Performance of K-edge subtraction tomography as application of the X-ray source based on parametric X-ray radiation

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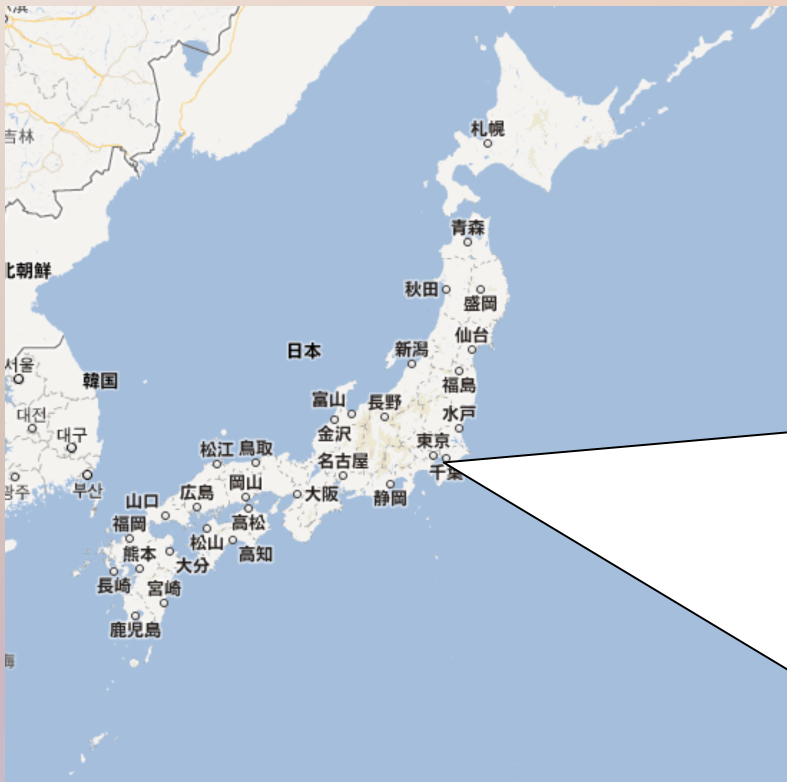
Outline

- Status of LEBRA-PXR source
- Advanced applications using the PXR source
- Computed Tomography using PXR
- Simultaneous-KES method based on PXR
- Quantitative performance of PXR-based KES
- Summary

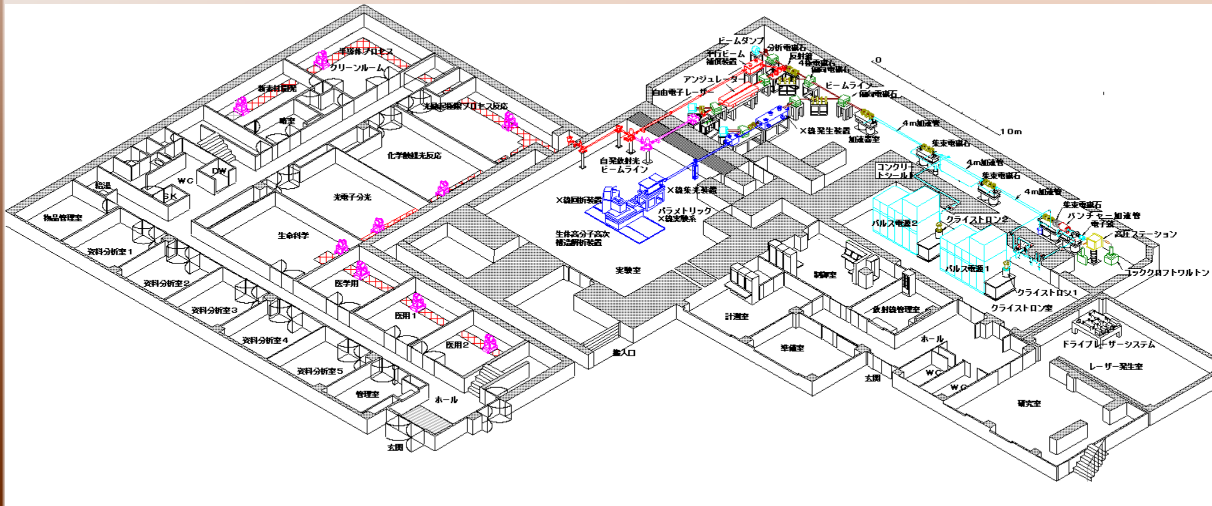
Nihon University



Funabashi, Chiba

LEBRA facility

LEBRA: **L**aboratory for **E**lectron **B**eam **R**esearch & **A**pplication



Coherent light-source facility based on
a conventional S-band electron linac

elctron energy: 125MeV(max.), 100MeV(typ.)
average current : 5μA (max.), 1 – 3 μA(typ.)

Specification of LEBRA Linac

electron energy	50 – 100 MeV
accelerating frequency	2856 MHz
bunch length (rms)	0.5 – 3 ps
bunch charge	~ 40 pC
macropulse duration	4 - 20 μs
macropulse beam current	~ 130 mA
macropulse repetition rate	2 – 5 pps
average beam current	< 5 μA
beam emittance	< 20π mm mrad

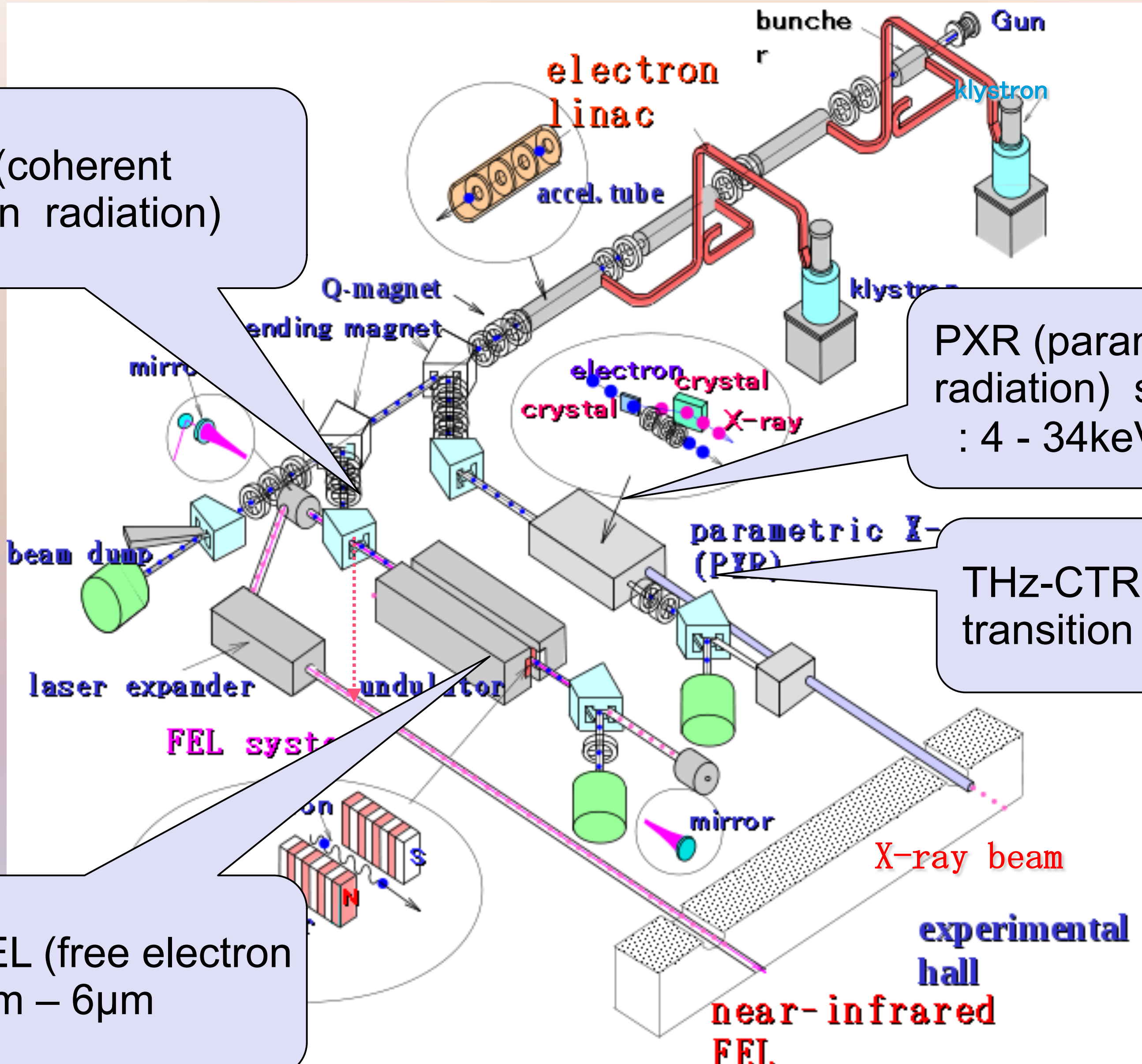
Tunable light source facility

THz-CSR (coherent synchrotron radiation)

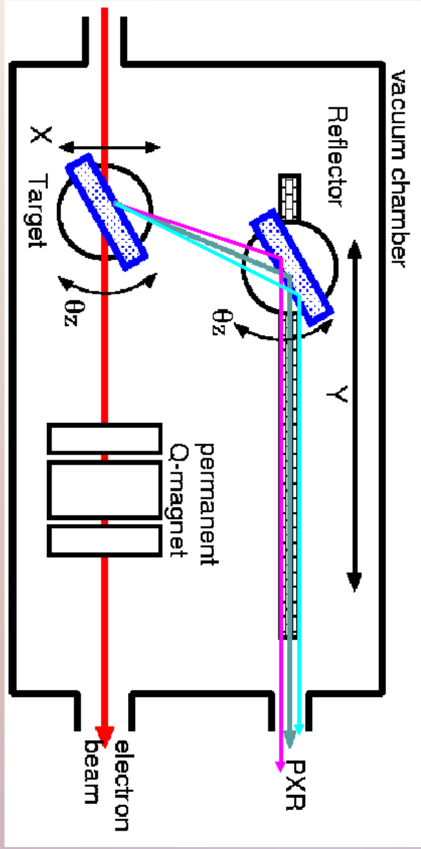
PXR (parametric X-ray radiation) source : 4 - 34keV

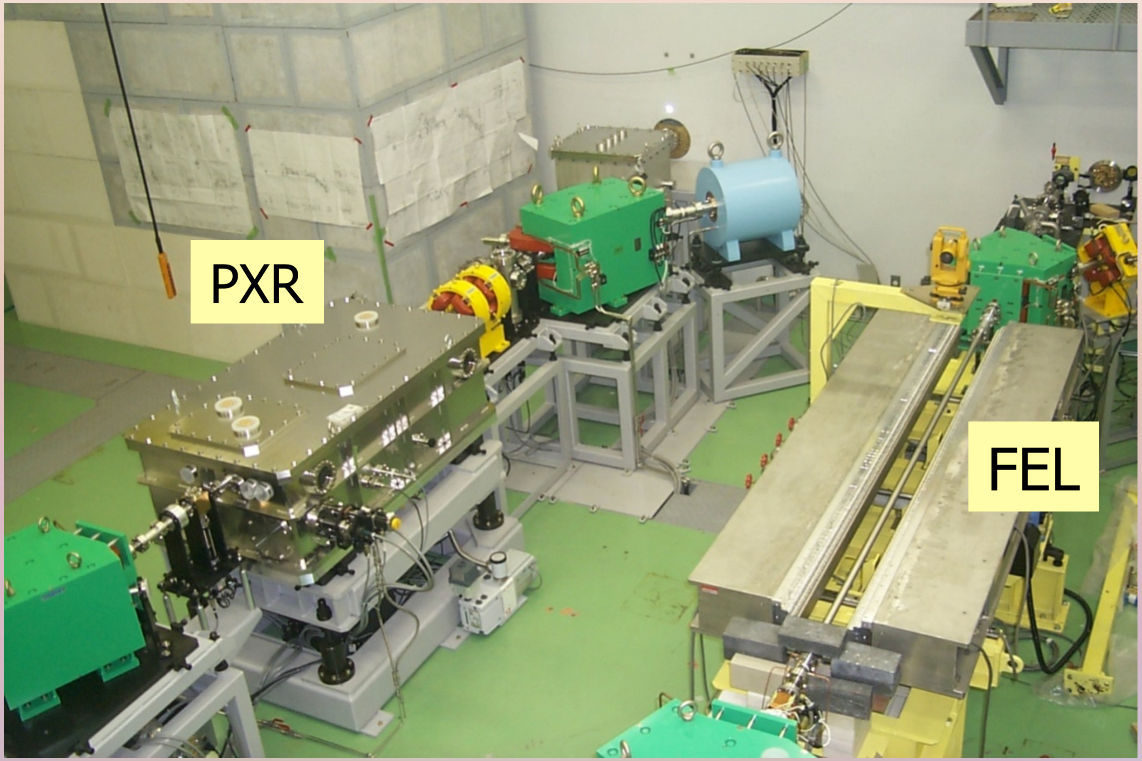
THz-CTR (coherent transition radiation)

infrared FEL (free electron laser) : 1μm – 6μm



LEBRA facility: beamlines (FEL & PXR)





Free electron laser (FEL): 1 ?m– 6 ?m (near-IR)

Parametric X-ray radiation (PXR): double-crystal system

X-ray beam is extracted using a (+, -) crystal optics

Status of LEBRA-PXR source

electron energy	100 MeV
X-ray radiator (target)	Si crystal plate
source size	
(e-beam spot on target)	0.5 – 1mm in dia.
X-ray energy range	Si(111): 4 – 20 keV
	Si(220): 6.5 – 34 keV
irradiation field	100 mm in dia.
total photon rate	$\geq 10^7$ /s @17.5keV

Feature of LEBRA-PXR

- Monochromaticity

  energy dispersion (spatial chirp) ~ 10%
  local band width ~ 0.1% (several eV)
- Tunability

  continuous selection of the center energy
- Large irradiation area

  at least 100mm in diameter after the extraction
  cone-beam depending on $1/\gamma$
- Spatial coherence

  phase-contrast imaging is actually possible
- Stability

  X-ray stability depends only on
  the linac condition

Application of LEBRA-PXR source

- Conventional imaging

  monochromaticity & tunability

- Diffraction-enhanced imaging (DEI)

  refraction (phase-gradient) contrast
  contrast based on small-angle scattering (SAXS)

