Science case for high-energy photons

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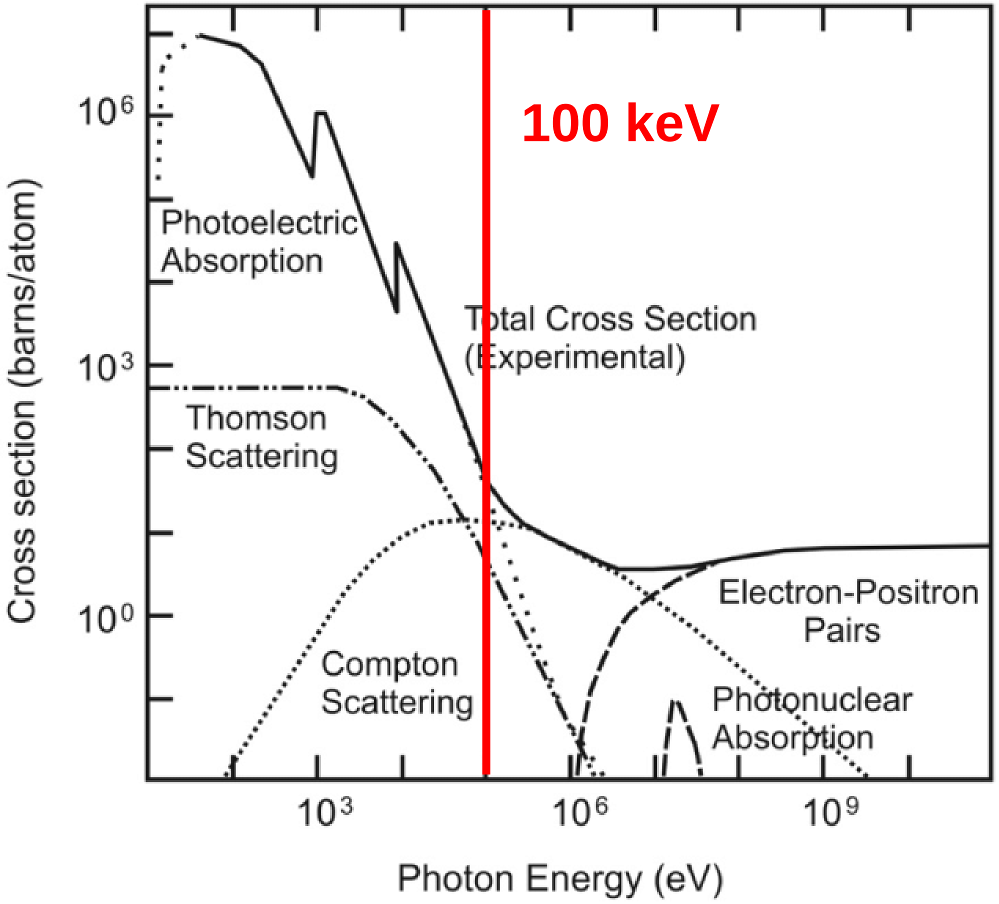
Outline

- **Introduction to hard X-rays for the experimental point of view**
- **Diffraction limited beams (yes, we like them!)**
- **Applications in X-ray experiments (quick tour)**
- **Conclusion and Outlook**

Introduction to hard X-rays

- Definition of “hard X-rays” depends on the facility and point-of-view
- For X-ray scattering and X-ray imaging experiments “hard” typically means E >~ 20 keV (λ <~ 0.62 Å)
- Scattering and imaging experiments are less interesting above E ~ 100 keV (0.12 Å), depending on the material
- Thomson scattering vs Compton scattering
- Photoelectric absorption vs Compton scattering
- Compton scattering produces unwanted bgnd in elastic scattering and imaging experiments, the lighter the element (smaller Z) the worse

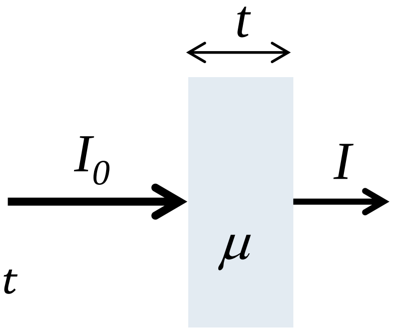
Photon-matter interactions (for Cu)



