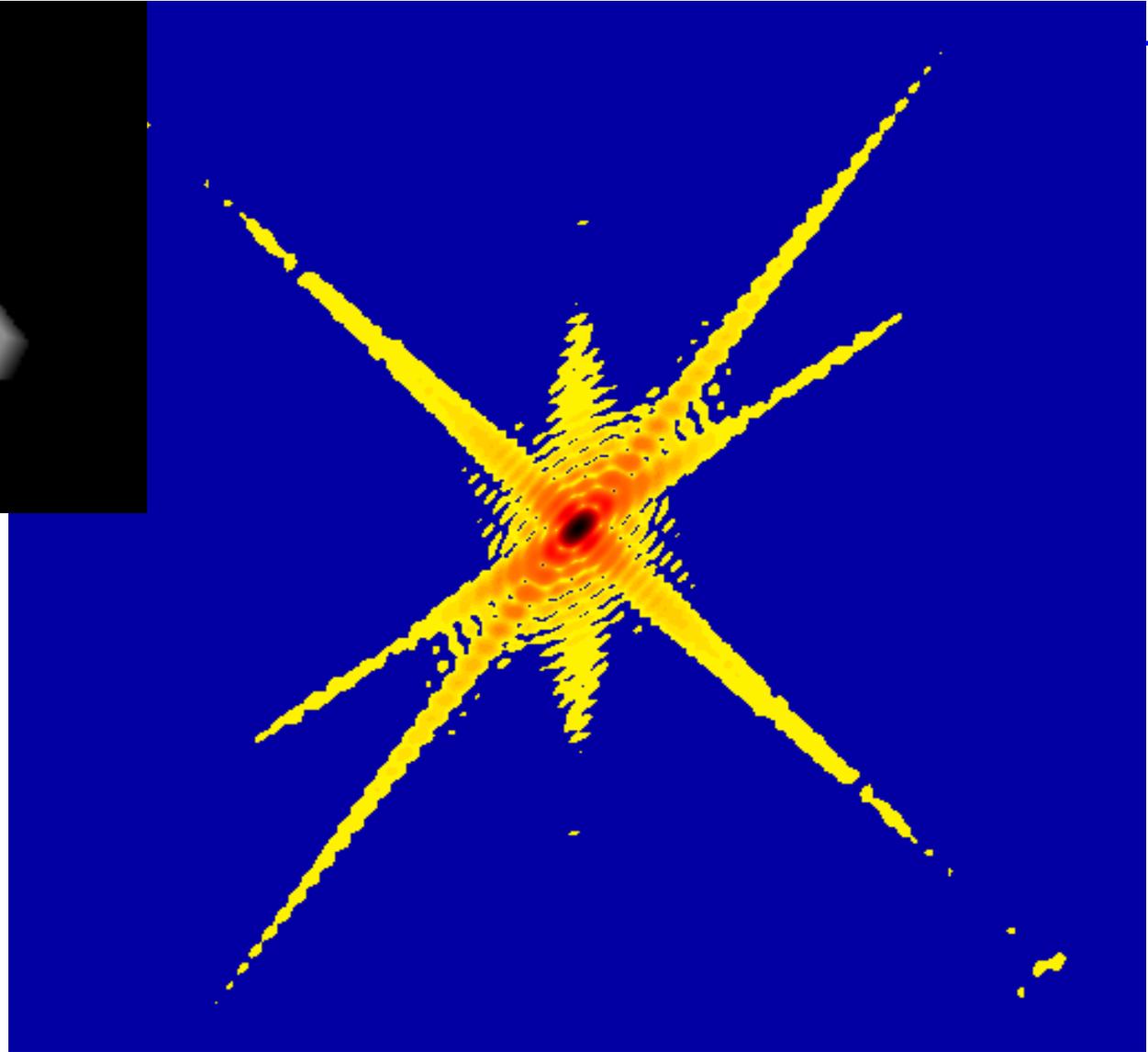
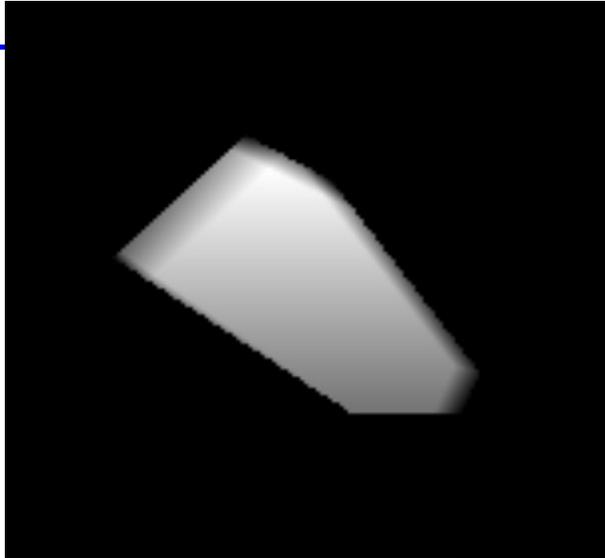


J. R. Fienup Appl. Opt. 21 2758 (1982)

R. W. Gerchberg and W. O. Saxton Optik 35 237 (1972)

# *Coherent Diffraction from Crystals*





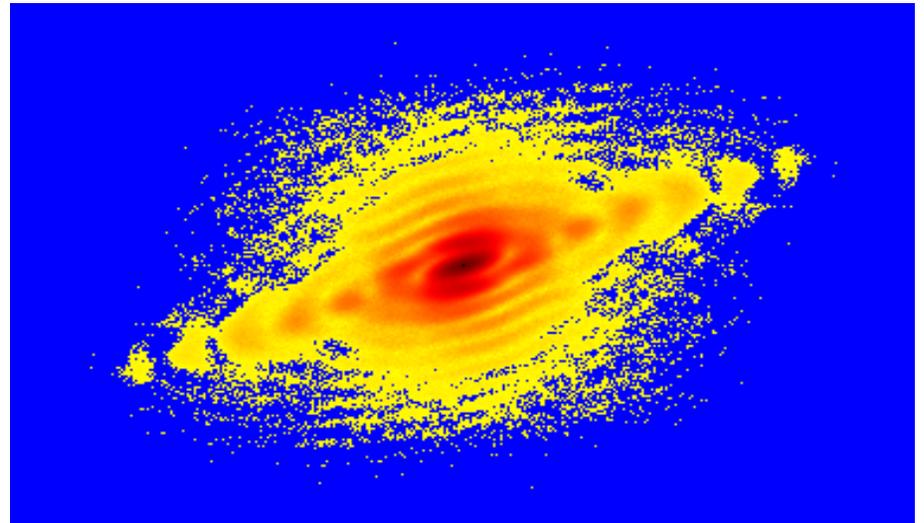
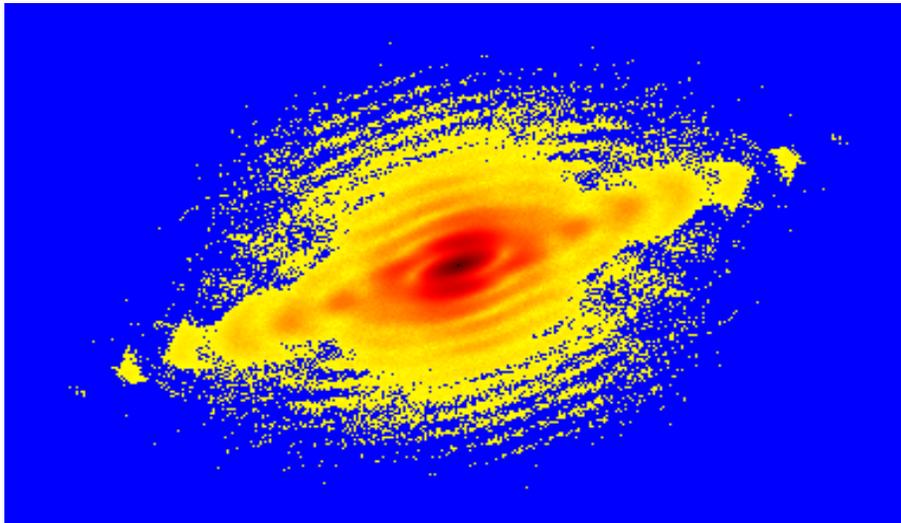
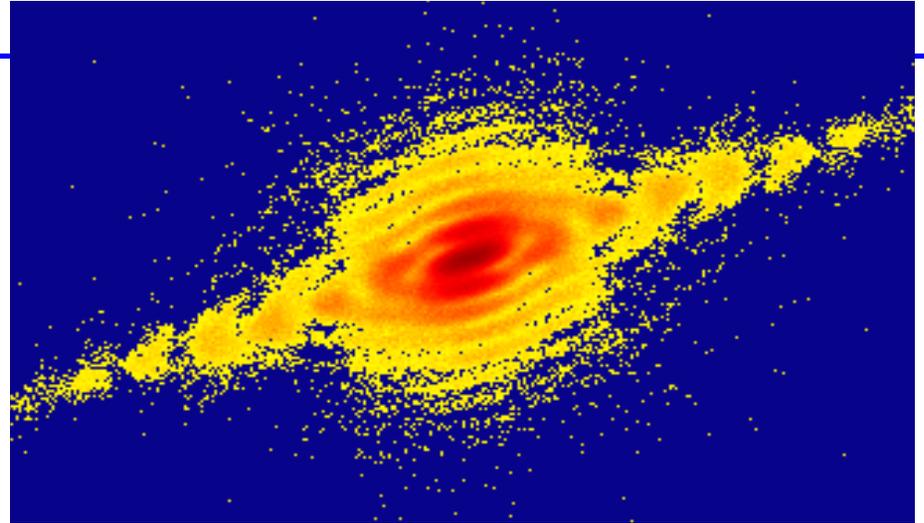
---