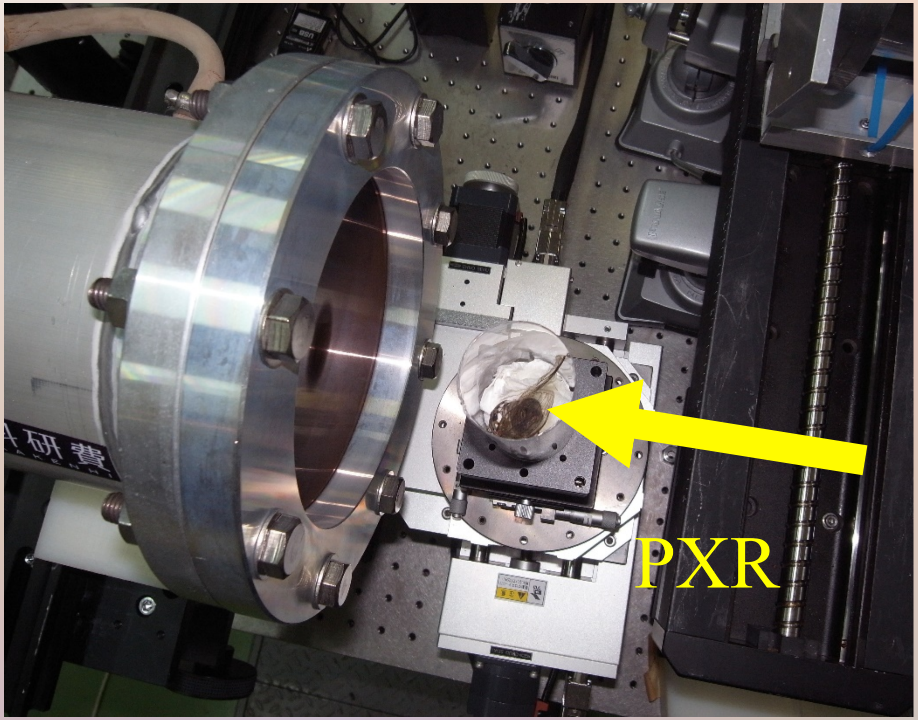
- X-ray absorption fine structure (XAFS)

  energy dispersive type XAFS analysis

- Computed tomography (CT)

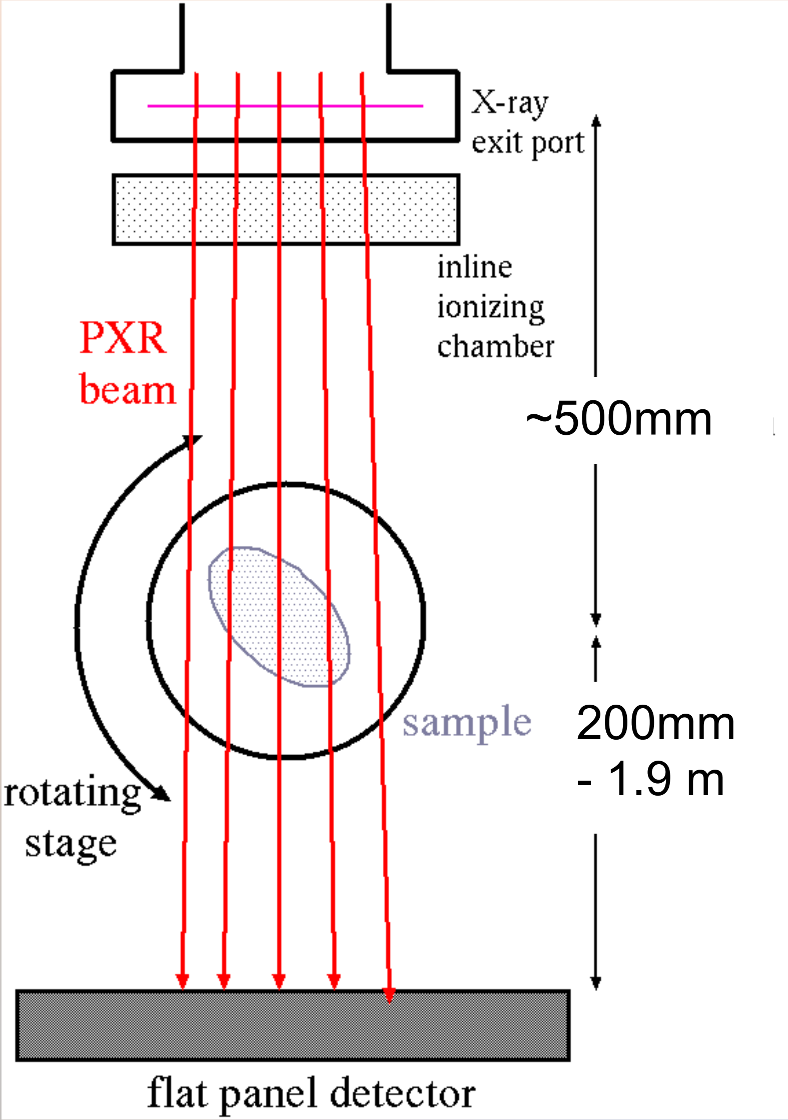
  monochromaticity & tunability
  propagation-based phase contrast effect

Setup for CT experiment using PXR

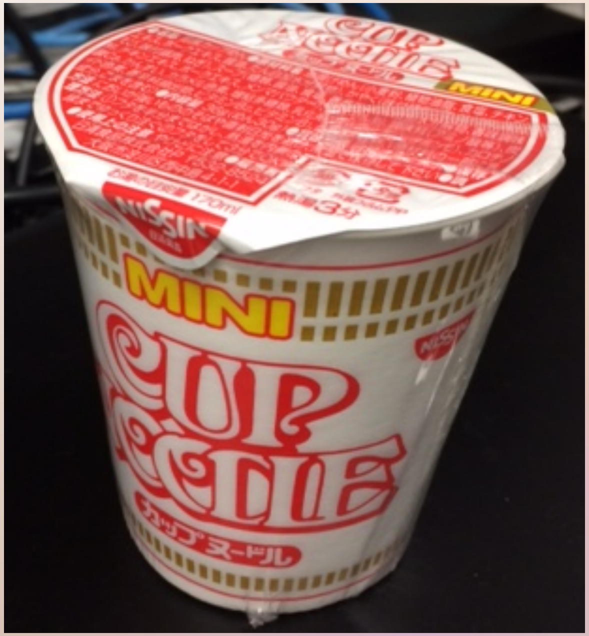


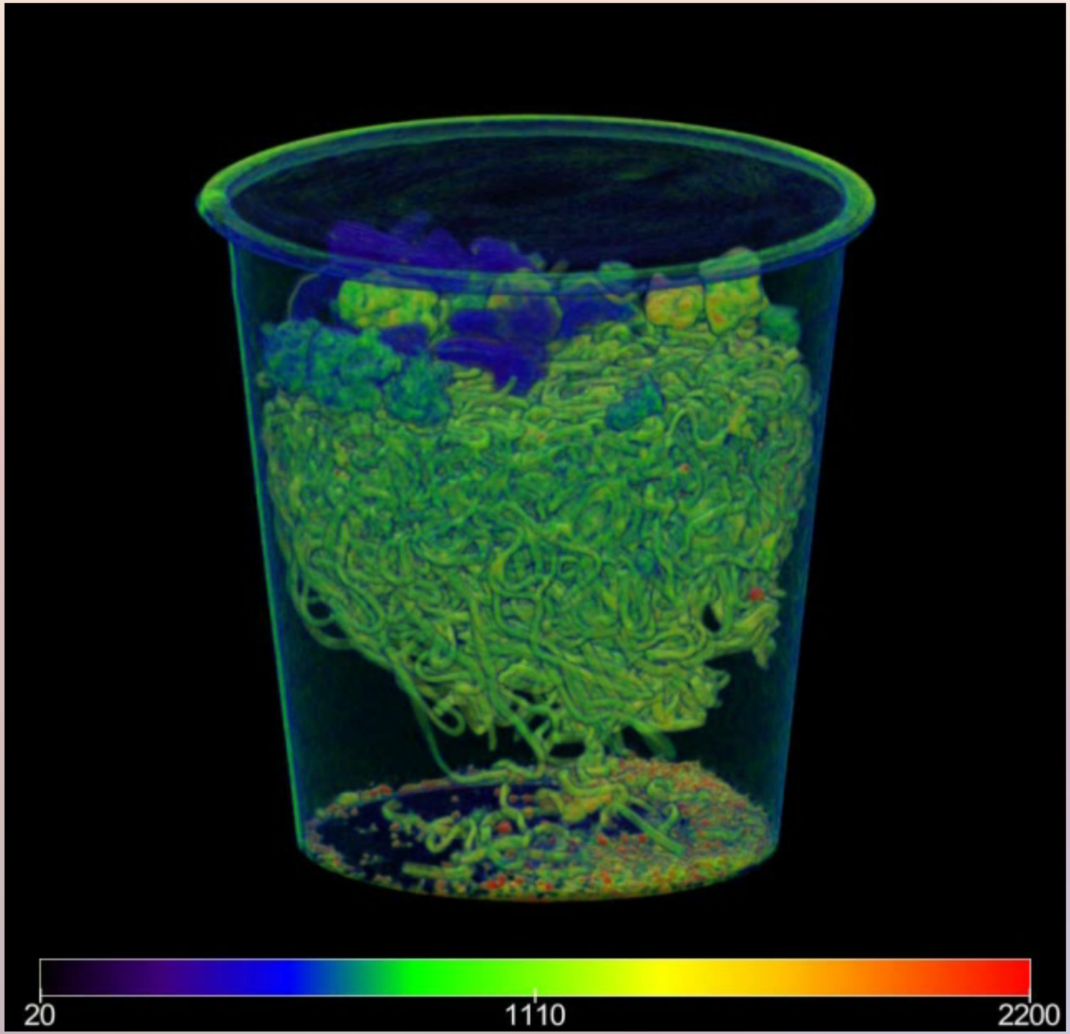
vacuum path

sample & rotating stage (0 – 180 deg.)



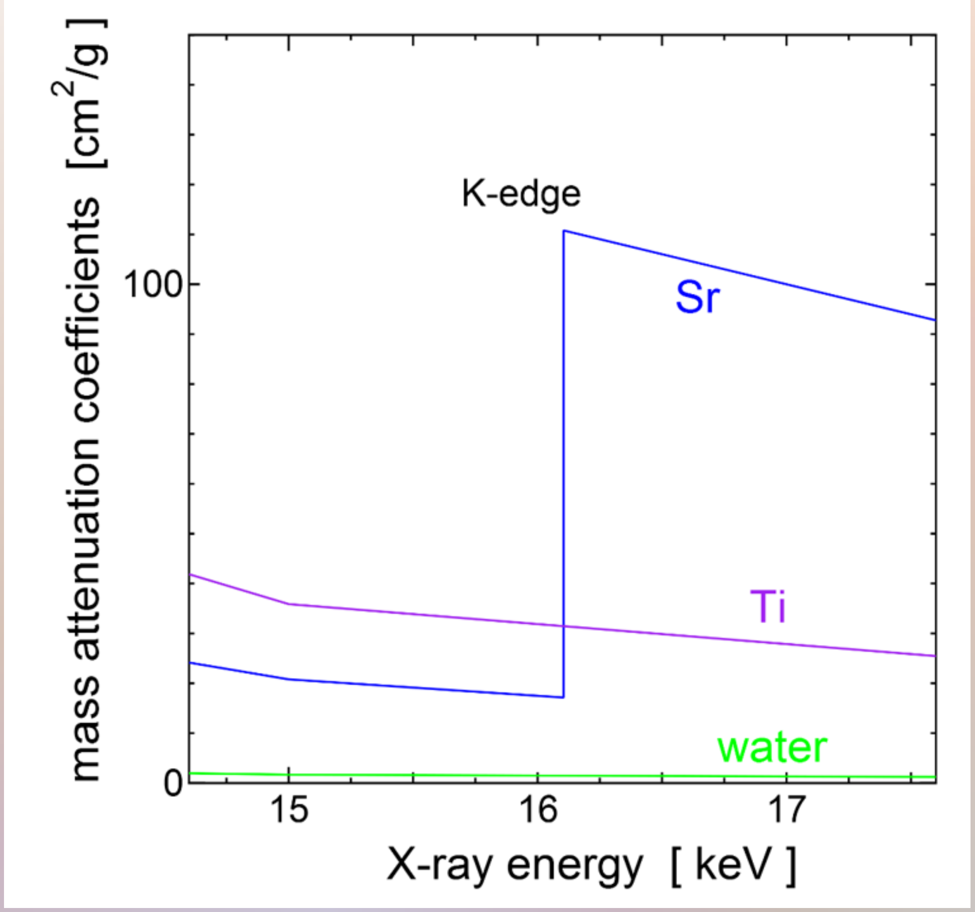
Result of CT using PXR





PXR energy: 22keV
sample: cup noodle
FPD: 100μm x 100μm
sample-FPD: 300mm
projection image: 500
each exposure: 25s
total measurement time: 3.5h (net)