Introduction to hard X-rays

Hard X-rays provide

- Penetration power



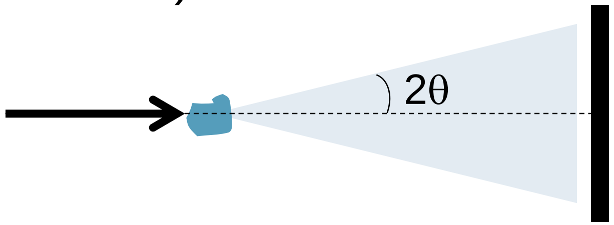
$$I = I_0 e^{-\mu t}$$

μ : absorption coefficient
$1/\mu$: absorption length

$1/\mu \propto E^n$ with n ~ 3
$1/\mu \propto Z^{-m}$ with m ~ 4

- Smaller scattering angles (2θ) for the same q (momentum transfer)

$$q = \frac{4\pi}{\lambda} \sin\theta$$



$q_{max} \propto E$

- Phase contrast in addition to absorption contrast in X-ray imaging experiments

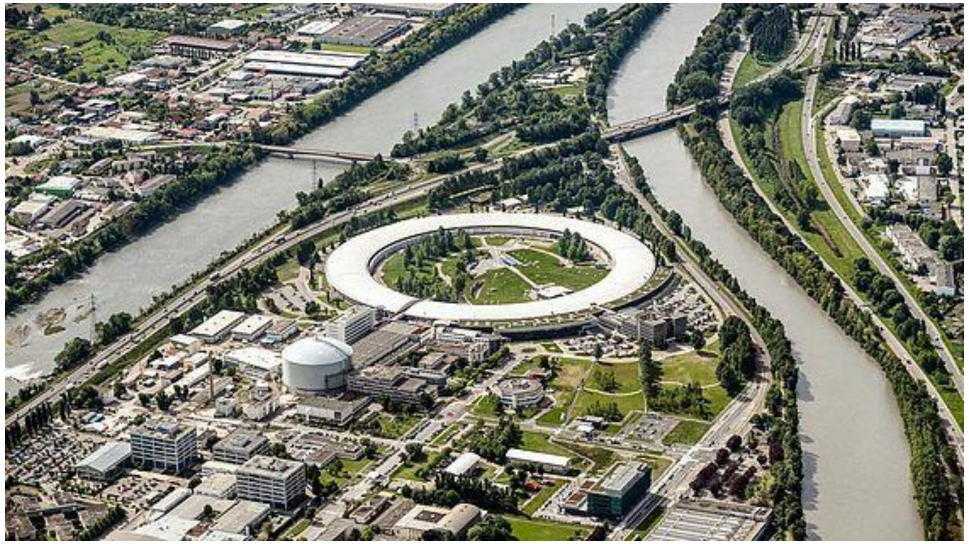
$$E(\boldsymbol{r}, t) = e^{i(n\boldsymbol{k}\cdot\boldsymbol{r} + \omega t)}$$

refractive index
n = 1 - δ + iβ

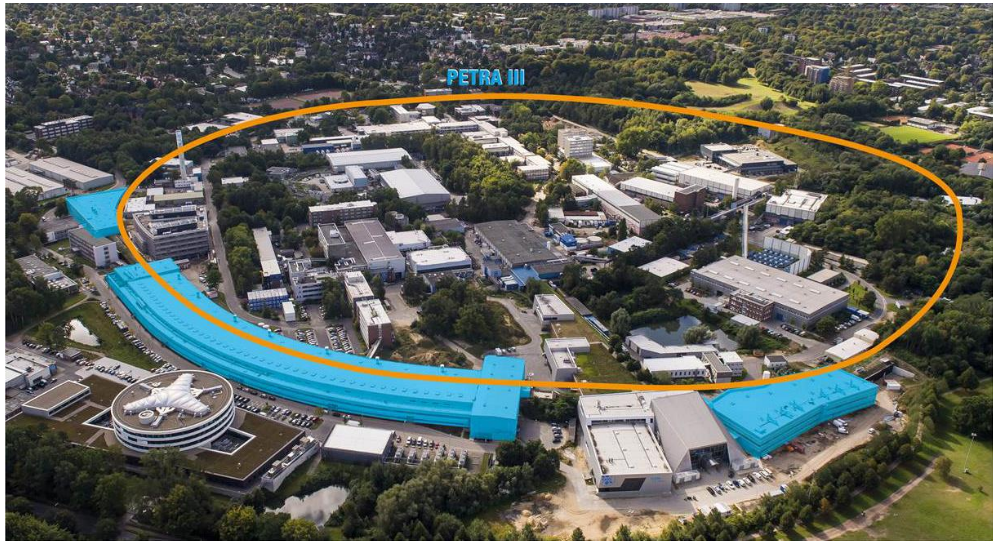
δ >> β for hard X-rays and light elements