*Ian Robinson -- Medical Imaging Seminar -- March 2006.*

---

*Symmetrized Data  
and two best fits*

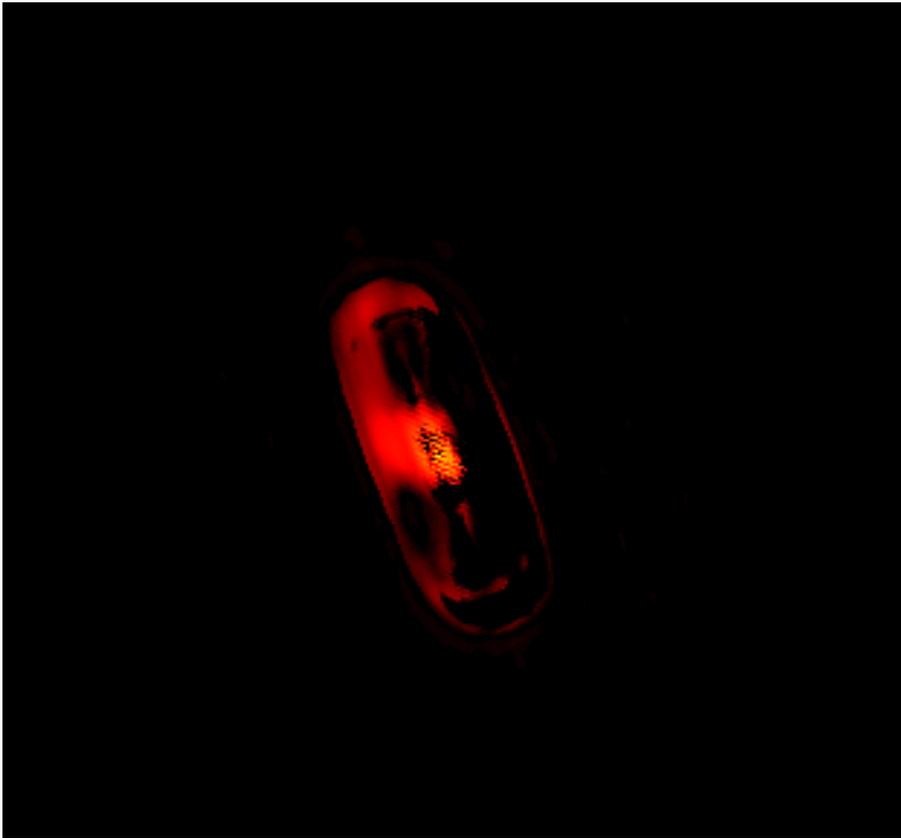
*Chisq=0.0005*

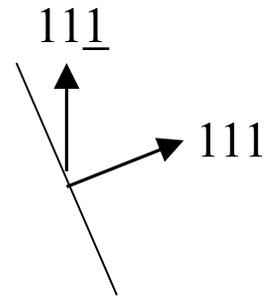
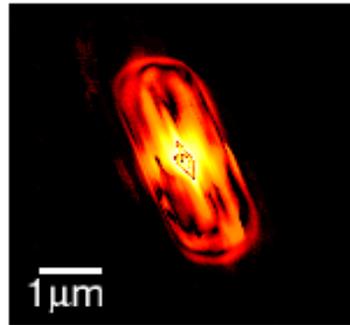
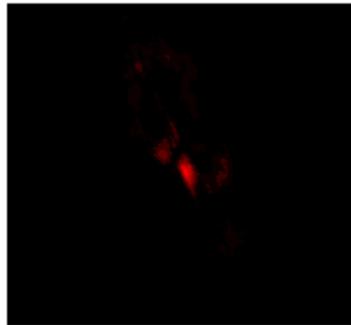


# *2D Reconstructions*

---

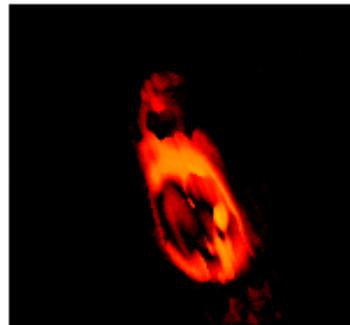
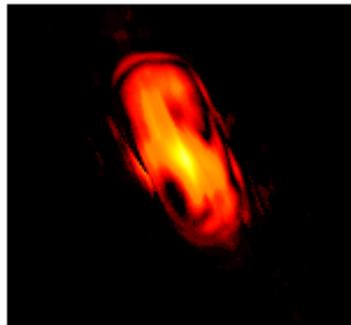
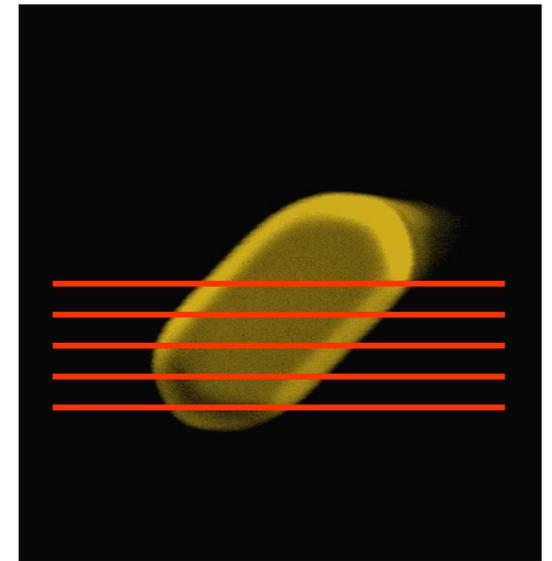
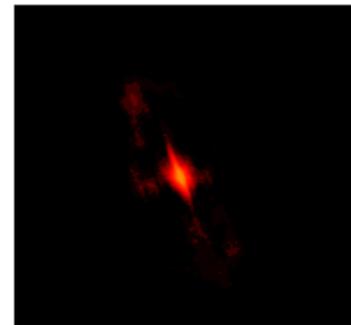
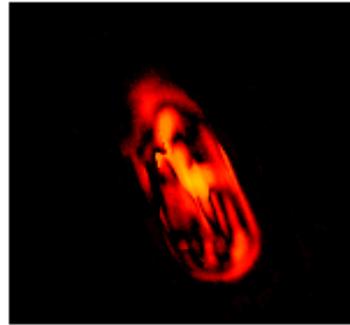
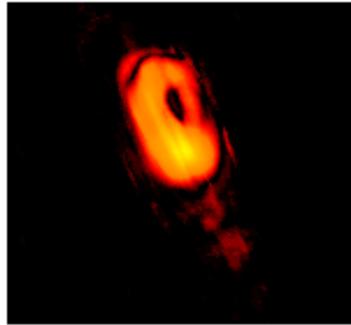
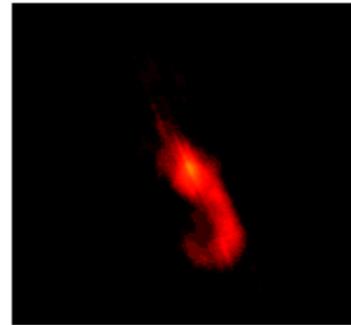
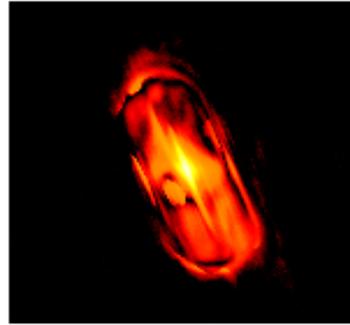
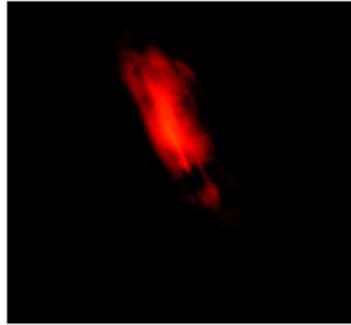
*chisquare = 0.0005*