K-edge subtraction for element imaging



Sr K-edge: 16.105 keV

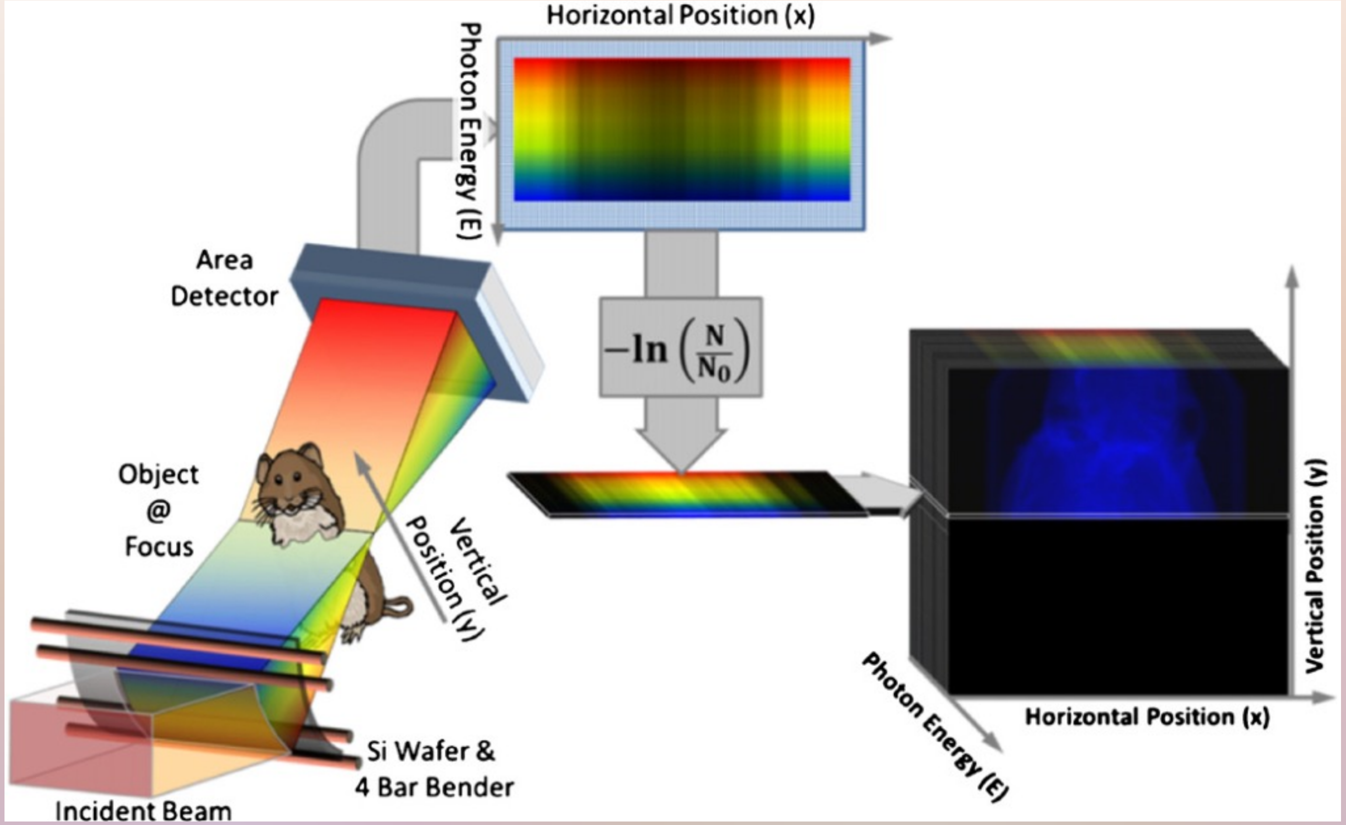
At the K-shell absorption edge of strontium, the X-ray absorption power drastically changes at only the place where strontium exists.

⇩

Subtraction between X-ray images on opposite sides of the K-edge energy can provide a 2D distribution of the Sr element.

KES: K-edge subtraction

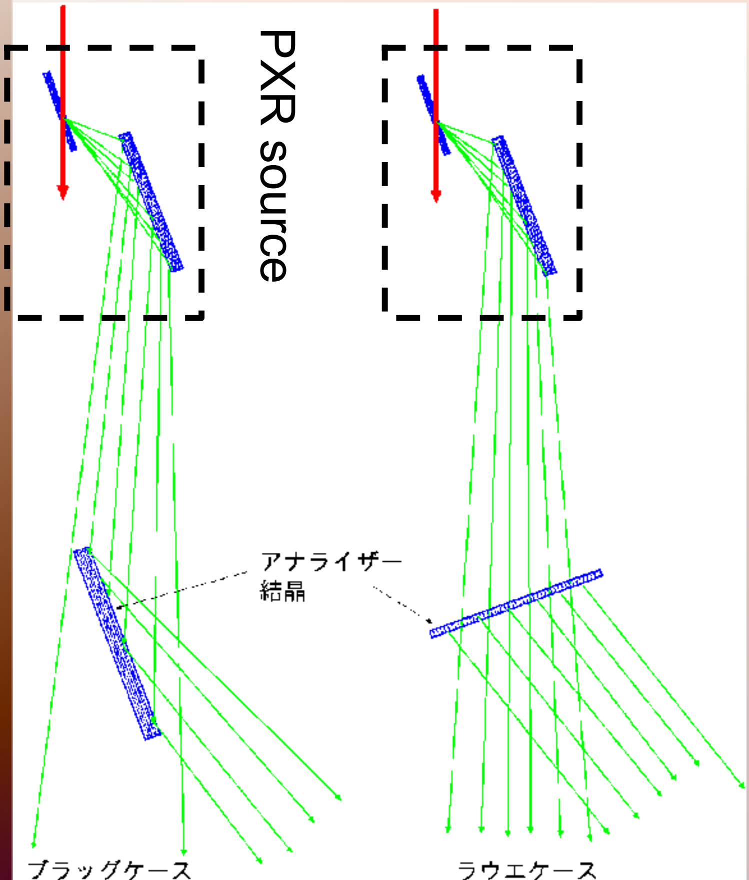
Spectral-KES using SR source



Y. Zhu, et al., Phys. Med. Biol. 59 (2014) 2485–2503.

Simultaneous KES method is developed at Canadian Light Source using bent crystal optics.
They call the method “spectral-KES method”.

(+, -, +) arrangement optics

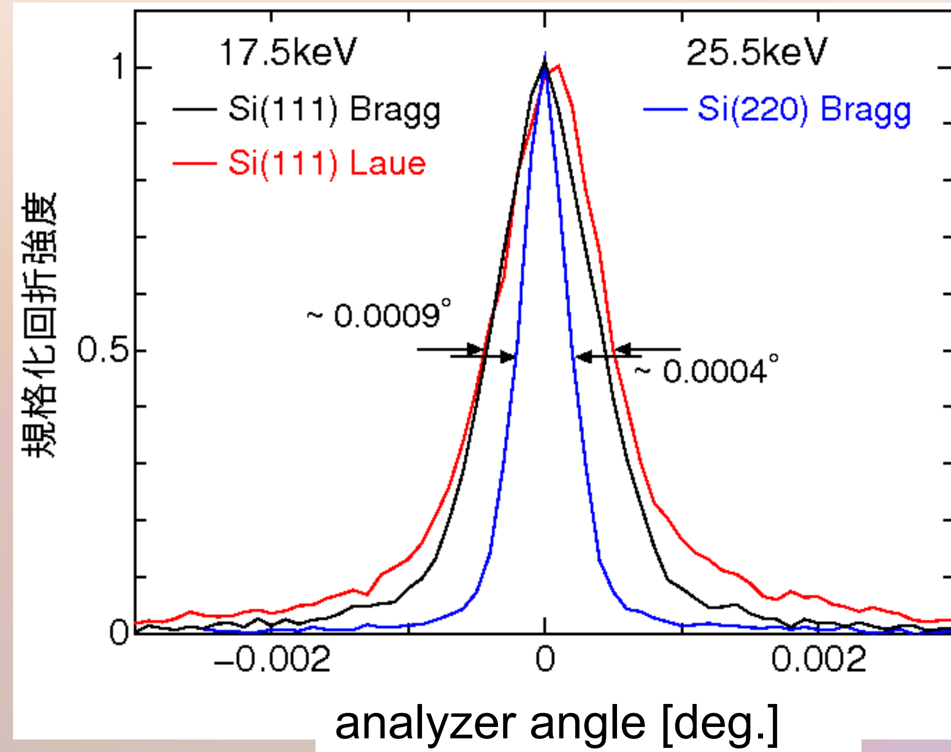


Bragg case Laue case

Bragg angle:

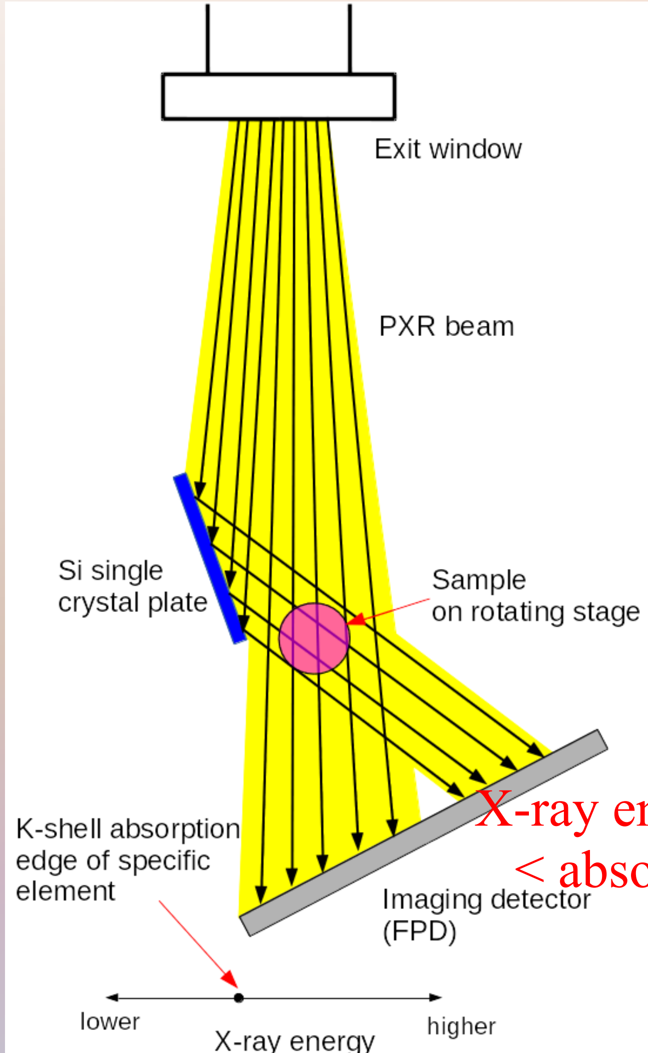
larger for longer wavelengths

smaller for shorter wavelengths



Using a 3rd analyzer crystal in the (+,-,+) arrangement, a PXR beam can be diffracted like a plane wave despite the cone-beam, because of the spatial chirp property.

Simultaneous KES-CT using PXR

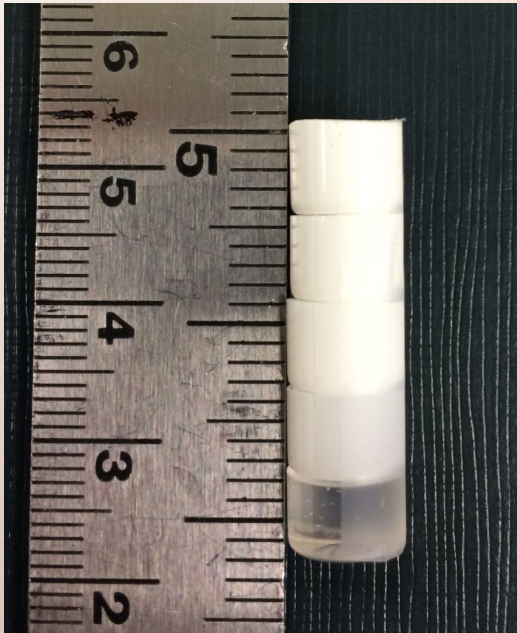


Using the spatial chirp property of PXR, crossing 2-color beams having slightly different energies can be formed using a plane crystal.

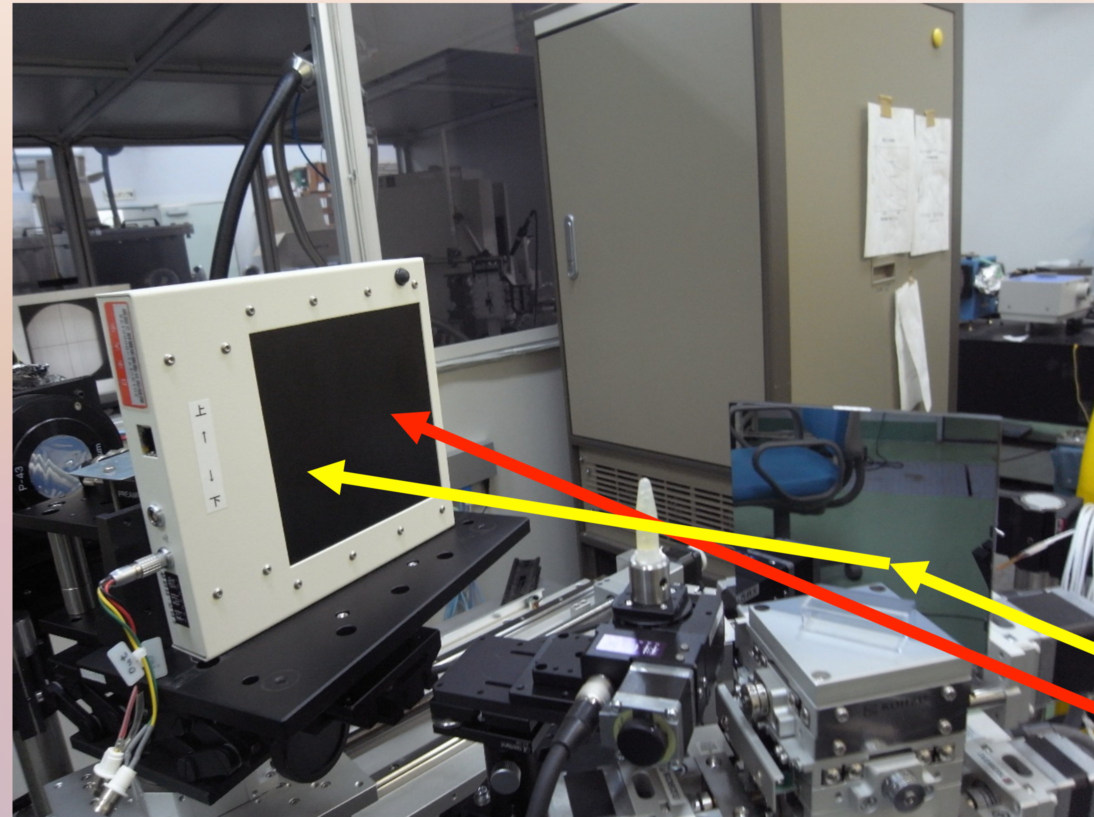
When the center energy of the PXR beam is adjusted to the K-edge energy of a specific element, the 2-color beams can be used for simultaneous KES imaging.