High Brilliance and hard X-rays in Europe

ESRF, Grenoble



Petra III @ DESY, Hamburg



Free-Electron lasers: up to ~25 keV on the fundamental at European XFEL (but SC-U plans are underway),
High-harmonic lasing at other FELs but with reduced photon flux

Diffraction limited beams

Diffraction limited beams, low emittance (ε), large coherent flux (Fc), high Brilliance (B)

$$\lambda_{h,v}^{diff} \sim 4\pi\epsilon_{h,v} \qquad B = \frac{I}{(2\pi)^2\epsilon_h\epsilon_v} \qquad F_C = B\lambda^2/4$$

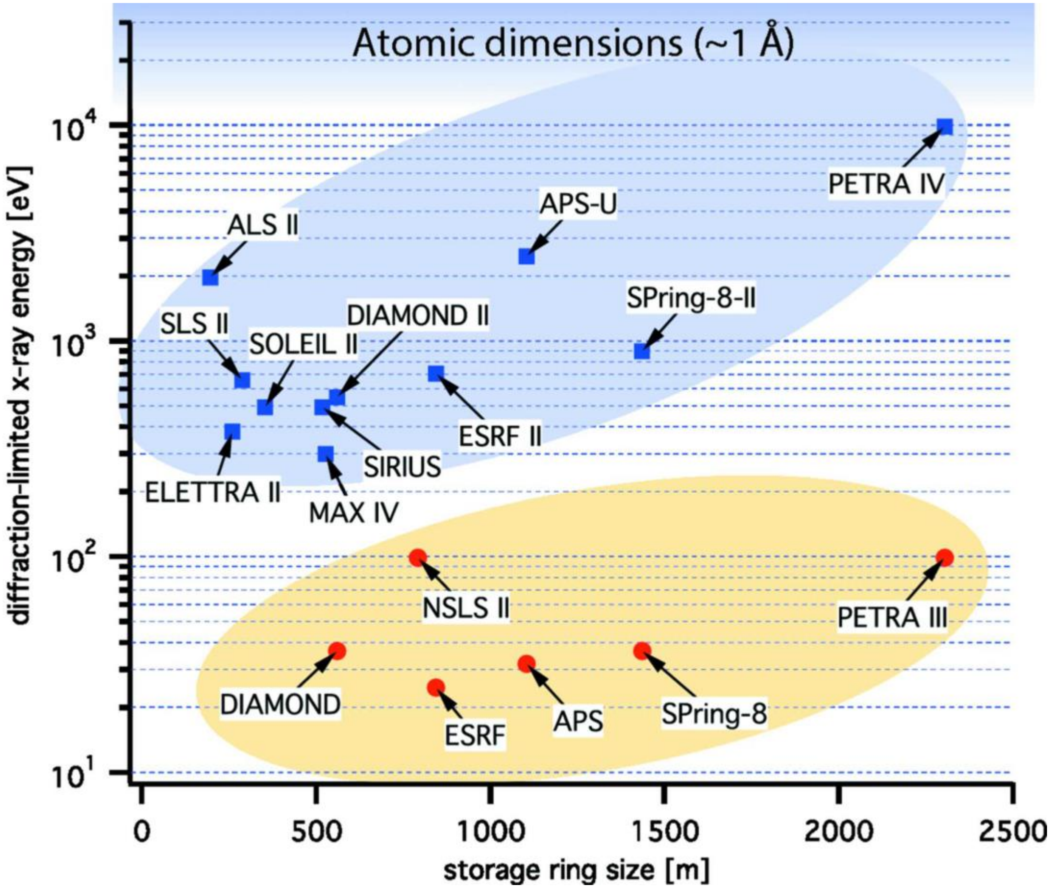
Great advantages for experimental X-ray methods, for instance in terms of