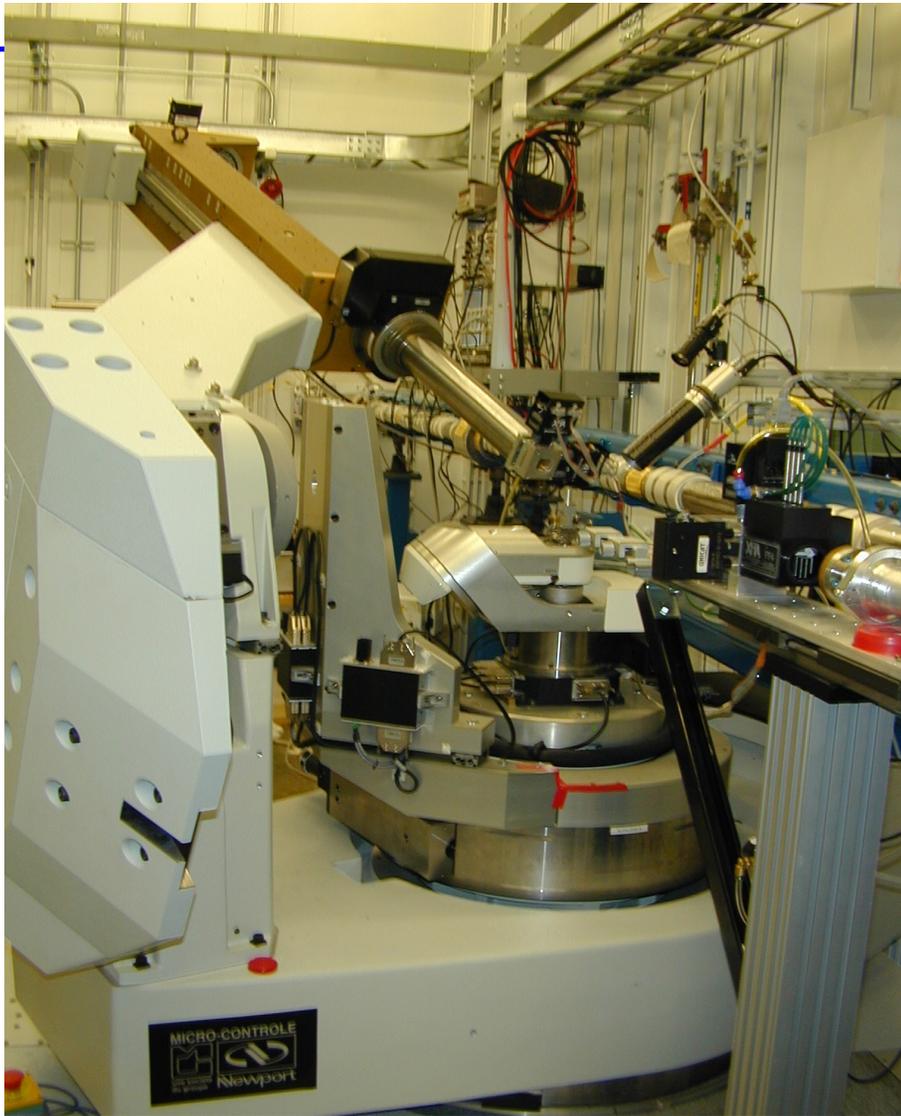




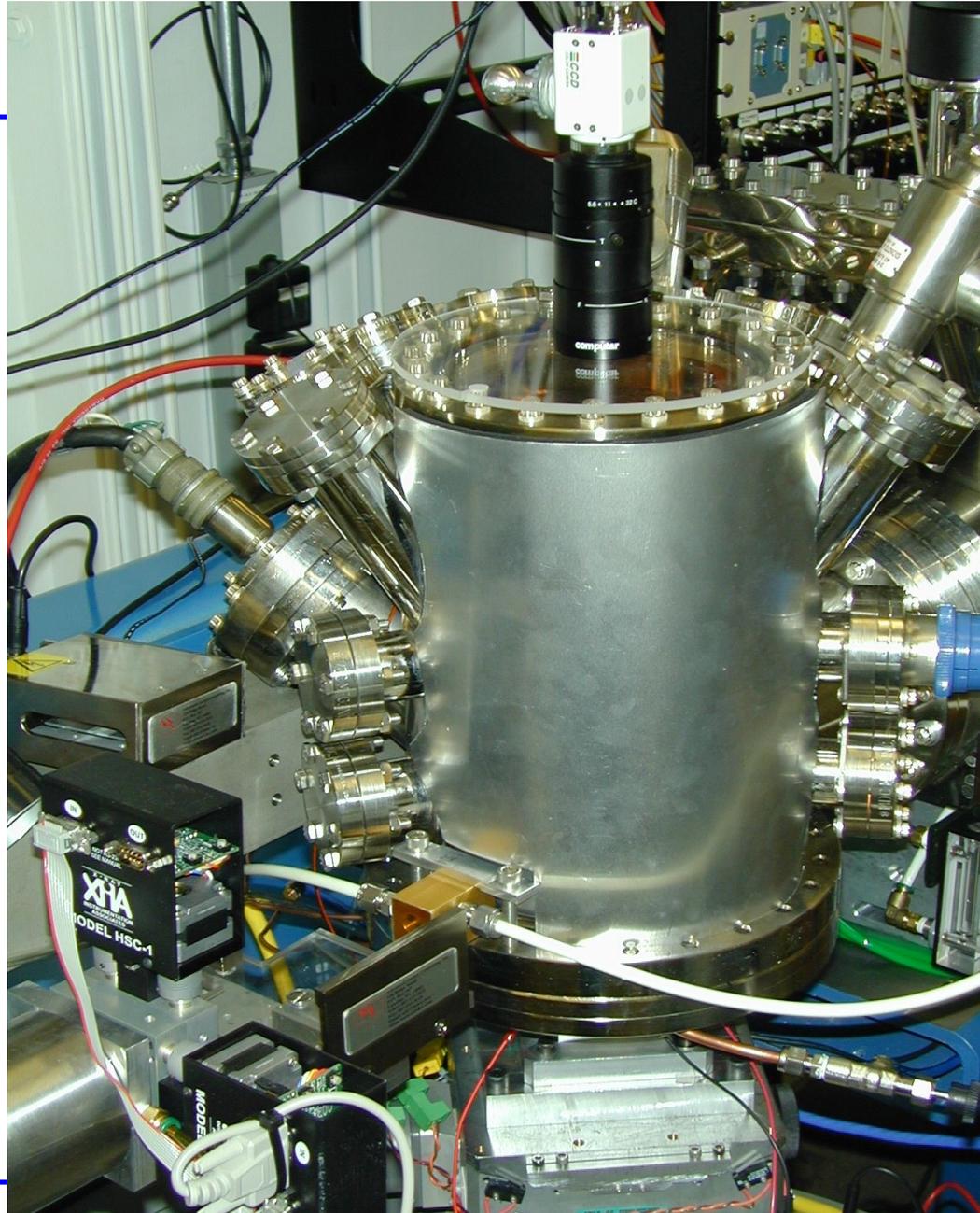
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Slices through  
plan view SEM:





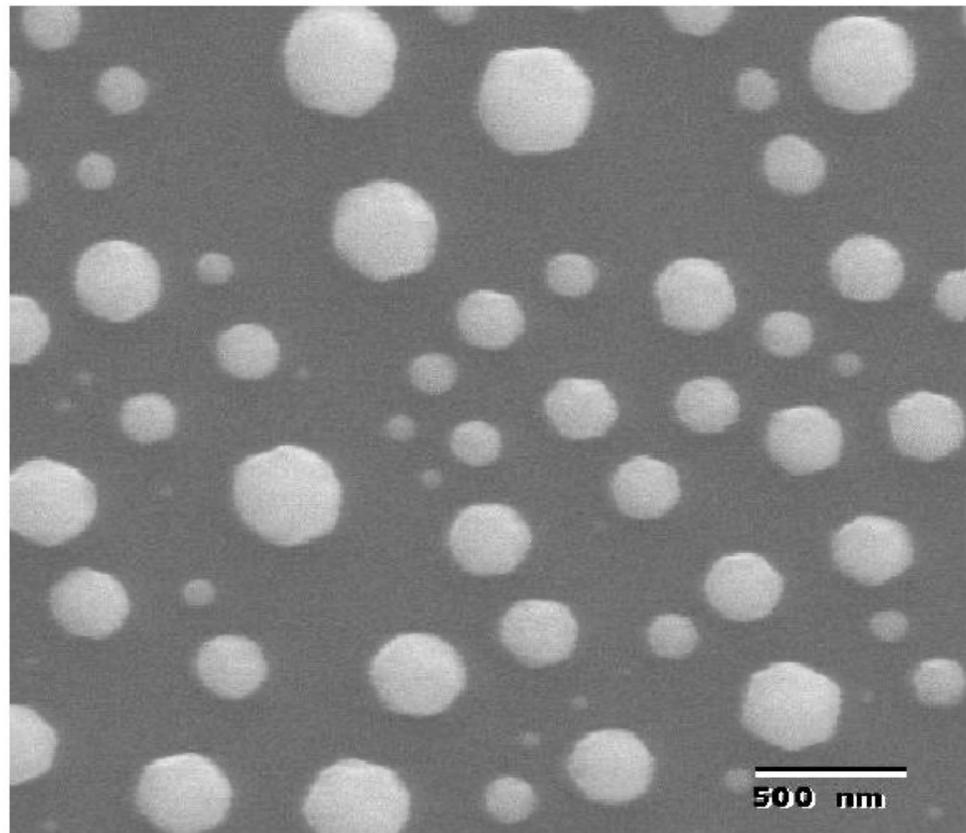
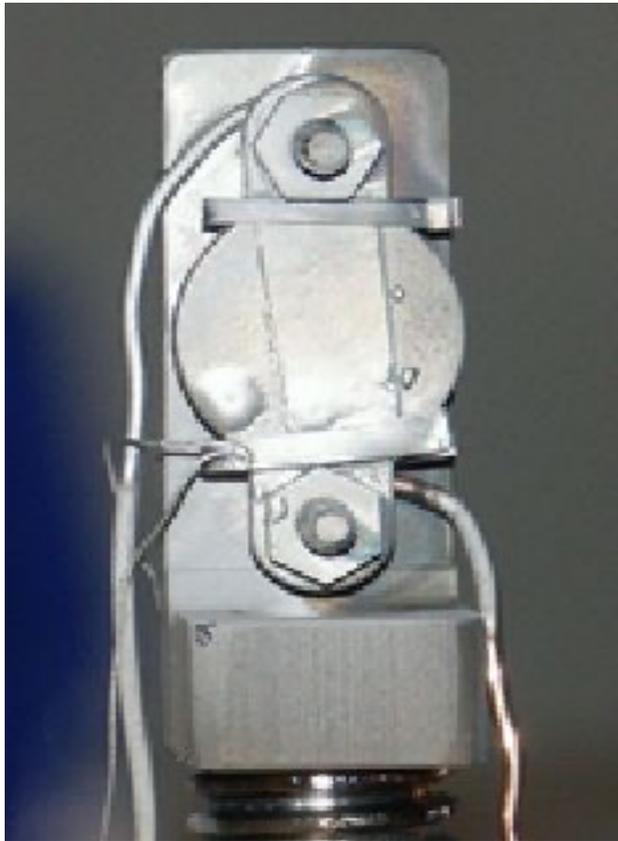
*Ian Robinson -- Medical Imaging Seminar -- March 2006.*