Furthermore, KES-CT is possible by rotating the sample.

Setup for simultaneous KES-CT

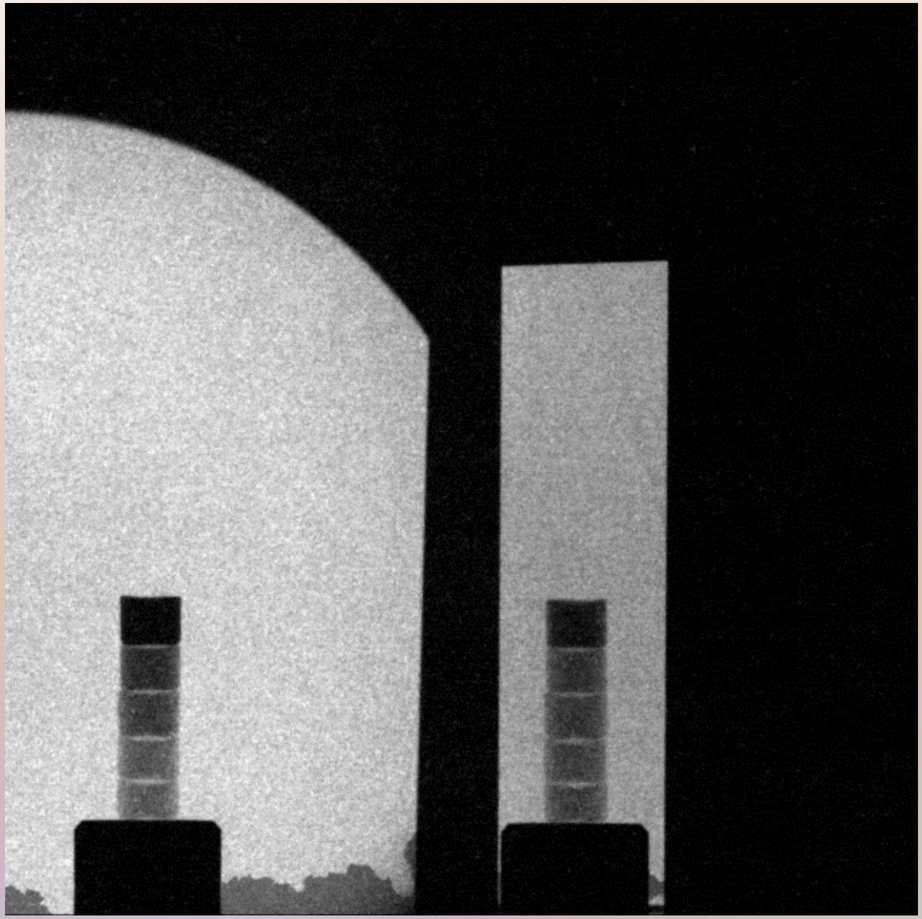


sample:
epoxy resin colored with $SrTiO_3$ (STO)
Sr concentration
5%, 1%, 0.5%, 0.1%, 0%
from the top



PXR source & DEI analyzer: Si(220)
PXR energy: 16.105 keV
FPD: Shad-o-Box 1280HS
(pixel size: 100μm)

Result of simultaneous KES-CT



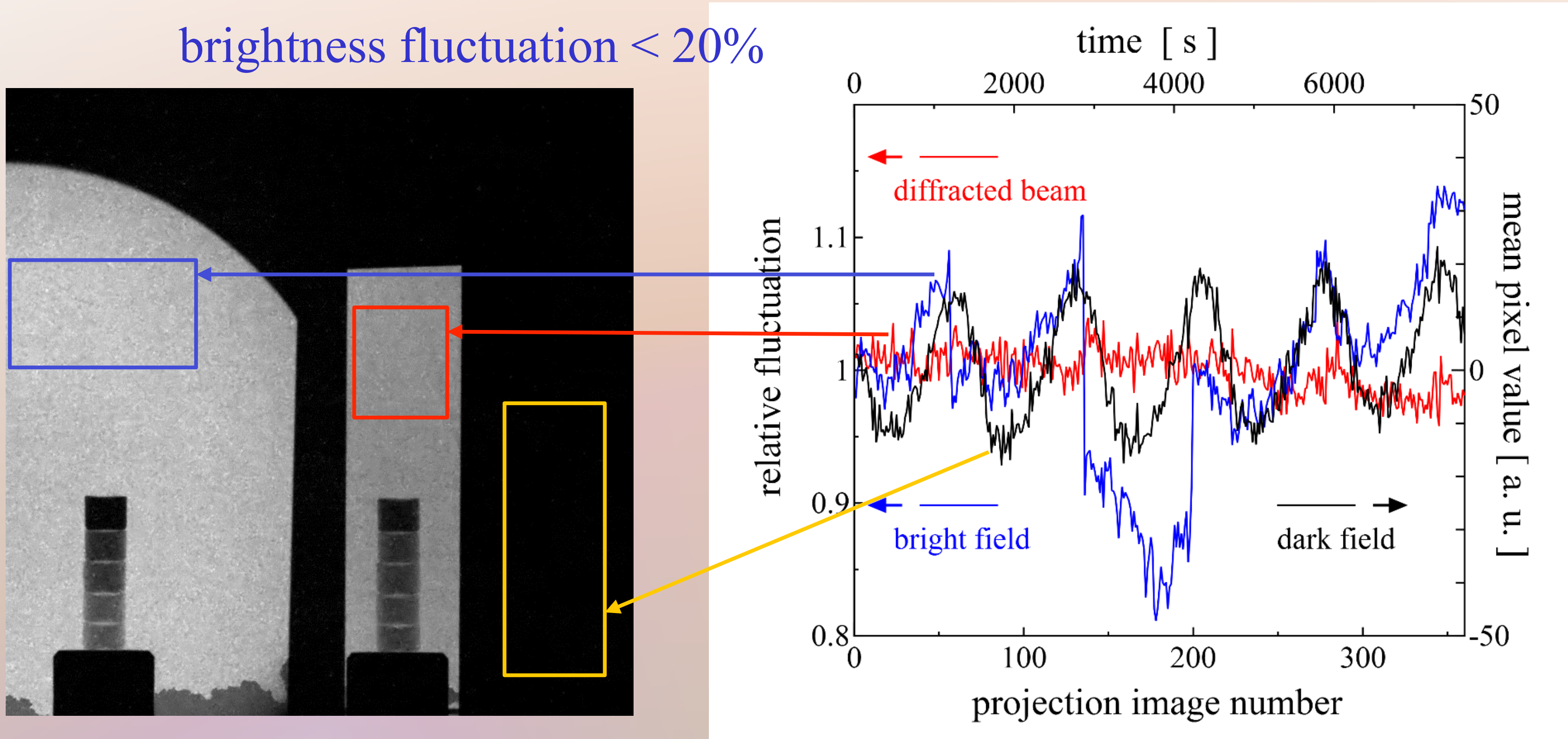
X-ray reflectivity of the Si(220) analyzer crystal ~ 75%

The quality of the diffracted-beam image is comparable to that of the direct-beam image.

projection images: 360 (angular step: 0.5 deg.)
each exposure time: 20s
total measurement time: 7632s ~ 2 hours (gross)

PXR fluctuation during KES-CT

brightness fluctuation < 20%



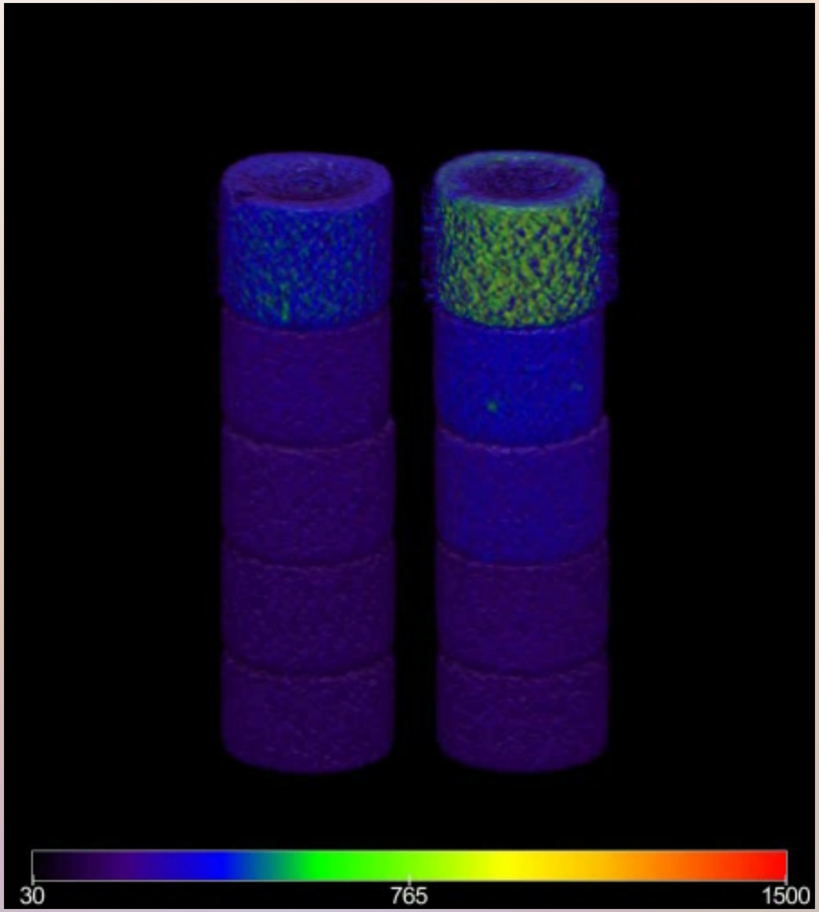
blue line: fluctuation of the bright field in the projection images

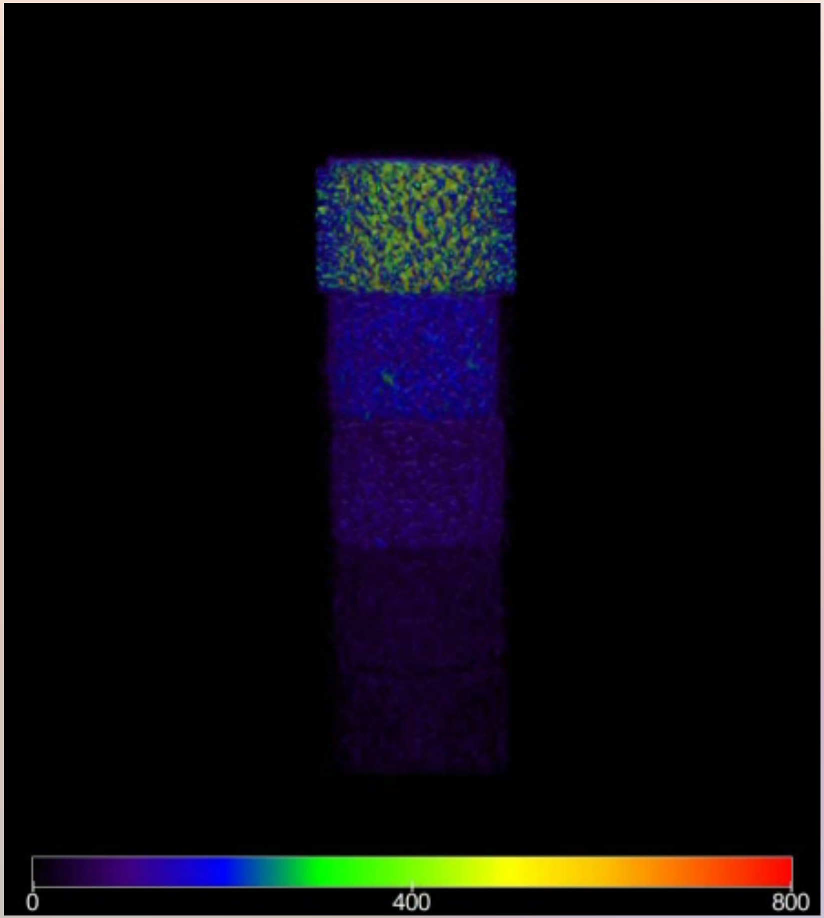
black line: fluctuation of the dark noise of the FPD

red line: diffracted beam stability after the brightness compensation

The measurement system including the PXR source is sufficiently stable during the KES-CT scanning.