- High degree of beam coherence (large coherent flux F_C)
- Focusing to nanometer spot sizes, Abbe's limit: $d \sim \lambda/(2NA)$
- More flux → shorter integration times (time-resolved exp)

Structural investigations by X-rays (real space vs reciprocal space):
Bridging the length scales between X-ray microscopy (imaging) methods and X-ray diffraction

Studies of dynamics by X-rays (time domain vs frequency domain):
Bridging the time scales between time domain methods (XPCS) and inelastic X-ray scattering

Diffraction limited beams



Schroer *et al.* (2018)

Petra IV (planned):

$\varepsilon \sim 10$ pm rad → E(diff) ~ 10 keV

Upgraded ESRF (existing):

$\varepsilon_h \sim 110$ pm rad → E(diff) ~ 0.9 keV

30 keV (U18, 2m, 3rd harm)
Brilliance [ph/s/0.1%/mm^2/mrad^2] ~ 3.5×10^{21}

50 keV (U18, 2m, 5th harm)
Brilliance [ph/s/0.1%/mm^2/mrad^2] ~ 1.4×10^{21}

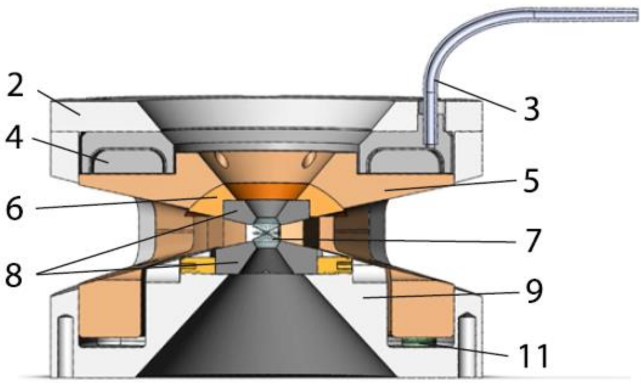
None of the existing or planned(?) storage ring upgrades provide diffraction limited hard X-ray beams!

FCC-ee booster: 0.5 pm rad ???

Applications of Hard X-Rays

Examples from X-ray Scattering

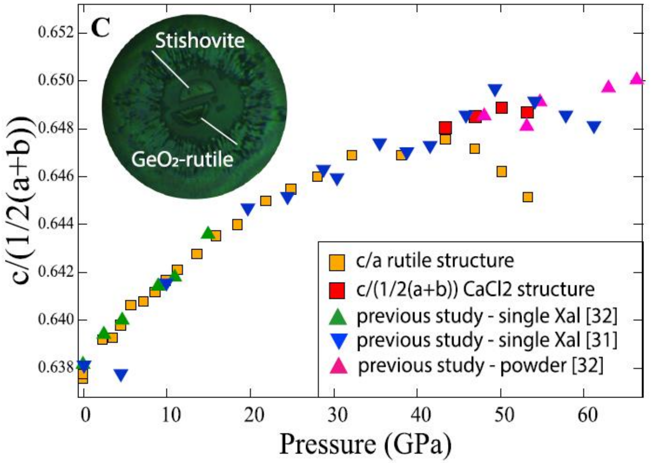
- **High pressure by Diamond Anvil Cell (DAC)**



- Conical diamonds and pressure cell
- Up to 100 GPa pressure for X-ray exp
- X-rays need to penetrate several mm of diamond