*Pat Robinson - Medical Imaging Seminar - March 2000.*

# *In situ growth of Pb crystals*

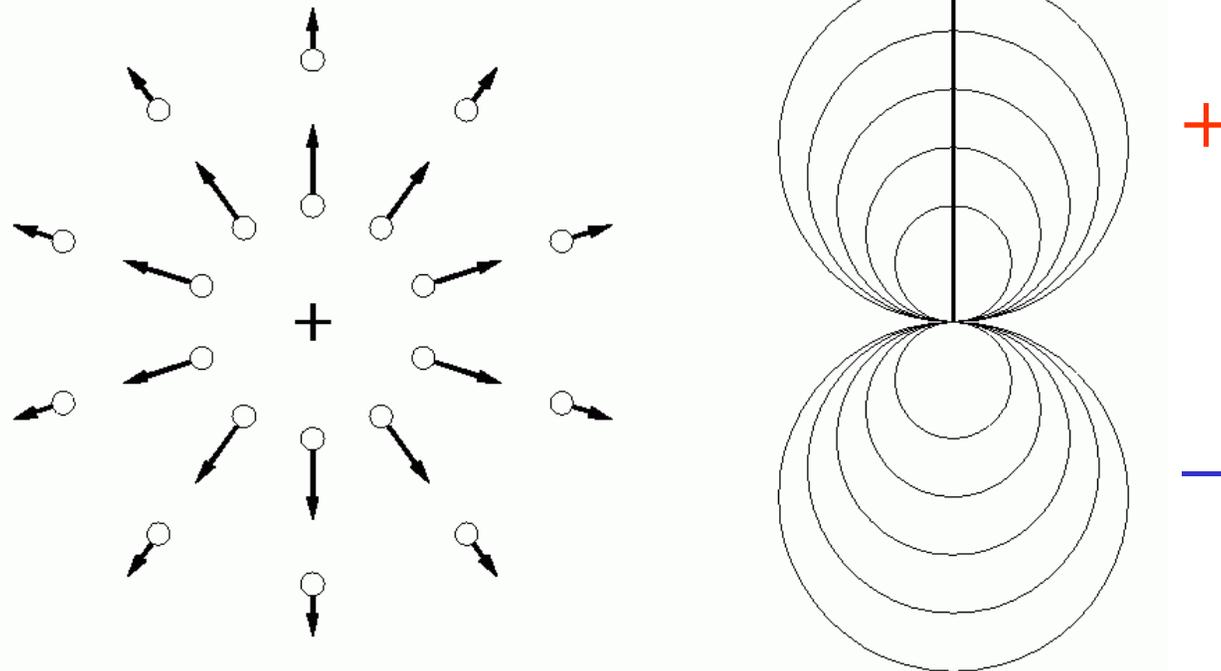
---



# *Diffraction by Strain of Point Defect*

$$A \sim \sum e^{i\mathbf{Q}\cdot(\mathbf{R}_j+\mathbf{u}_j)}$$
$$\approx \sum e^{i\mathbf{Q}\cdot\mathbf{R}_j} (1 + \mathbf{i}\mathbf{Q}\cdot\mathbf{u}_j)$$

Imaginary density



## *Good statistics, 3D diffraction data*

---

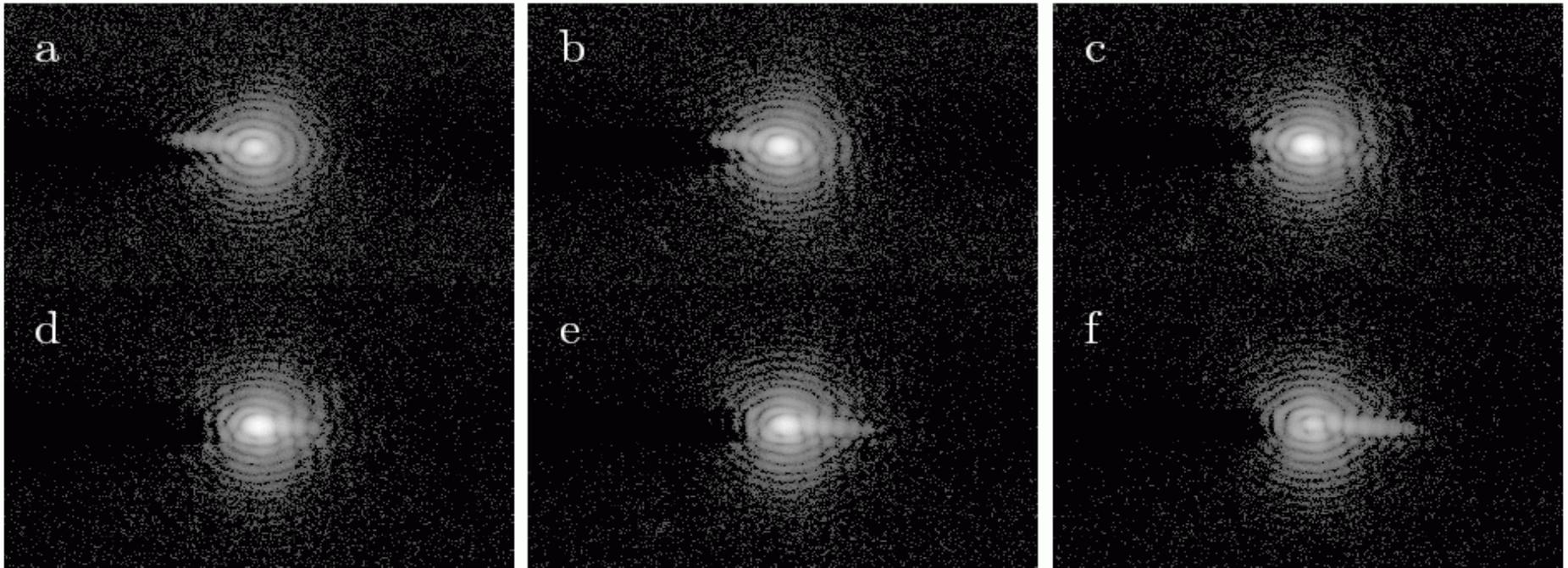
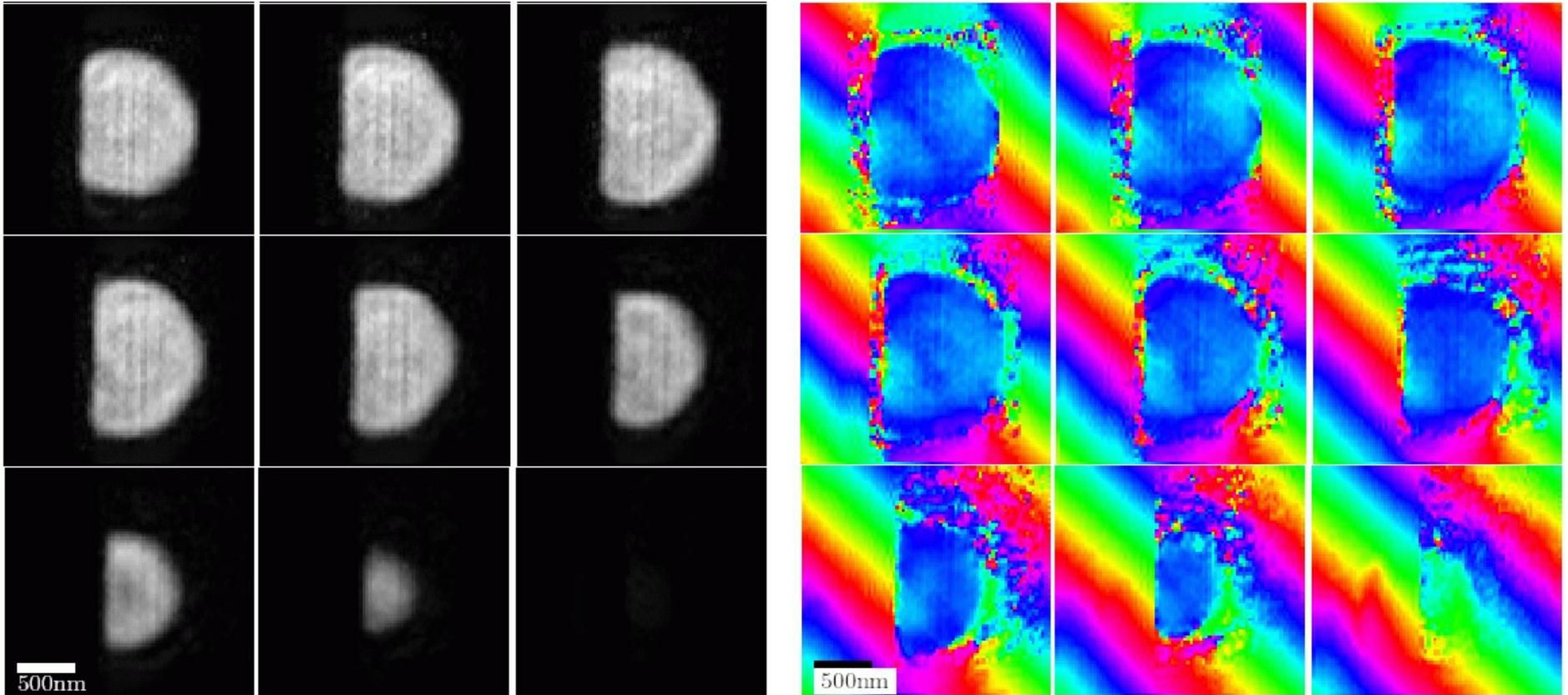
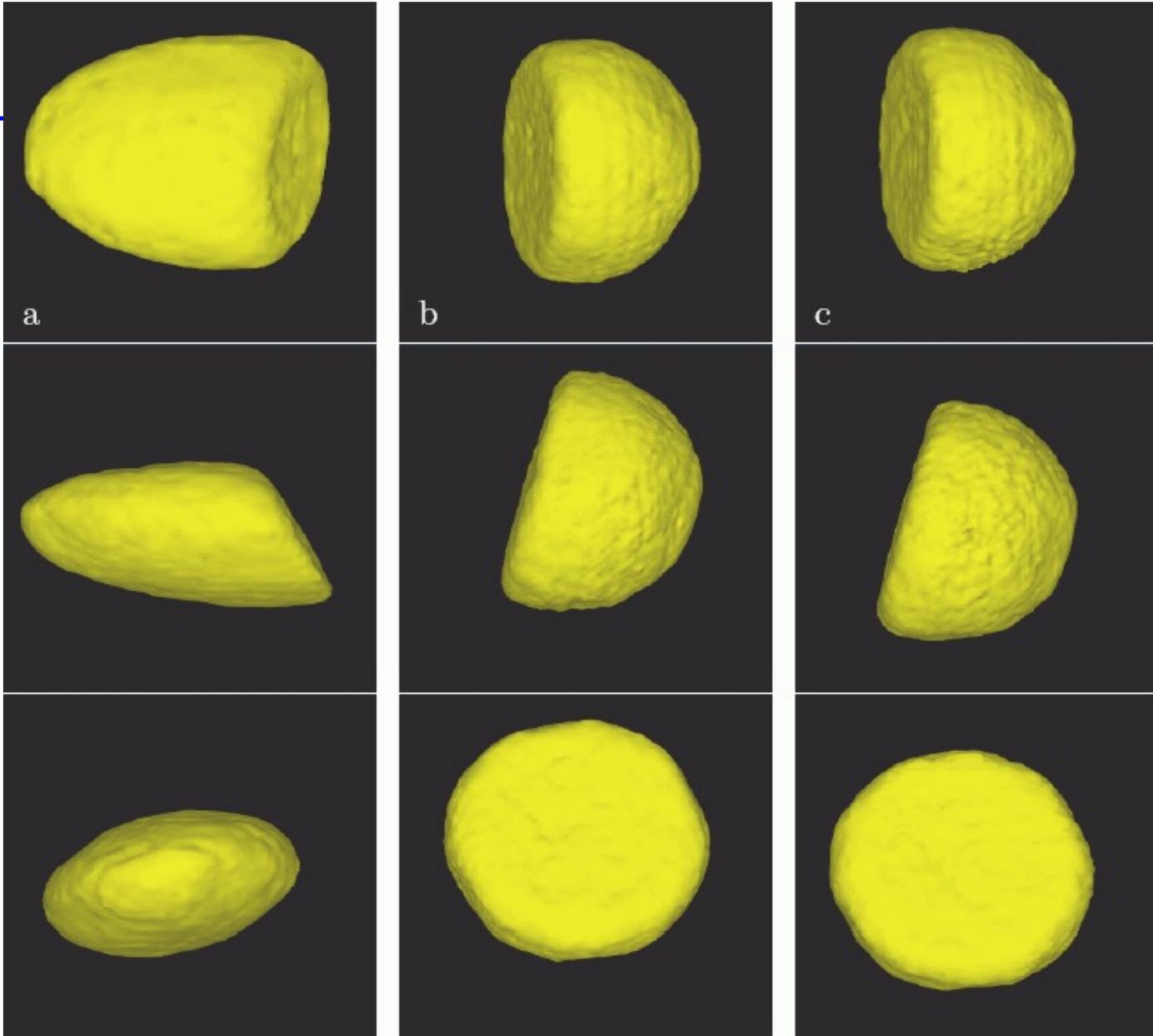