3D reconstruction from KES-CT data





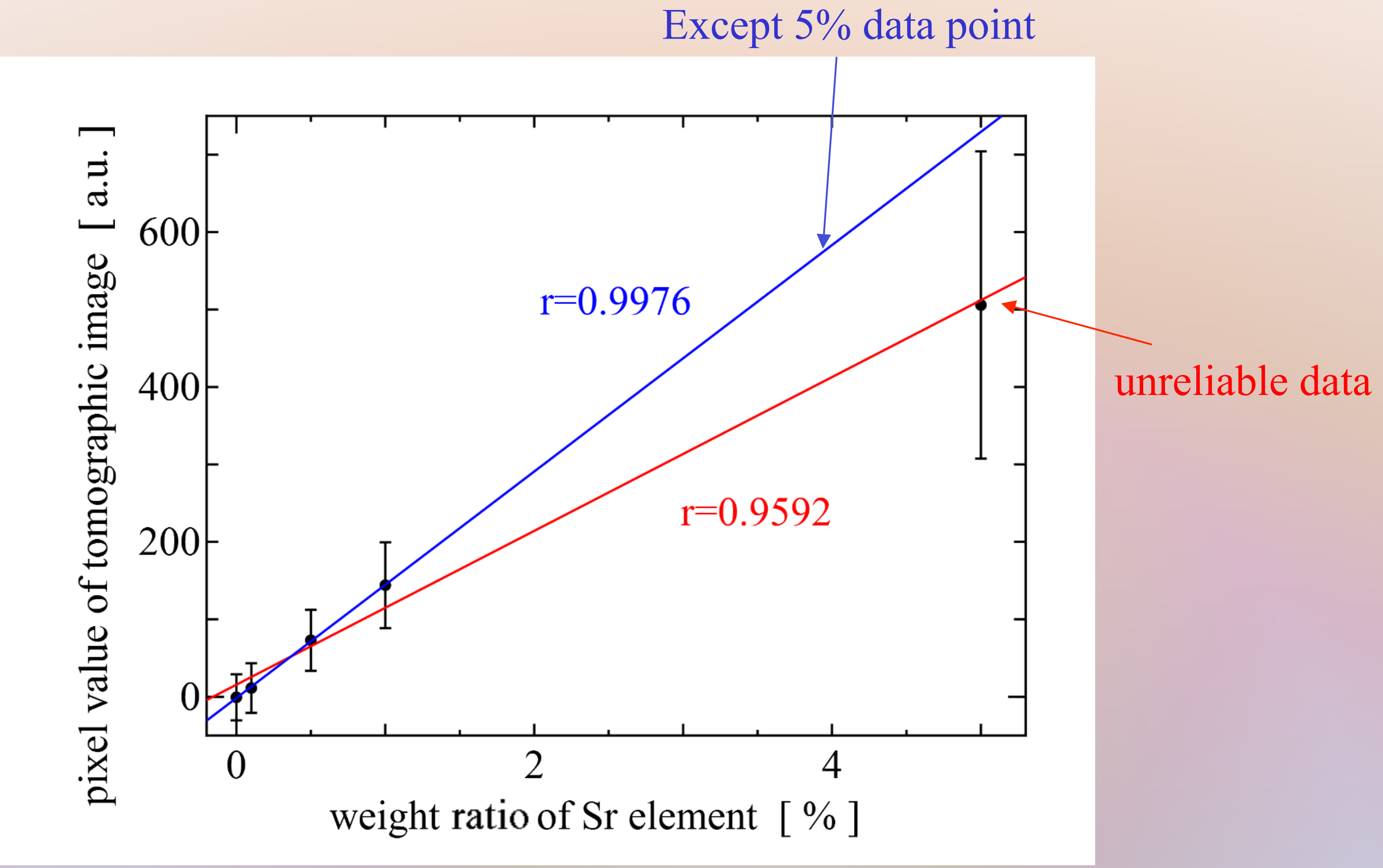
(left) lower energy (~ 16.0 keV)

(right) higher energy (~ 16.2 keV)

3D Sr distribution as a subtraction between tomographic images

Both image contrasts are normalized at the region of epoxy resin

Linearity to Sr concentration



The pixel values (brightness) of the KES tomographic image linearly depends on the Sr concentration.

Summary

- LEBRA-PXR source has a long-term stability sufficient to perform CT experiments.
- Element detection based on KES method is one of the advanced applications of PXR.
- Simultaneous KES-CT using PXR is very unique compared to similar applications of SR sources.
- Simultaneous KES-CT has a significant sensitivity to 0.5% concentration of Sr in the sample at least.
- Although the absolute sensitivity to the element concentration is far inferior to that of X-ray fluorescence analysis, simultaneous KES-CT can treat samples having cm-scale thickness.

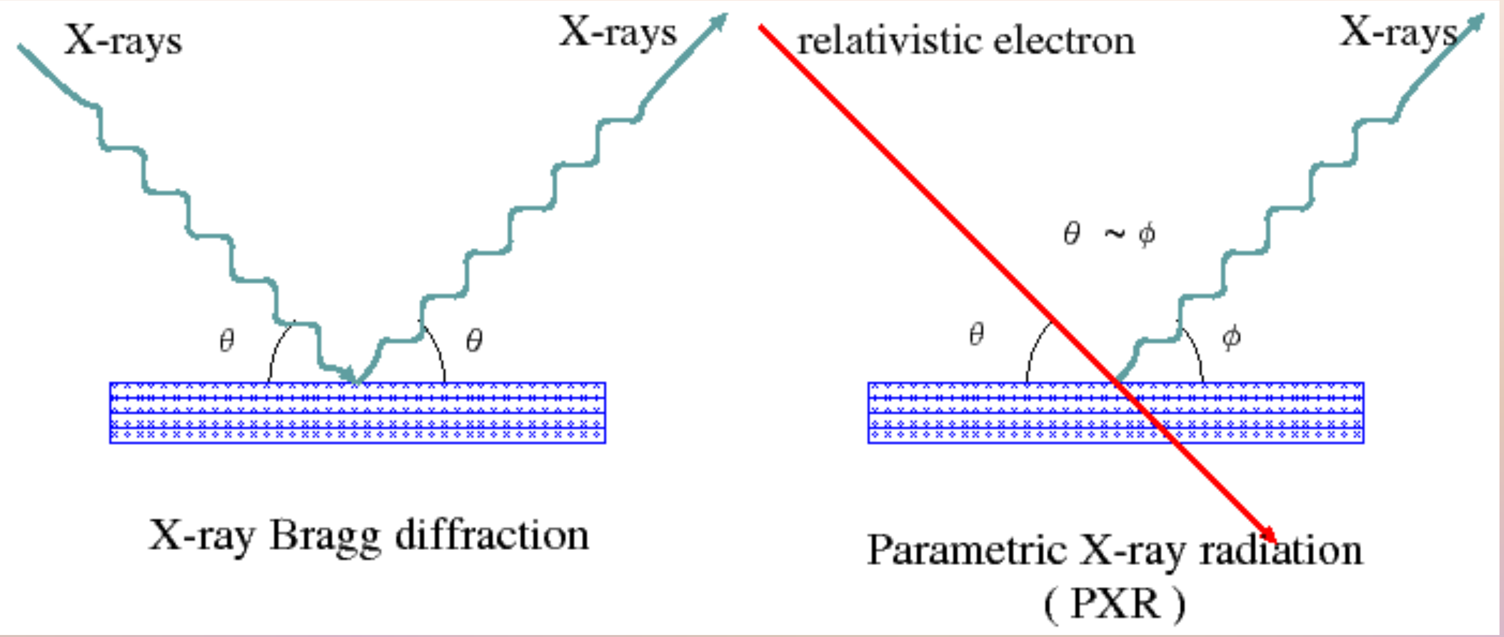
Acknowledgements

MEXT.KAKENHI (25286087&16K05008)

Thank you for your kind attention !!

Appendix

What is PXR?

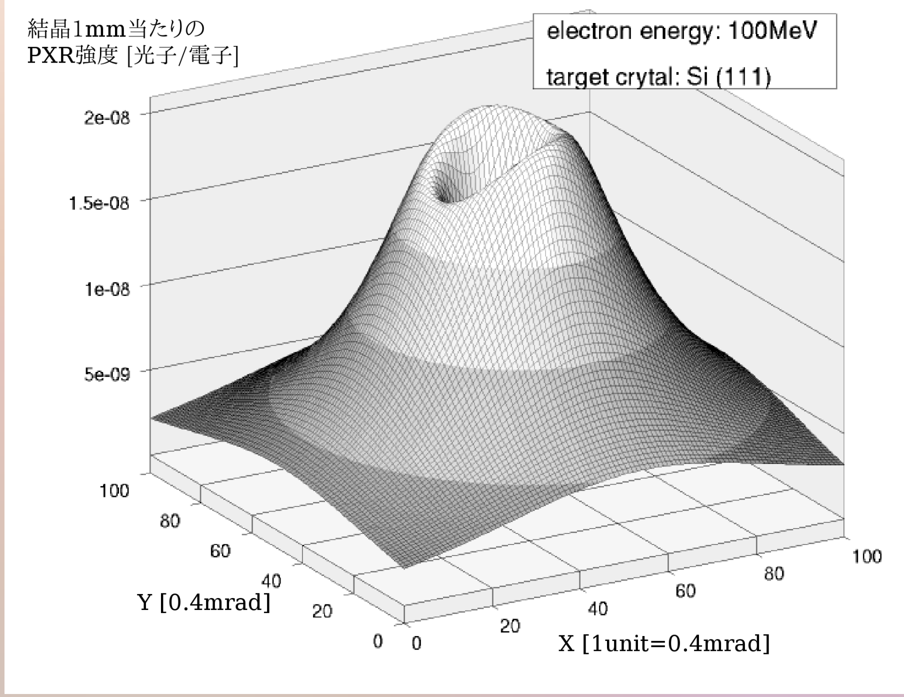


PXR: Parametric X-ray Radiation

PXR is apparently similar to X-ray Bragg diffraction.
The phenomenon corresponds to Bragg diffraction for virtual photons accompanying the incident electron.
The X-ray energy is tunable depending on the Bragg angle.

PXRの空間分布

PXRの空間・角度分布
- 中心に放射が無い
- 円錐状の広がり（1/γに依存）



$$\frac{\mathrm{d}N}{\mathrm{d}\Omega} = \sum_{|\boldsymbol{g}|\neq 0} \frac{e^2 \omega L |\chi(\omega)|^2}{2\pi\hbar\varepsilon^3 v(c - \boldsymbol{v}\cdot\boldsymbol{\Omega})}$$

$$\times \frac{\left|\frac{\omega}{c}\boldsymbol{\Omega} \times \left(\frac{\omega}{c^2}\boldsymbol{v} + \boldsymbol{g}\right)\right|^2}{\left\{\left|\frac{\omega}{c}\boldsymbol{\Omega}_\perp - \boldsymbol{g}_\perp\right|^2 - \left(\frac{\omega}{v}\right)^2 \left[\gamma^{-2} + \left(\frac{v}{c}\right)^2 (1-\varepsilon)\right]\right\}^2}$$

total cross section: 10^{-5} ～ 10^{-4} photon/electron @ Si(111) 1mmt

Characteristics of LEBRA-PXR source

- X-ray energy is controlled by the Bragg angle (almost independent of the electron energy)
- Wide and continuous tunability

  Si(111): 5 - 20keV, Si(220): 6.5 - 34keV
- Energy dispersion (spatial chirp)

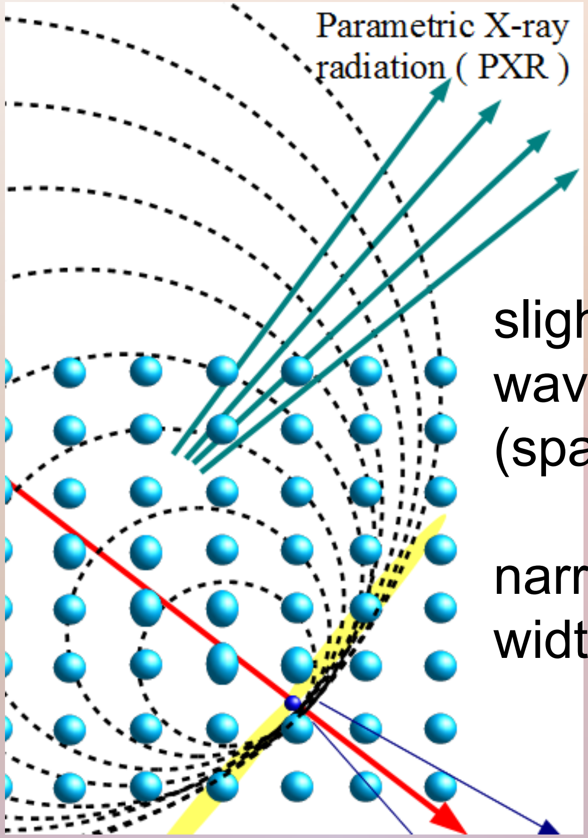
  local spectral width ~ several eV
- Spatial coherence

  wave front disturbance ~ 1 μrad
- Stability

  long-term (several hours) experiments
- Pulsed source

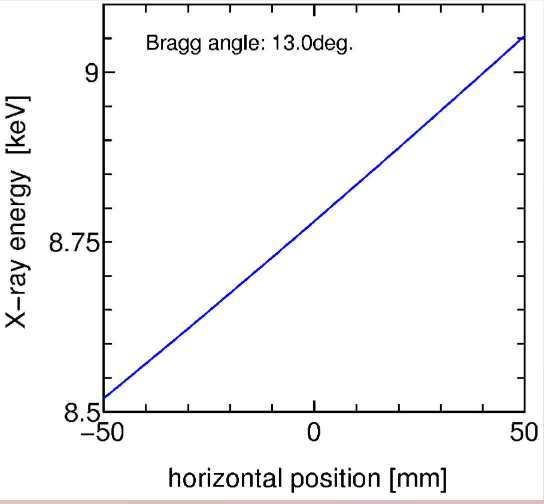
  macropulse: 5μs, michropulse: ~several ps

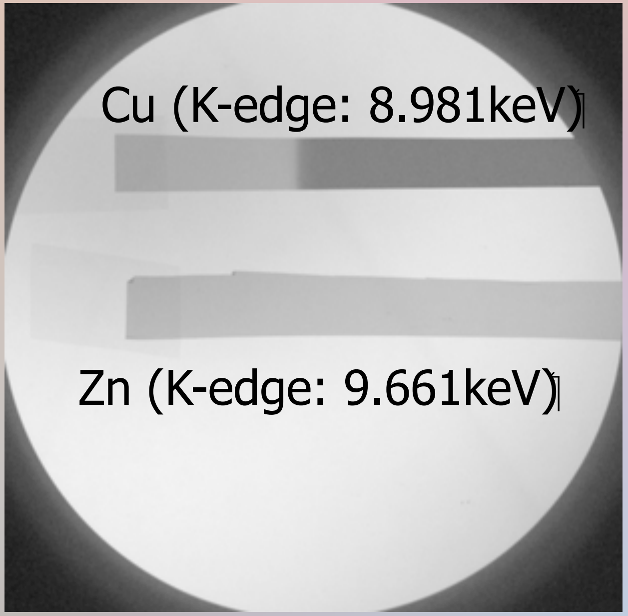
Spatial chirp of PXR beam



slight & continuous wavelength-shift (spatial chirp)

narrow local spectral width (several eV)