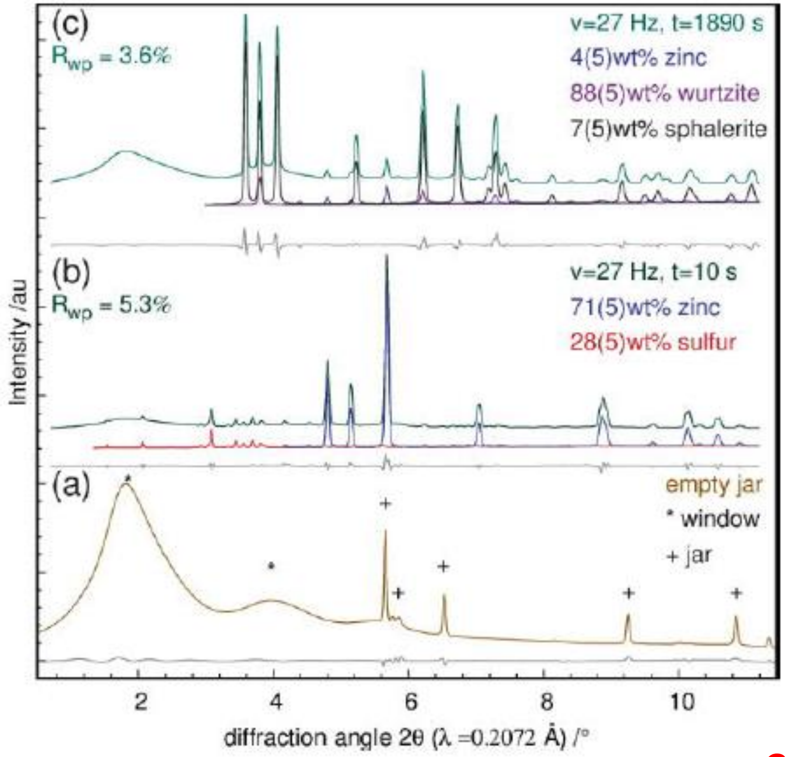
Petitgirard *et al.* (2019)

30 keV X-ray data (ESRF)



- **Powder diffraction and pair-distribution function analysis**

Mechanochemistry, ball milling of mixtures
60 keV data (Petra III)



$q = 6$ Å^{-1}

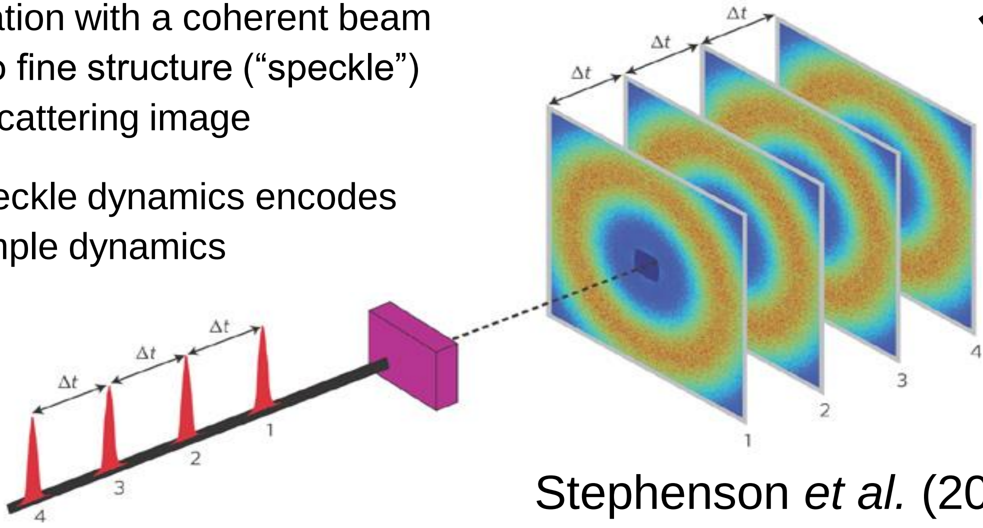
Petersen *et al.* (2021)