Figure 4.12: Center slices from 3D CXD pattern from Pb sample, on a log scale. Data file 296 from 10/03.

# *Then refine amplitude and phase*

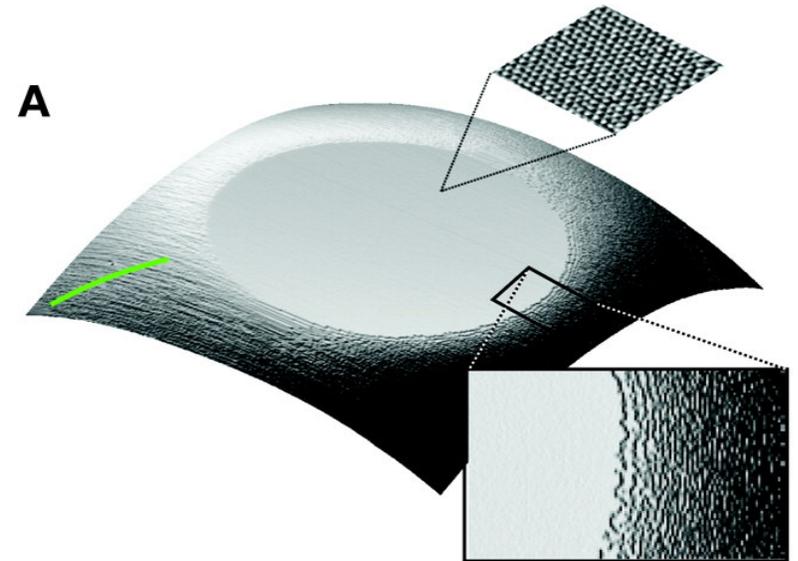
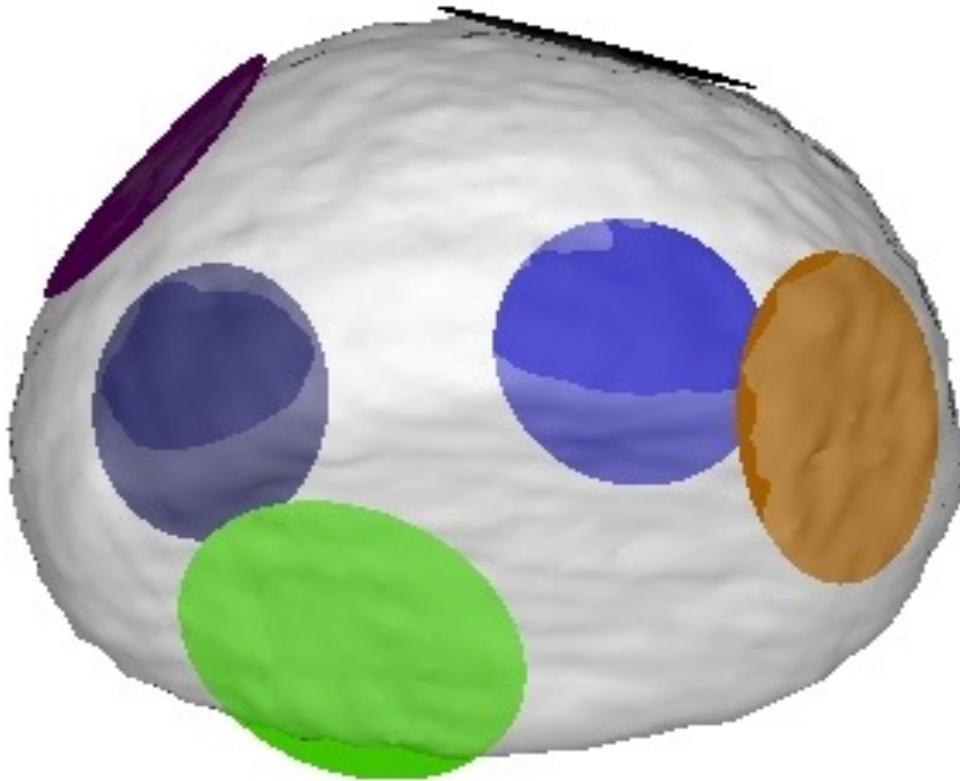
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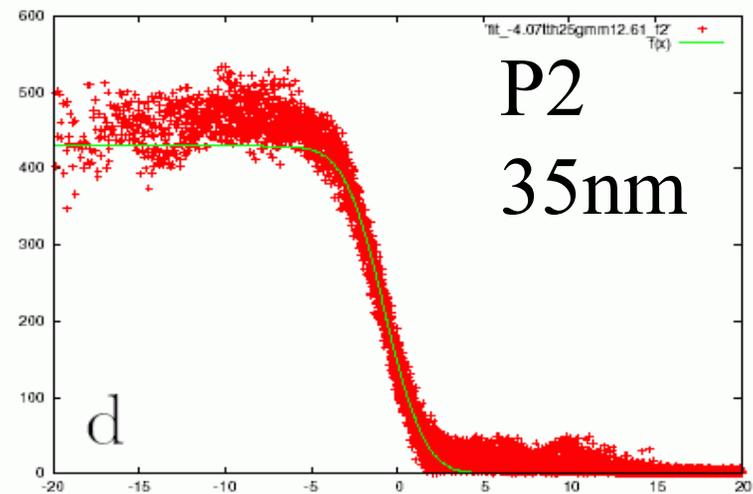
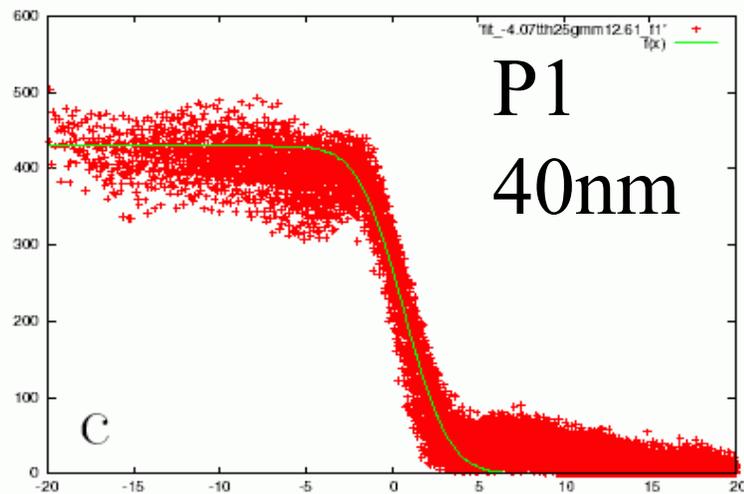
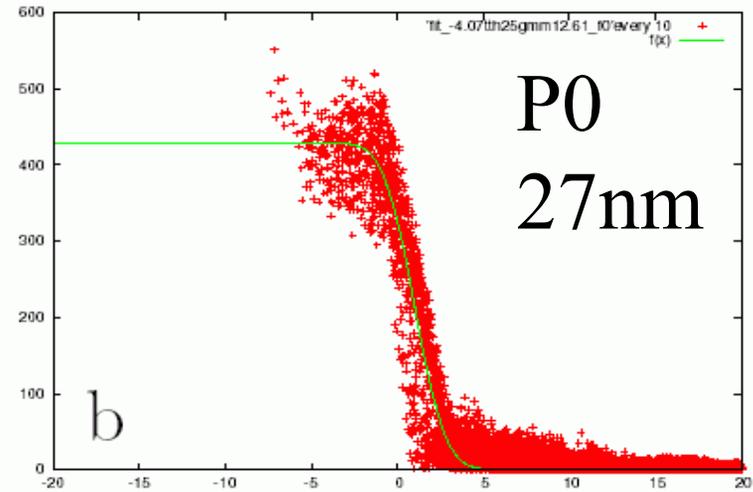
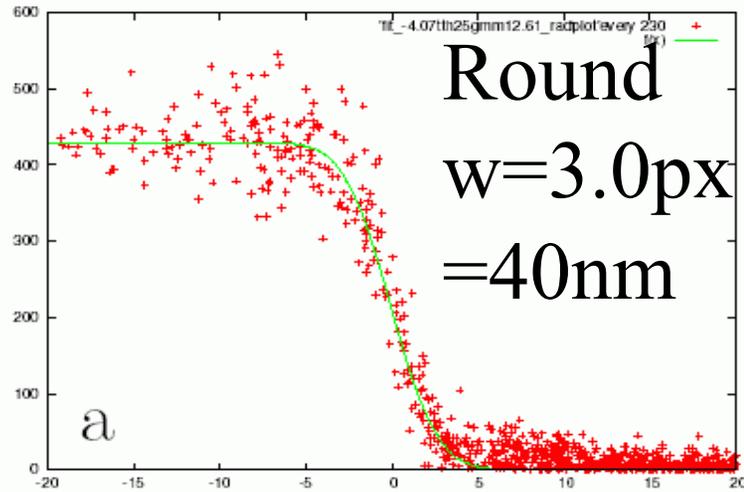
# *Facets of Equilibrium Crystal Shape*