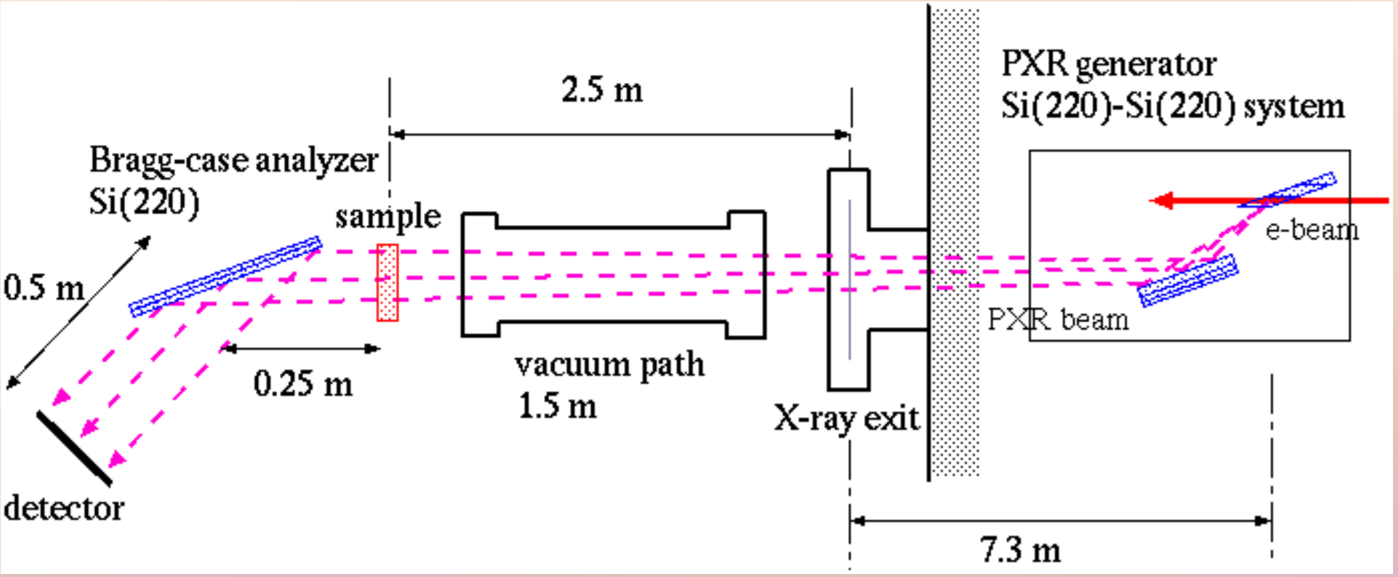


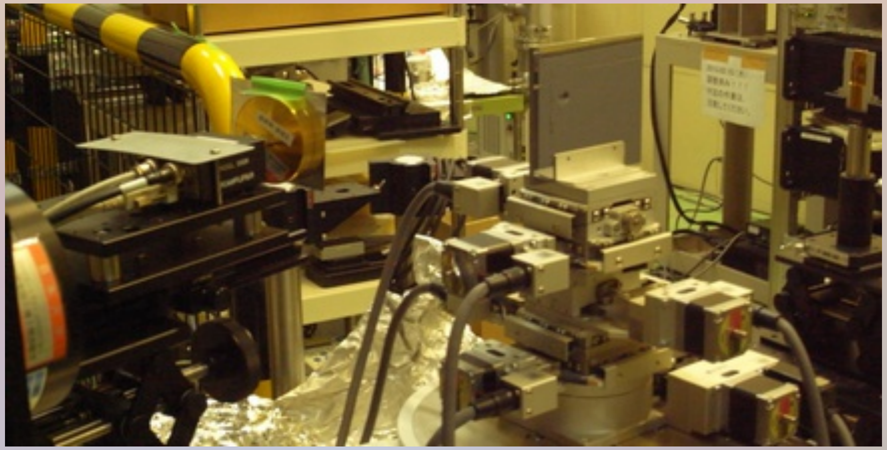


Wave front of PXR is different from both plane wave and spherical wave.

Setup of DEI experiments

top view

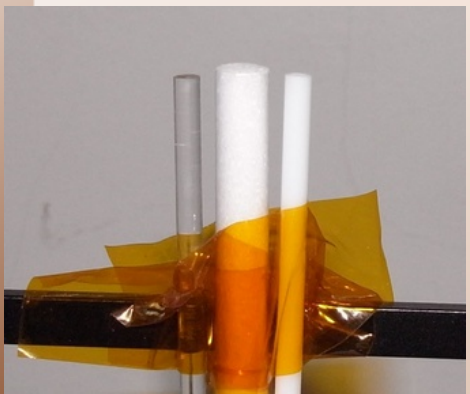




Due to the extension of cone-beam, a wide irradiation field can be obtained without asymmetric analyzer.

The distance between the PXR source and the sample is shorter than 10m.

Image contrast



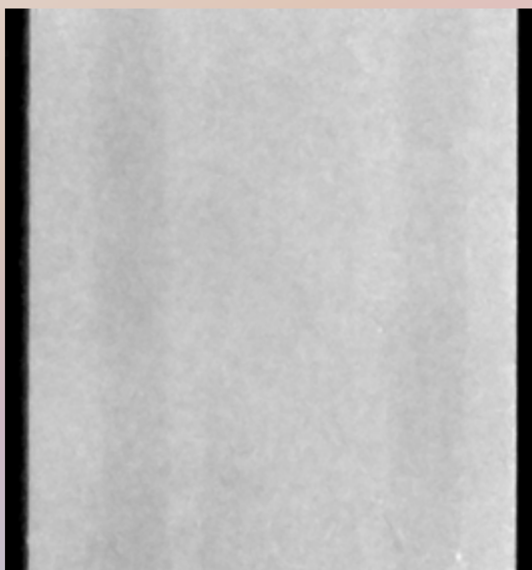
sample:

acrylic rod, styrene-foam rod, polystyrene rod

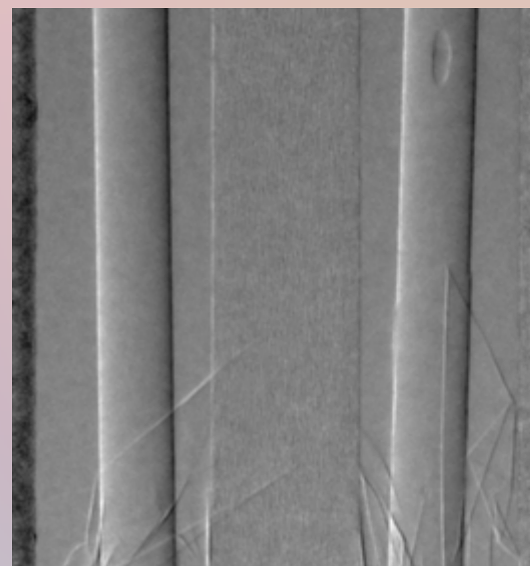
PXR energy: 25.5 keV

Phase contrast is much stronger than absorption contrast.

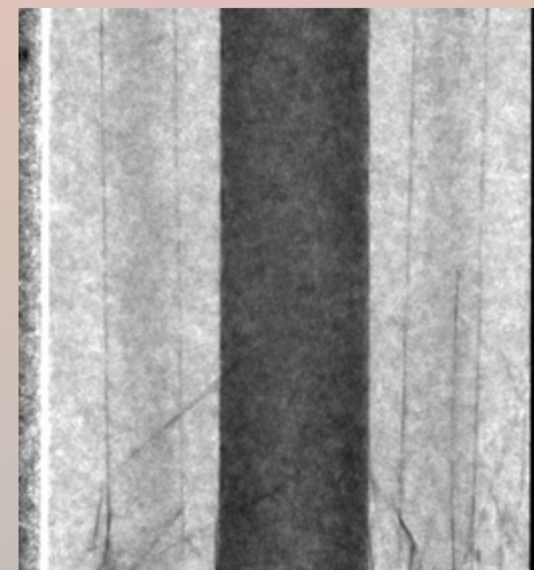
SAXS imaging is sensitive to micro structures of sample material smaller than 1-micron.



absorption



refraction
（phase gradient map）



small-angle scattering
（SAXS contrast）

Application of LEBRA-PXR source

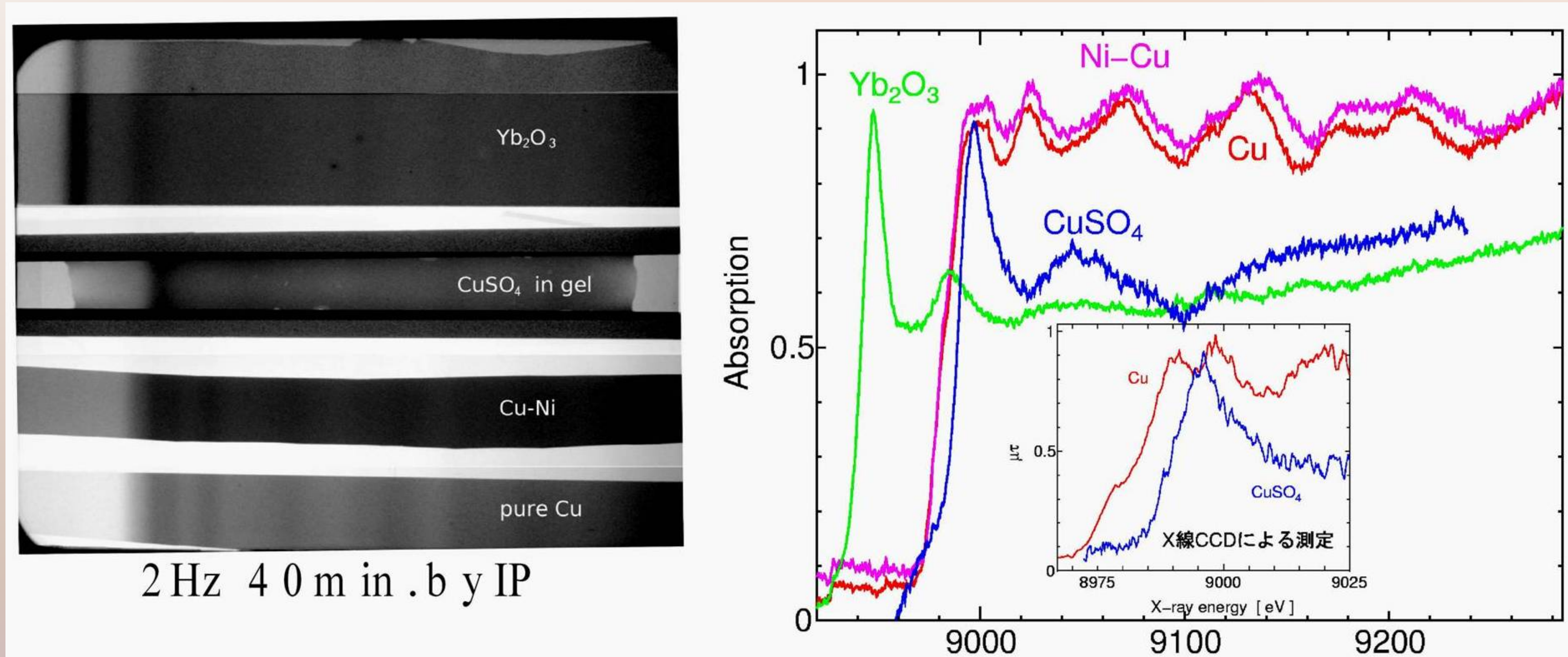
Imaging

- **Conventional imaging**
  - monochromaticity & tunability
  - propagation-based phase contrast effect
- **Computed tomography (CT)**
  - 3D analysis of element distribution
- **Diffraction-enhanced imaging**
  - refraction (phase-gradient) contrast
  - contrast based on small-angle scattering (SAXS)

X-ray absorption fine structure (XAFS)

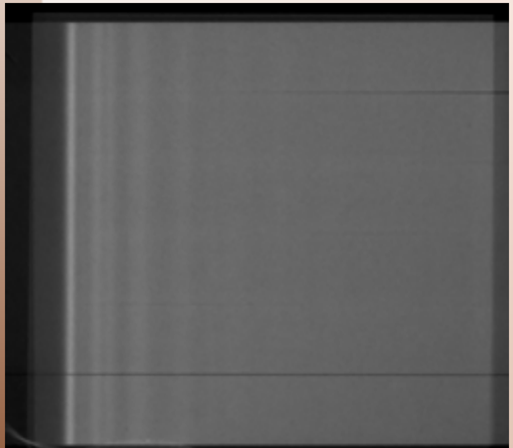
energy dispersive type XAFS analysis
(XANES & EXAFS)

Dispersive-type XAFS (X-ray Absorption Fine Structure) analysis using PXR



Application of the energy dispersion (spatial chirp) of PXR. Absorption spectra of several samples can be simultaneously obtained by this method.