Applications of Hard X-Rays

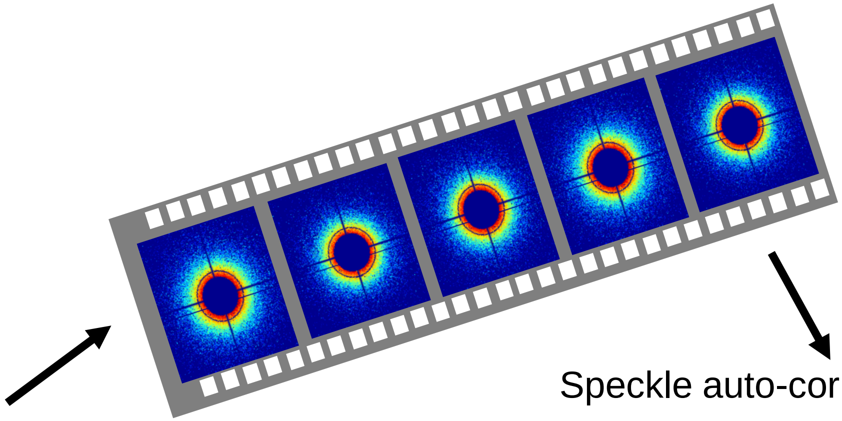
Examples from X-ray Scattering

- **X-ray Photon Correlation Spectroscopy (XPCS)**

- Illumination with a coherent beam leads to fine structure (“speckle”) in the scattering image
- The speckle dynamics encodes the sample dynamics

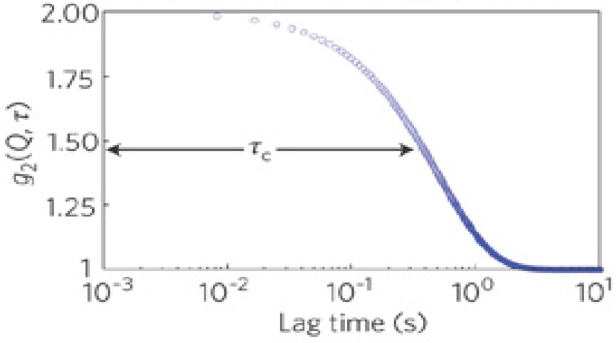


Stephenson *et al.* (2009)



“Speckle” movie

Speckle auto-correlation function



Advantageous SNR scaling for XPCS:
x10 in Fc → x100 in shorter timescales

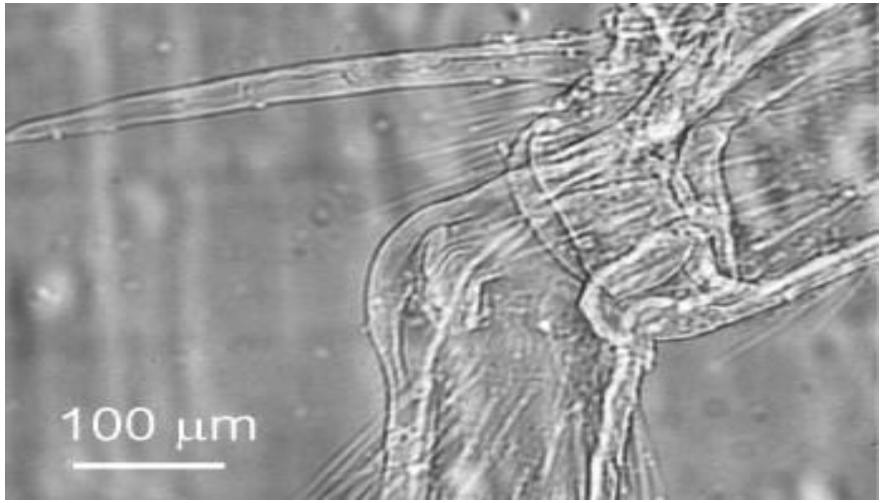
- Advantage to work at higher ph energy than today (7-10 keV) if sufficient coherent flux is available
- XPCS experiments at 30-50 keV also beneficial for radiation damage, e.g. to study soft and bio matter
- Would require a long (~30 m) sample-detector distance and an optimized detector (small pixels, high Z sensor)

Möller *et al.* (2019)