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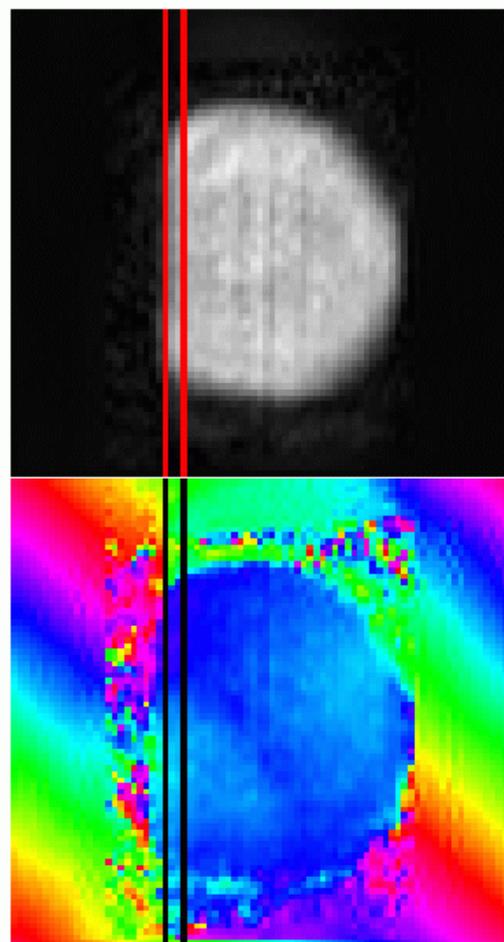
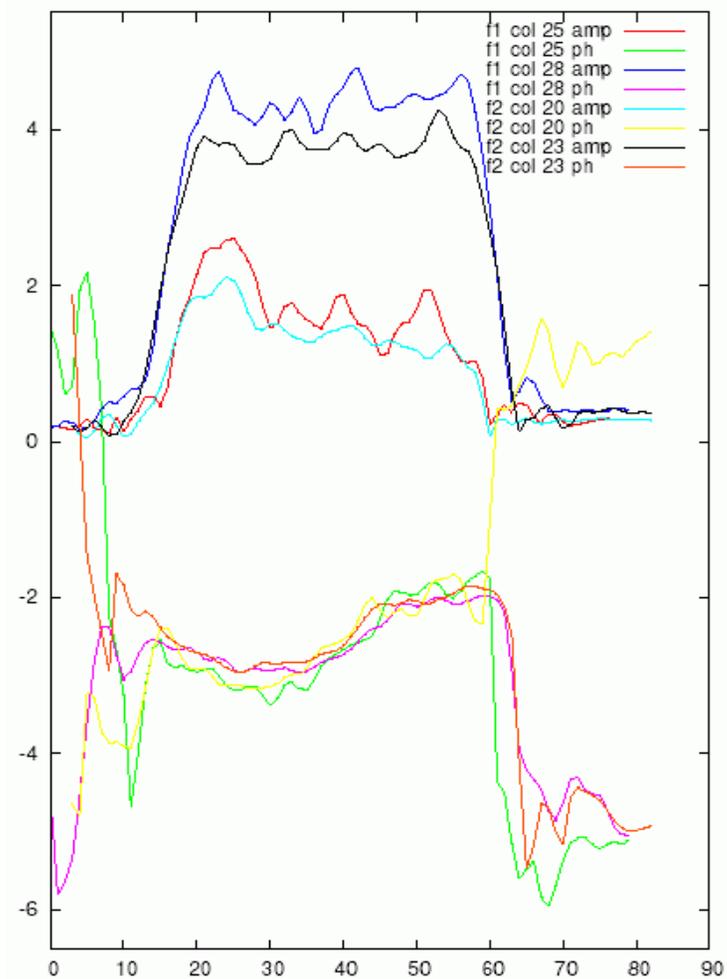
Thurmer K, Williams E, Reutt-Robey J  
Science **297** 2033 (2002)