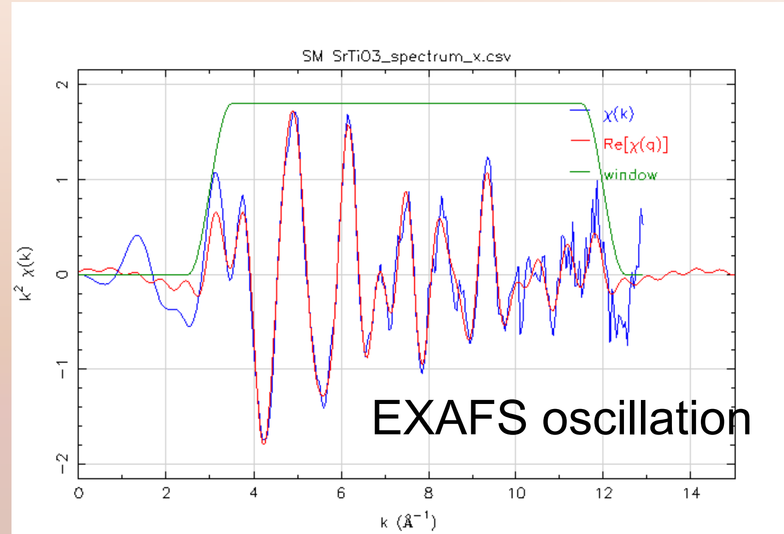
Typical result of DXAFS experiment

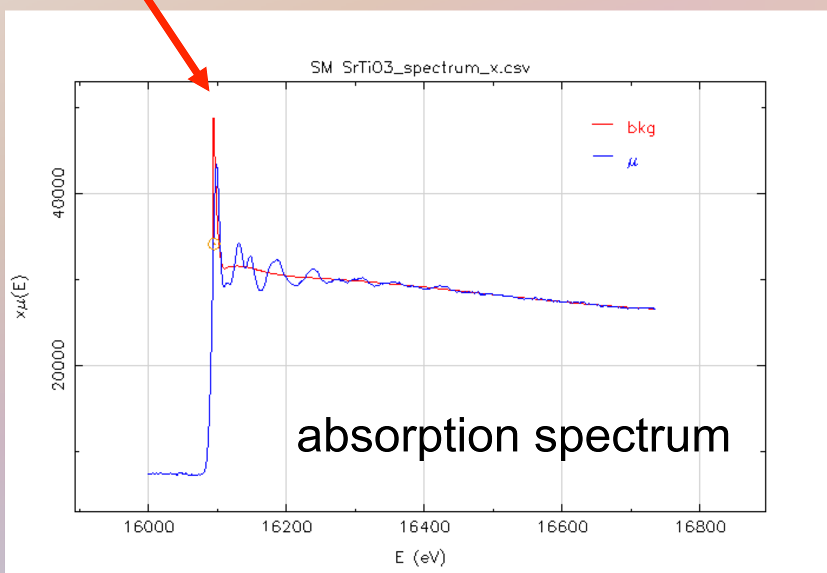


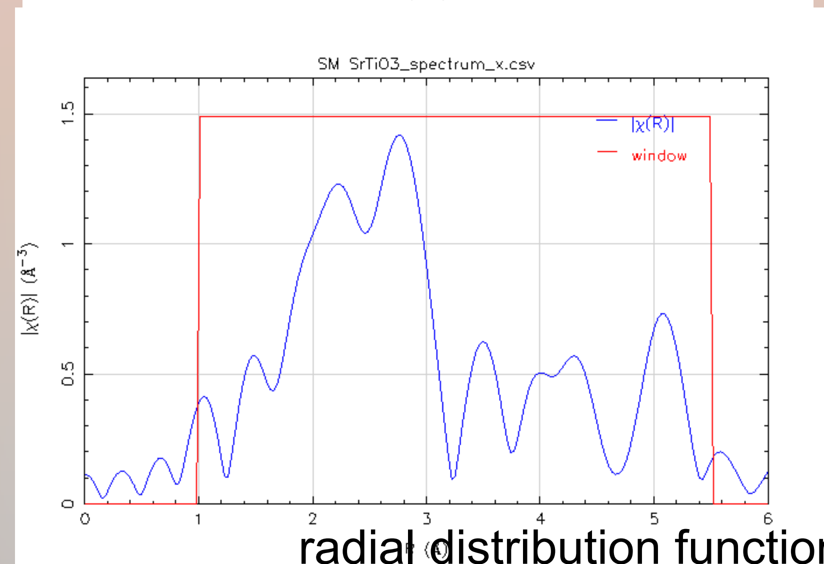
sample
$SrTiO_3$ (white pigments)

measurement time
30min

detector: Imaging plate



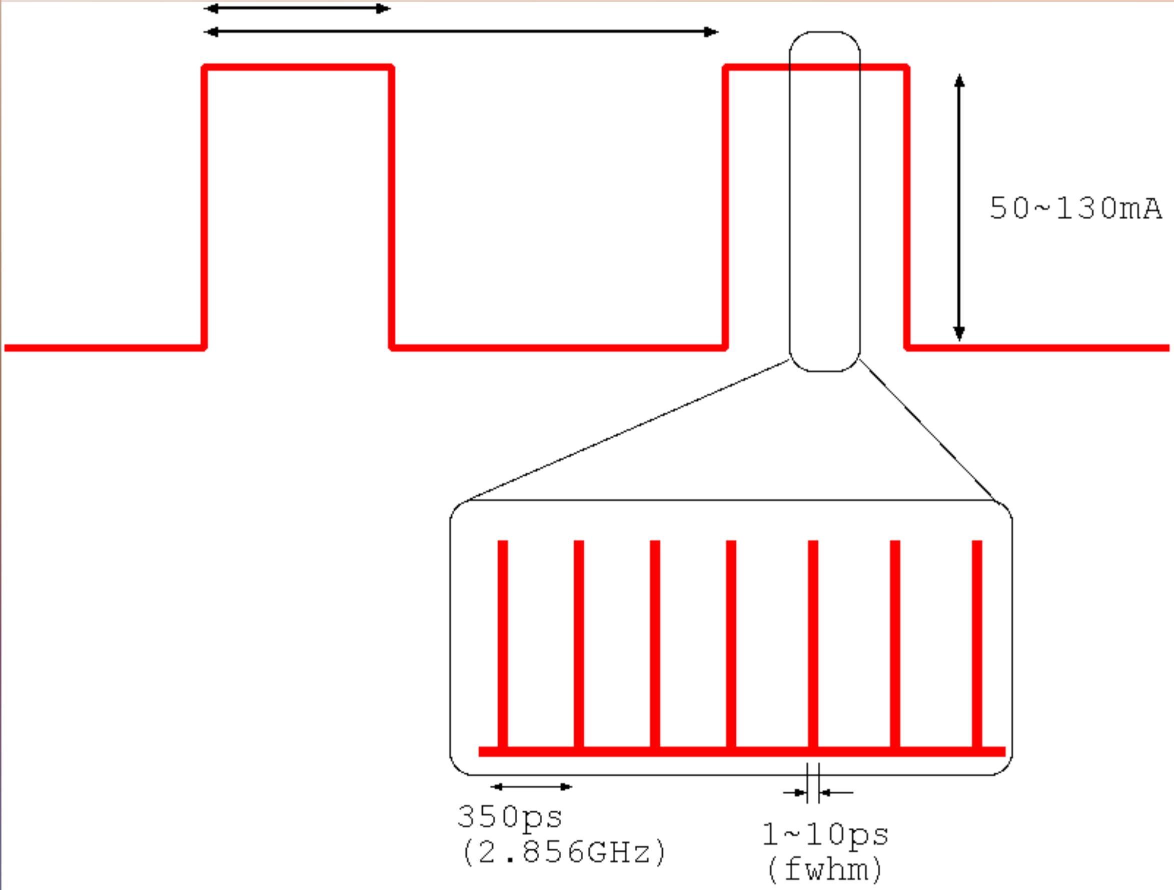


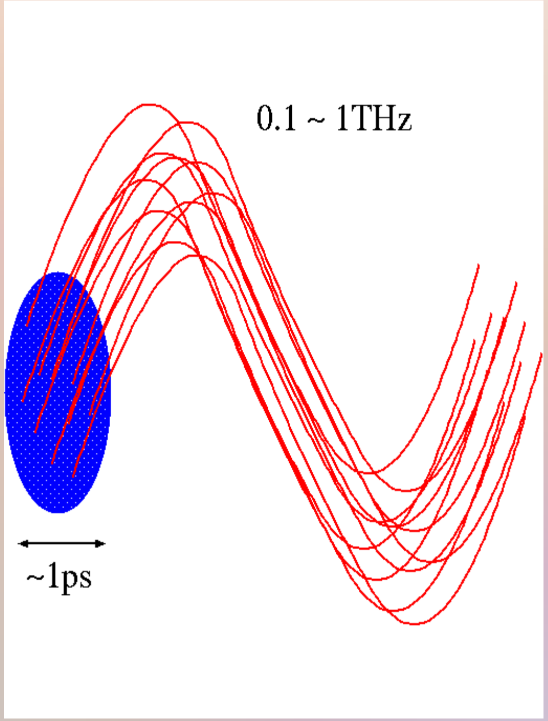


Time- resolved XAFS measurement can be expected using the linac-based source.

Pulse structure of LEBRA Linac

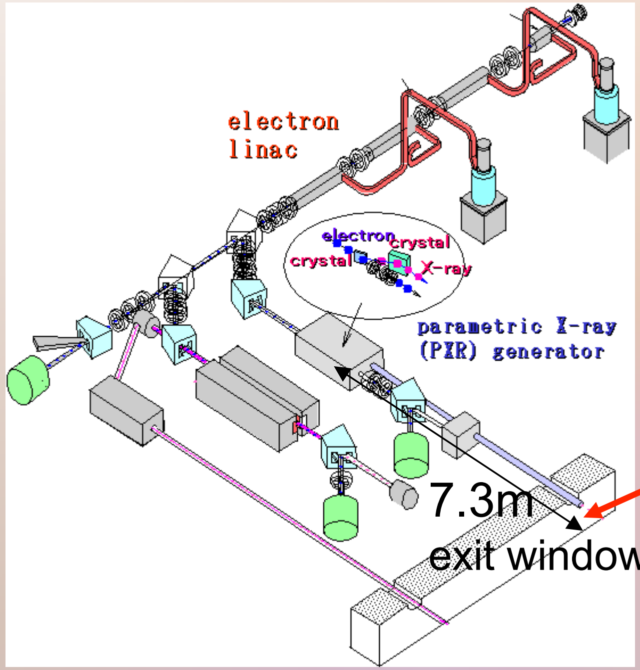
FEL: 20μs duration 2pps
PXR: 5μs duration 5pps



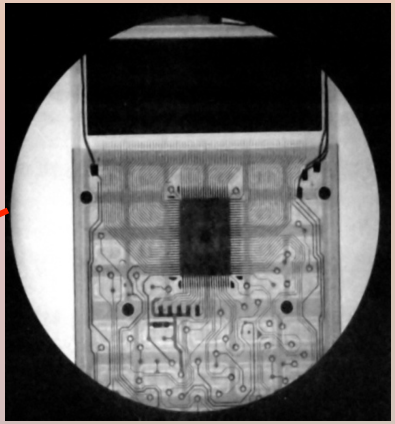


coherent radiation in THz region can be expected!

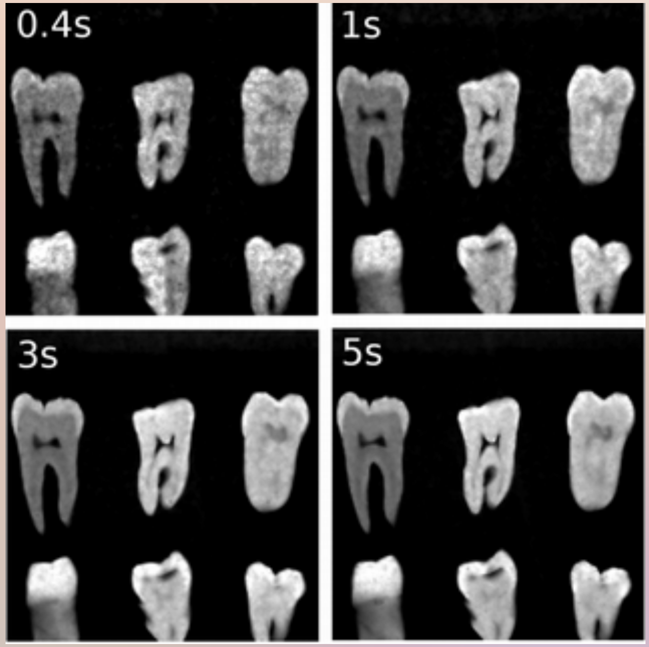
X-ray imaging (absorption contrast)



diameter: 100mm

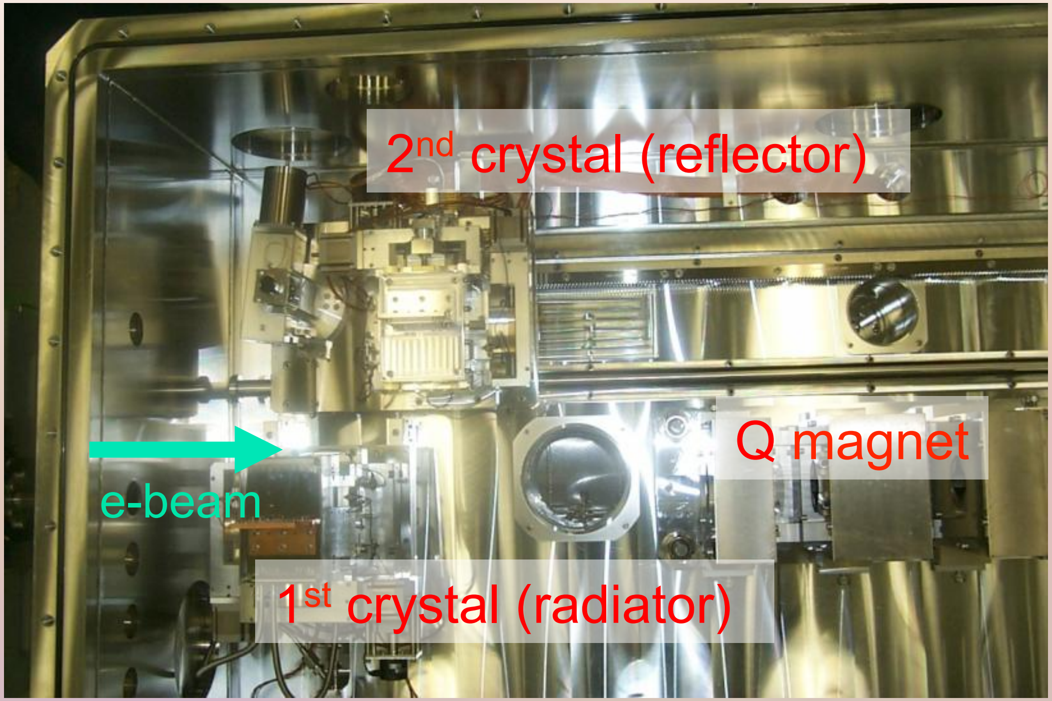


PXR radiator: Si(111)
PXR energy: 17.5keV (center)
e-beam: 2.6uA (average)
sample: calculator
detector: imaging plate (IP)
exposure: 10s



PXR radiator: Si(111)
PXR energy: 17.5keV (center)
e-beam: 2.6uA (average)
sample: human tooth
detector: flat panel detector (FPD)