Applications of Hard X-Rays

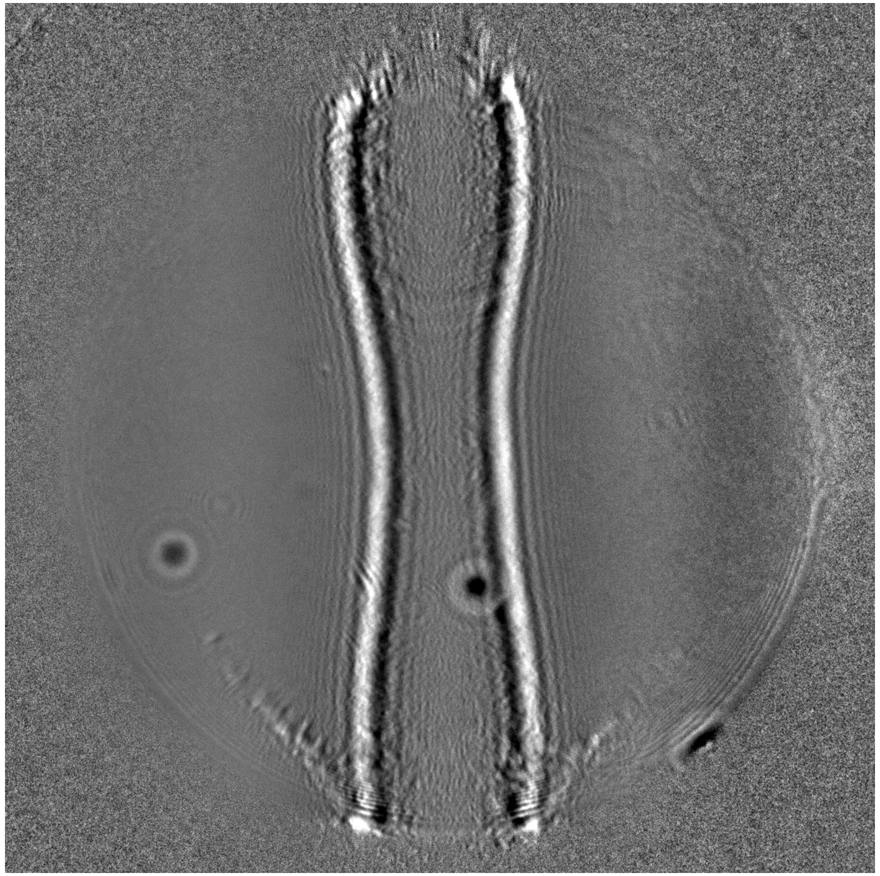
Examples from X-ray Imaging

- Phase contrast (“edge enhancement”)
- Stronger than absorption contrast
  at high photon energy and low-Z materials
- Can provide very high resolution in
  combination with phase retrieval methods



Phase contrast: Koch *et al.* (1998)

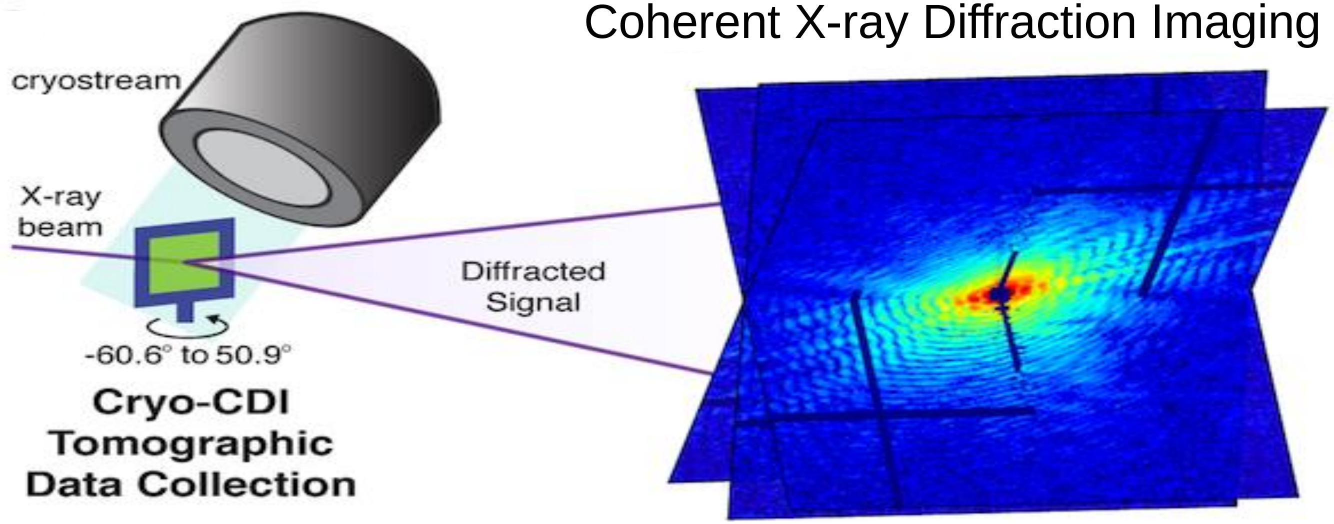
- State-of-the-art X-ray holography (cone beam)
  requires smallest focus (diffraction limited beam)