# *Density distribution across surface*



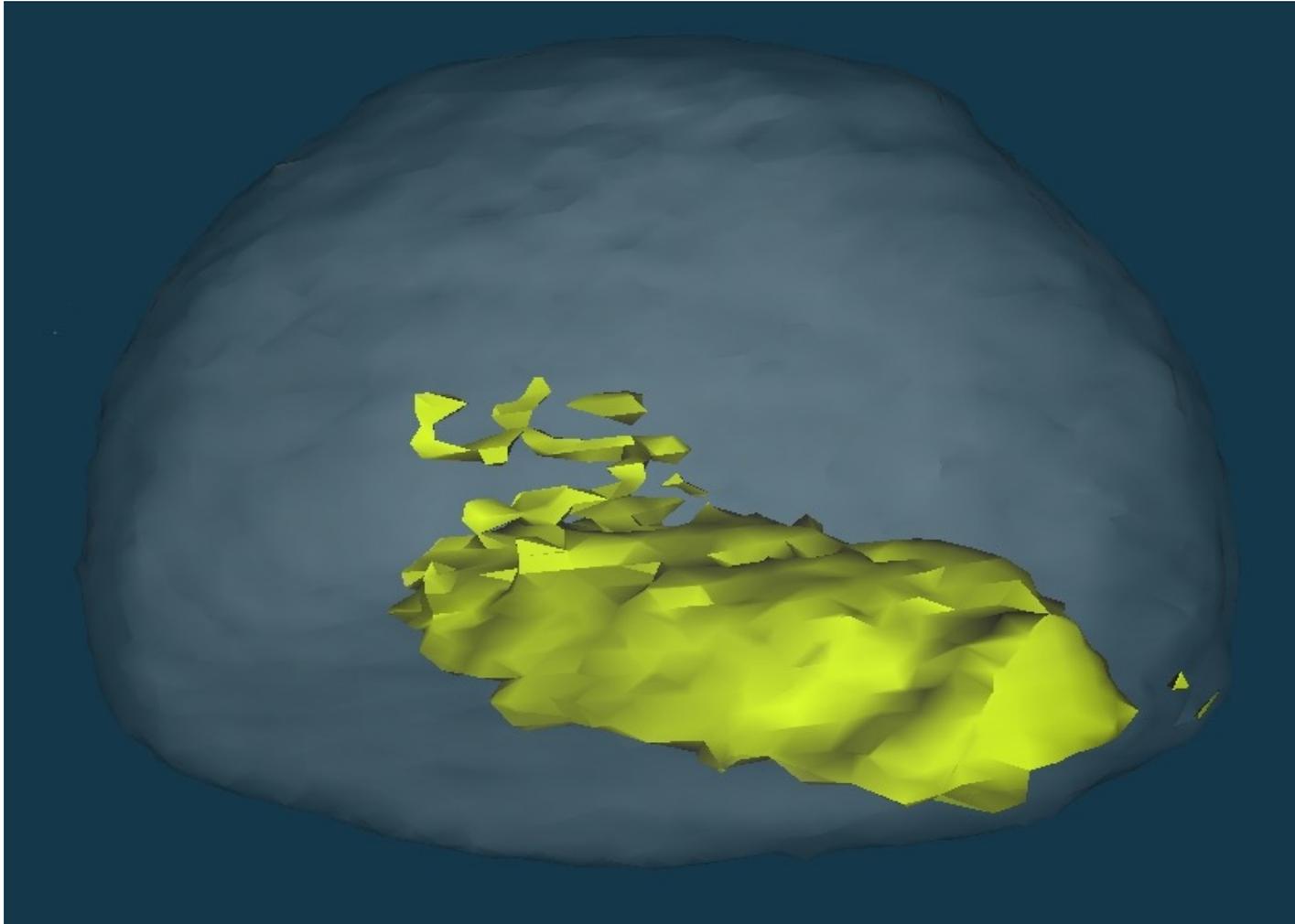
# *Phase structure near substrate interface*

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# *Modeling of 3D Phase Bump*

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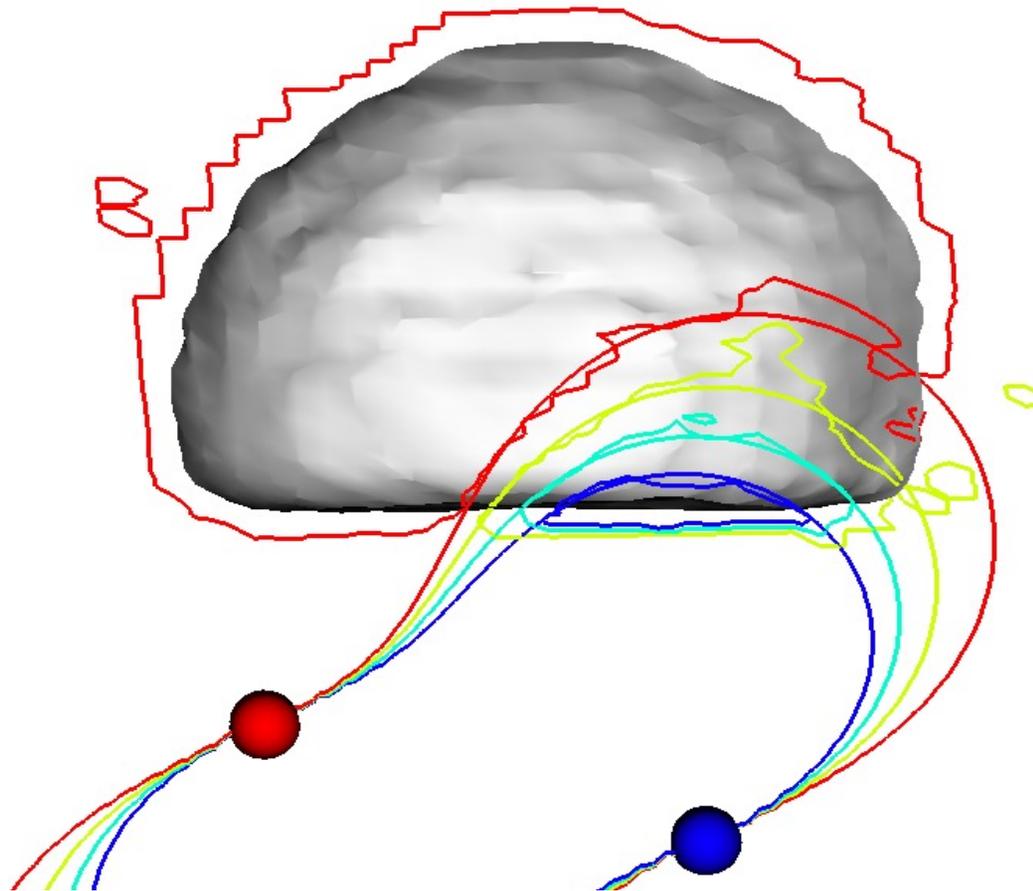


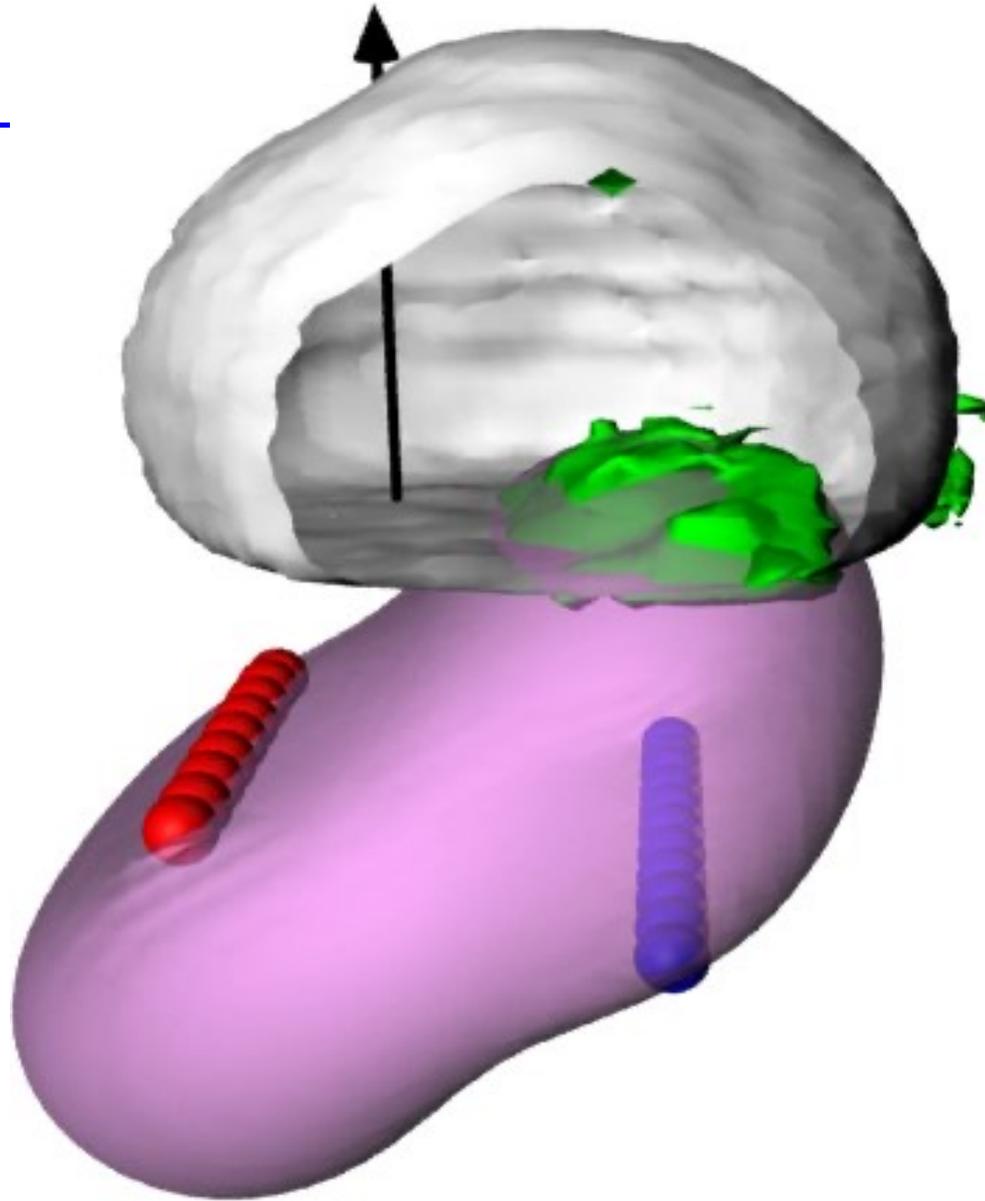
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*Ian Robinson -- Medical Imaging Seminar -- March 2006.*