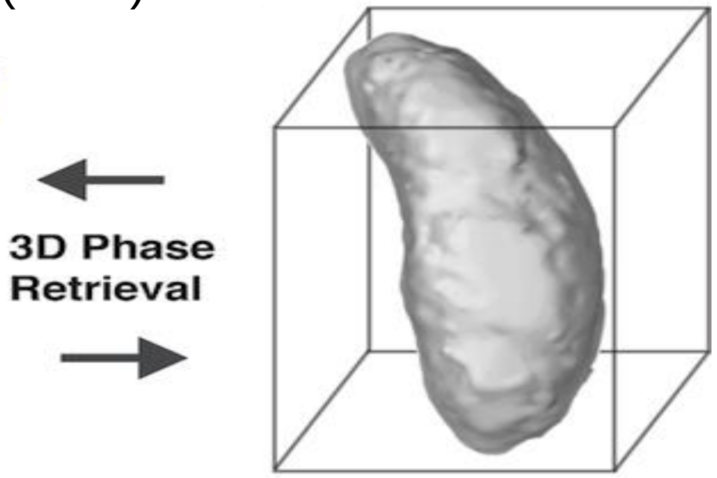


Hagemann *et al.* (2021)

Applications of Hard X-Rays

Coherent X-ray Diffraction Imaging (CXDI)



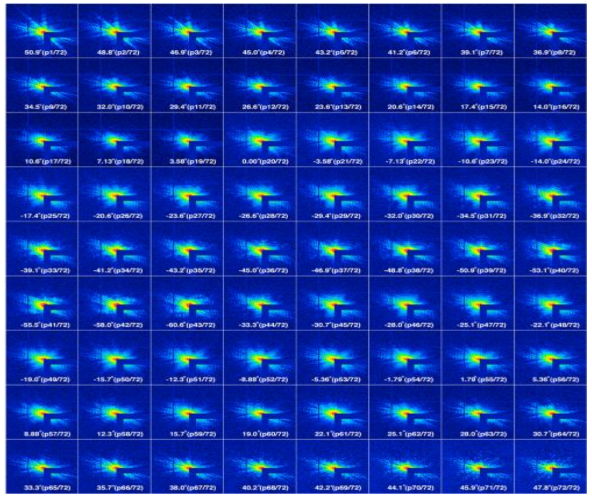


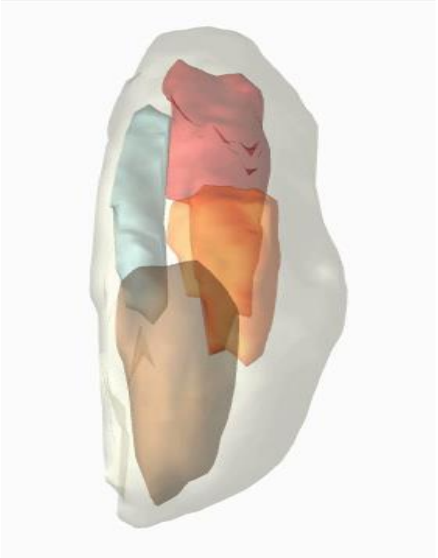
More than 100 different 2D projections necessary for 3D phase retrieval

Radiation damage is a problem. Probably better done with hard X-rays if sufficient coherent flux

Rodriguez *et al*. (2015)

ESRF data, 8 keV





Neospora caninum parasite

Conclusion and Outlook

- No doubt that a 0.5 pm rad source would revolutionize the X-ray world, particularly in the hard X-ray range
- Applications of hard X-ray scattering could be combined with ultra-small beams, higher time-resolution and coherence techniques
- High Brilliance techniques, e.g. coherent scattering, coherent imaging and nano-focus beams could be extended to the hard X-ray domain with benefits
- Enabling technologies at experiments also required, e.g. fast, high-resolution area detectors optimized for the 30-100 keV range