# *Field lines of Point Charges*

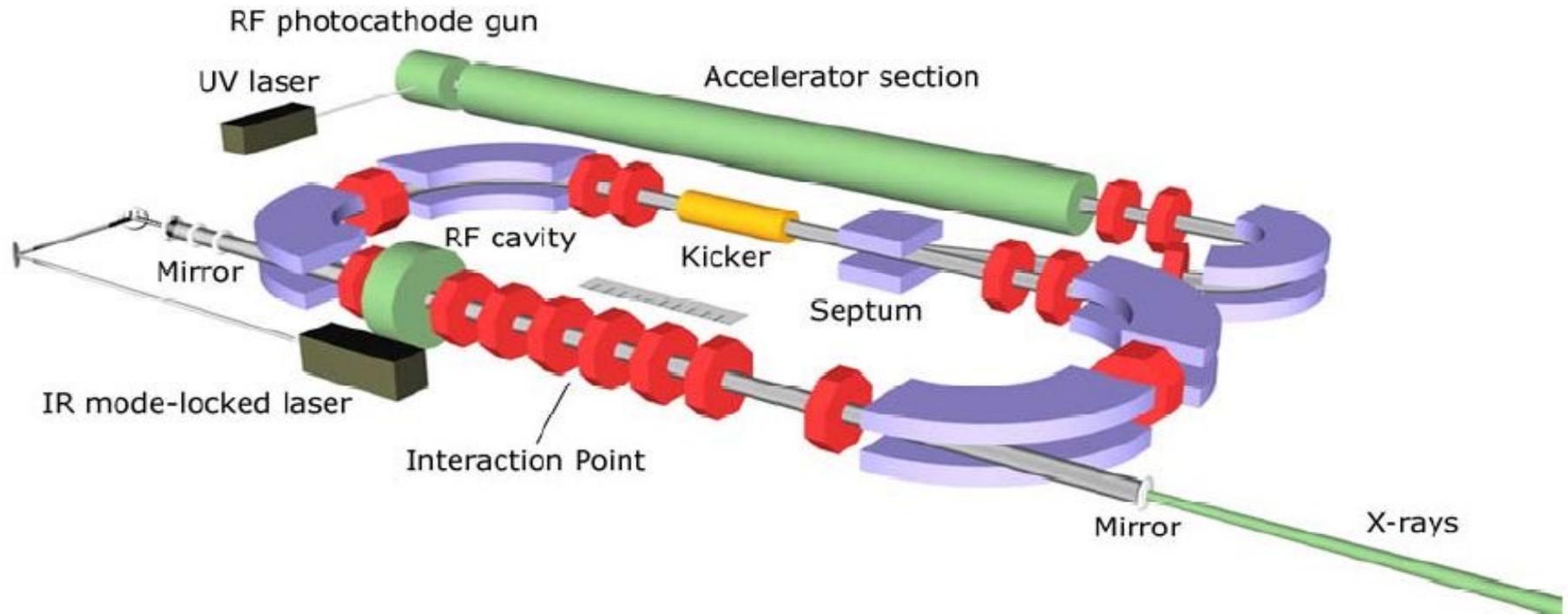
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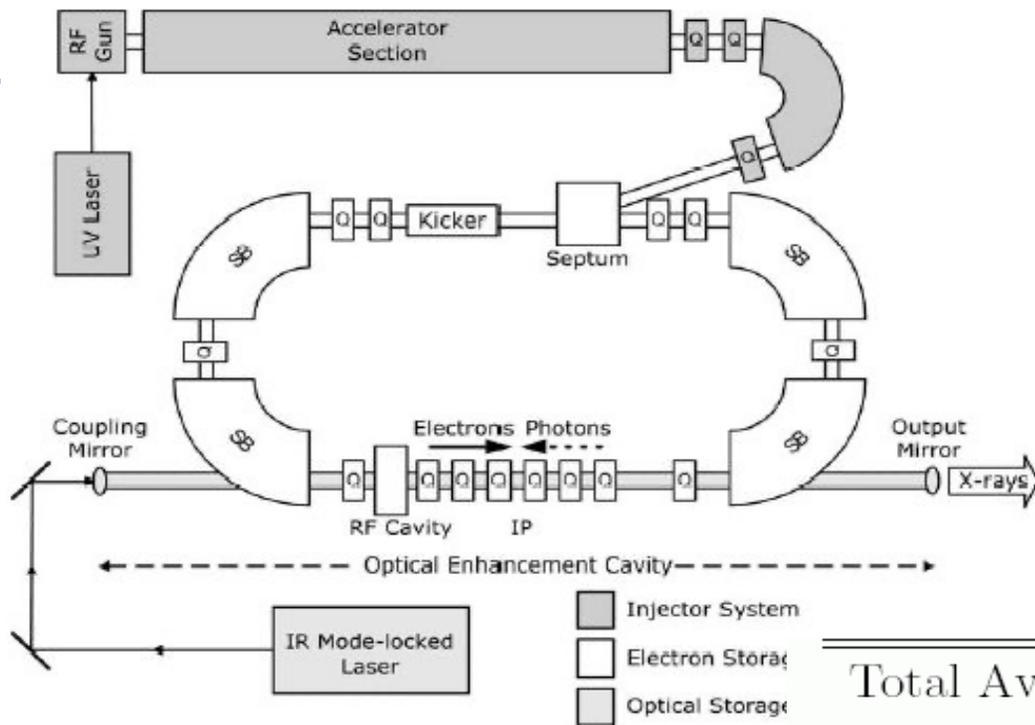




# Compact Light Source

Ron Ruth, Lyncean Technologies





# CLS Specifications

R. J. Loewen, Ph.D. Thesis

SLAC (2003)

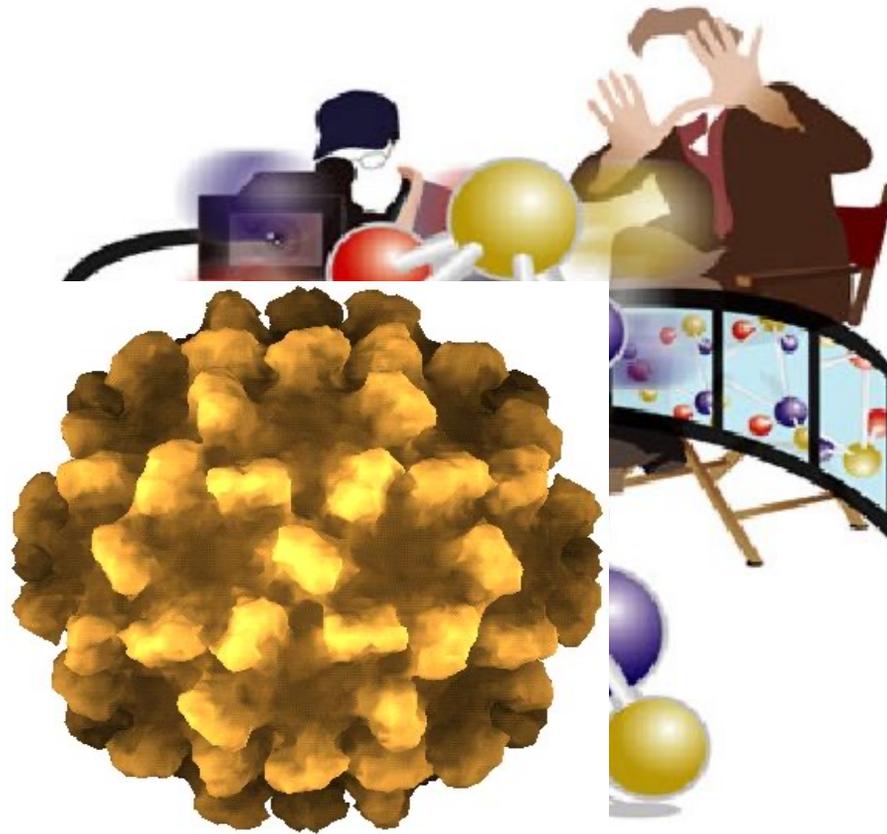
50MeV ( $\gamma=100$ ) + 1 $\mu$ m laser

$$\omega = \frac{4\gamma^2}{(1 + \gamma^2\theta^2)} \omega_0$$

Total Average Flux	$\gtrsim 10^{13}$ ph/s
Avg. "Monochromatic" Flux*	$\approx 10^{10}$ ph/s
Source Spot Size <sup>†</sup>	30 $\mu$ m radius
Source Divergence <sup>†</sup>	$\approx 3$ mrad
Source Brightness	$\gtrsim 10^{11}$
X-ray Energy Range <sup>‡</sup>	12 keV $\pm$ 6 keV

# *Molecular Movies using XFEL*

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## *Conclusions and Outlook*

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*Franz Pfeiffer* [pfeiffer@psi.ch](mailto:pfeiffer@psi.ch)

- Phase contrast imaging has medical applications
- Achievable and practical using gratings
- Diffraction phasing by computation instead of lens
- Strain fields imaged as phase objects
- Single molecules one day using XFEL
- Medical imaging opportunity now using CLS

# *Acknowledgements*

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**Christian Grünzweig, Jens Bruder, Ana Diaz, Christian David, Oliver Bunk, Ian Johnson, Marco Stampanoni, Xavier Donath, Gabriel Frei, Henrik Rønnow, Eberhard Lehmann,**  
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**Timm Weitkamp,**  
*ANKA, Forschungszentrum Karlsruhe, Germany*

**Peter Cloetens,**  
*ESRF Grenoble, France*

**Ivan Vartanyants**  
*HASYLAB, DESY, Germany*

**Ian Robinson**  
*University of Illinois, USA => University College London, U.K.*

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