Radiator of the PXR source



PXR radiator: 0.2mm thick Si perfect crystal wafer

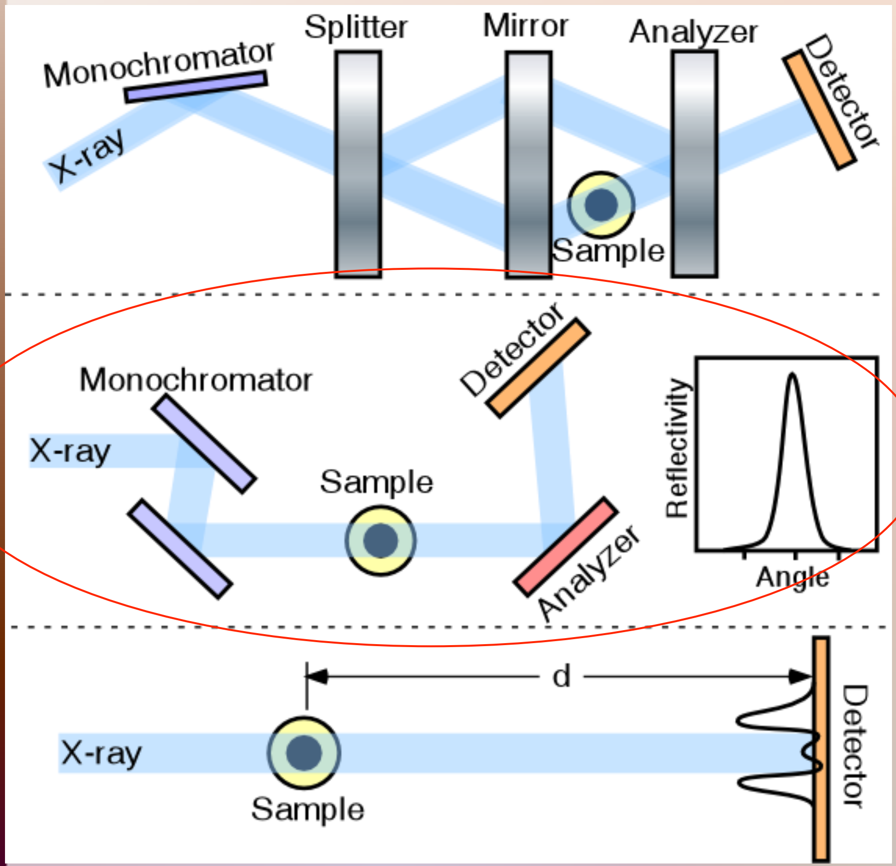
reflector: 5mm thick Si perfect crystal plate

crystal plane:

Si(111) for 4 – 20keV

Si(220) for 6.5 – 34keV

Phase-contrast X-ray imaging



R. Fitzgerald: Phys. Today 53 (2000) 23

interferometer-based technique

Si perfect crystal interferometer

Talbot interferometer

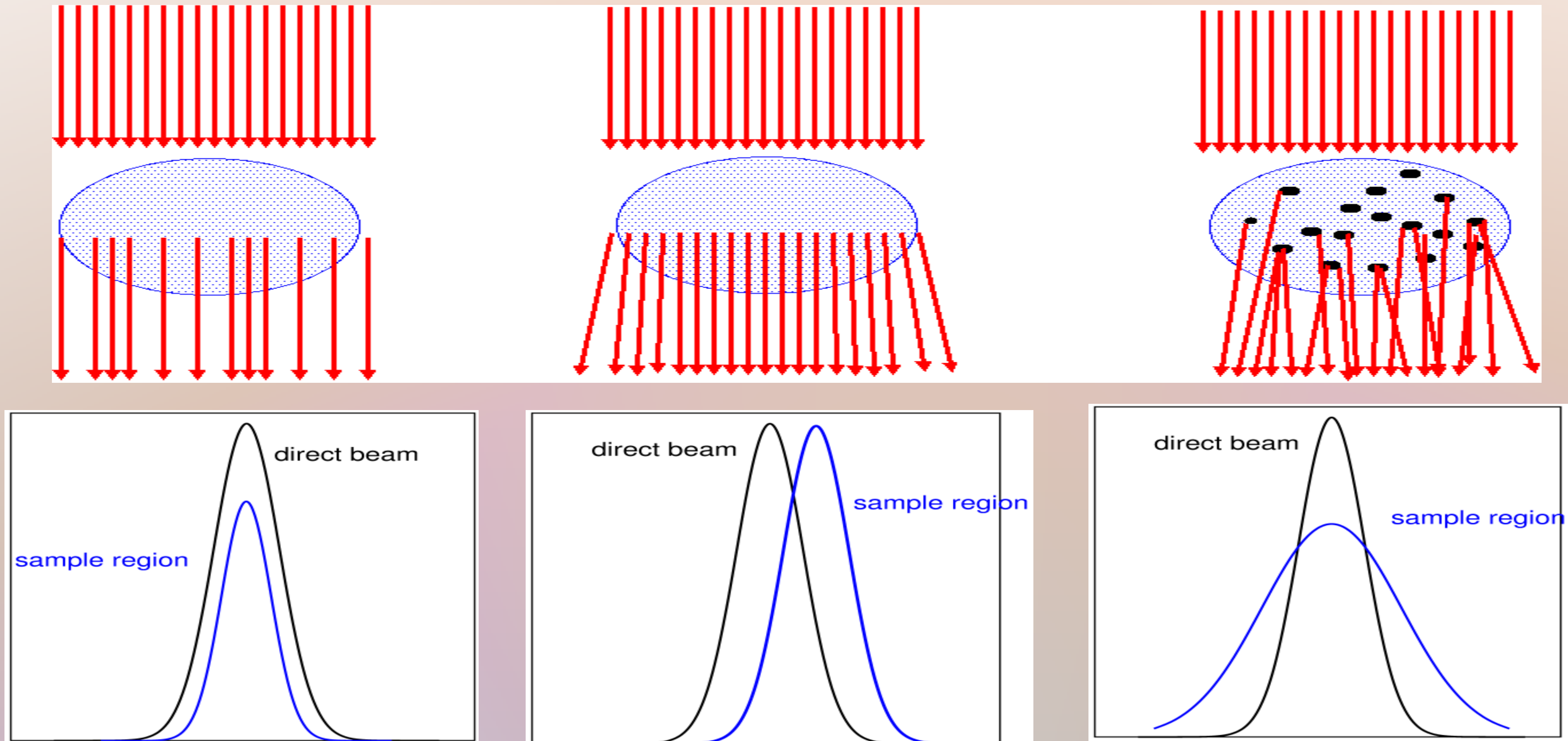
analyzer-based technique

DEI: diffraction-enhanced imaging

propagation-based technique

The narrow diffraction width means that DEI is possible using PXR.

Interaction between X-rays and material

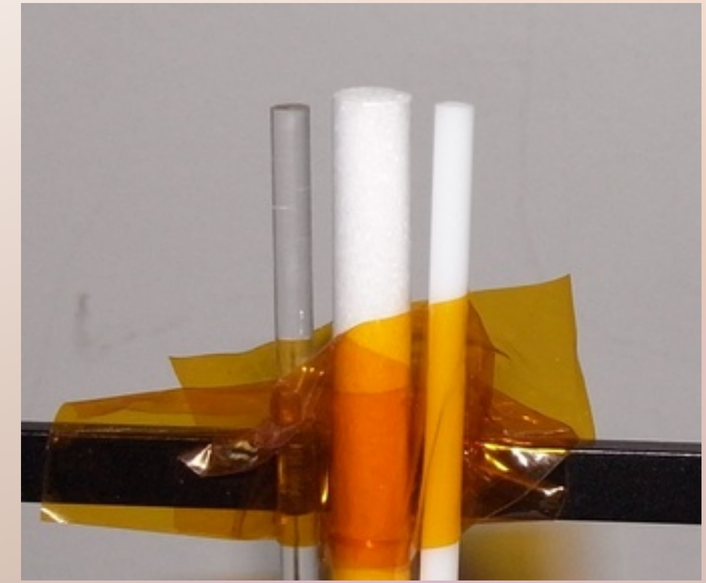


absorption (amplitude attenuation): reduction of the peak area

refraction (phase shift): shift of the center position

small-angle scattering (SAXS): reduction of the peak height (or peak broadening)

Experiment for demonstration



Sample:
acrylic rod (3mm in dia.)
density: 1.17 g/cm^3

styrene-foam rod (6mm in dia.)
density: 0.16 g/cm^3

polystyrene rod (3mm in dia.)
density: 0.986 g/cm^3

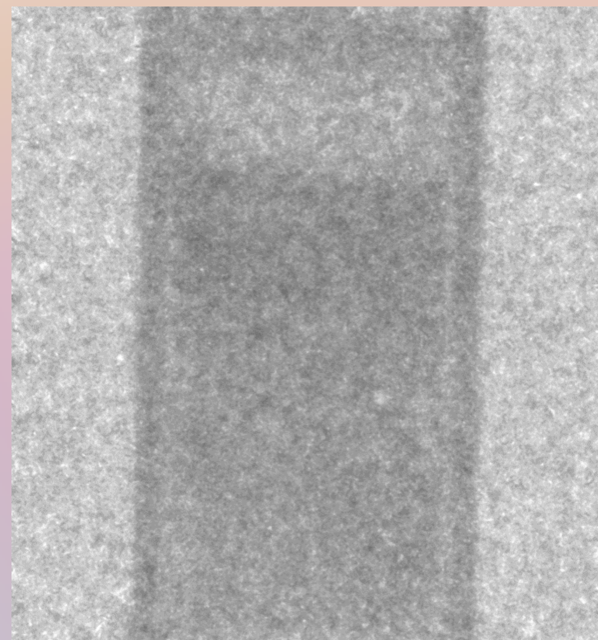
PXR source:
radiator-reflector: Si(220)-Si(220)
electron energy: 100MeV
average beam current: 3μA
PXR energy: 25.5keV
photon rate: ~ 10^6 /s /100mm in dia.

DEI measurement setup:
analyzer: Si(220)
160mm x 35mm x 5mm
angular step: 0.4625 μrad
image sensor: X-ray CCD
(Q.E. @25.5keV ~ 10%)
pixel size: 24μm x 24μm

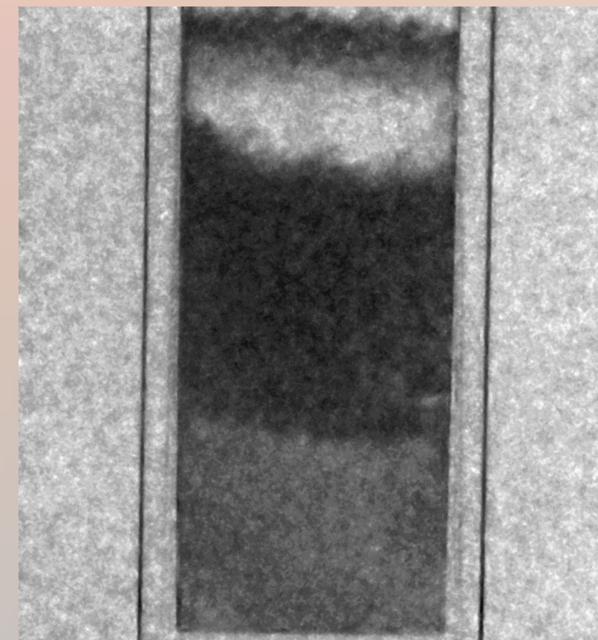
SAXS contrast image

experimental condition:
PXR radiator: Si(220)
PXR energy: 23keV
sample: silica standard particles（φ1μm, φ0.2μm）
X-ray camera: I.I. CCD （QE ≲ 10%）

silica powder
upper layer:
0.2μm in dia.
lower layer:
1.0μm in dia.



absorption contrast image



SAXS contrast image

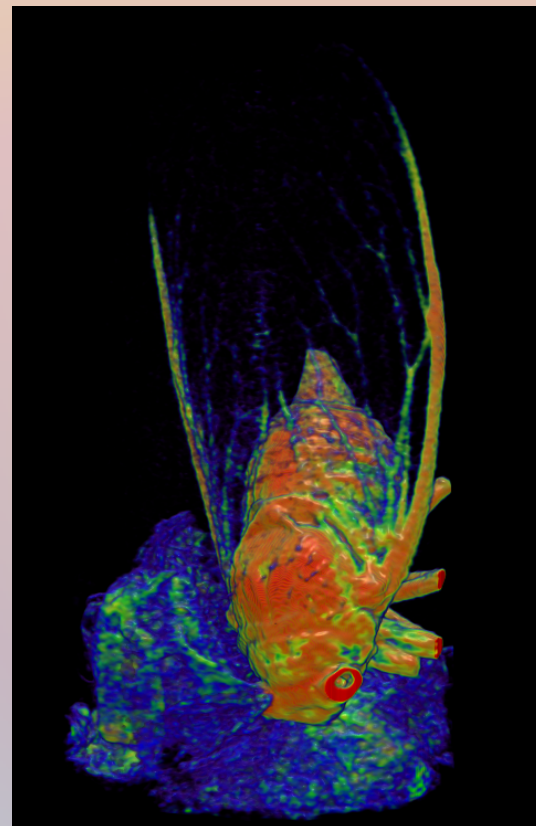
CT image using PXR

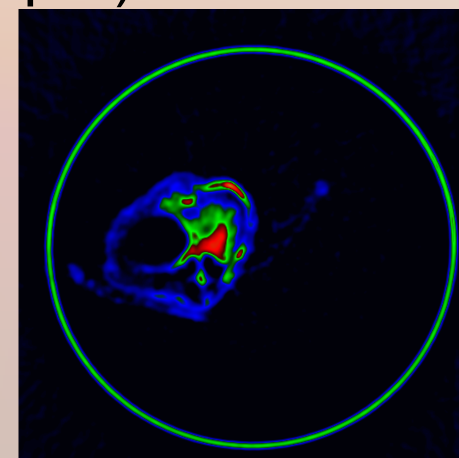
PXR source: Si(220)　　PXR energy: 15keV

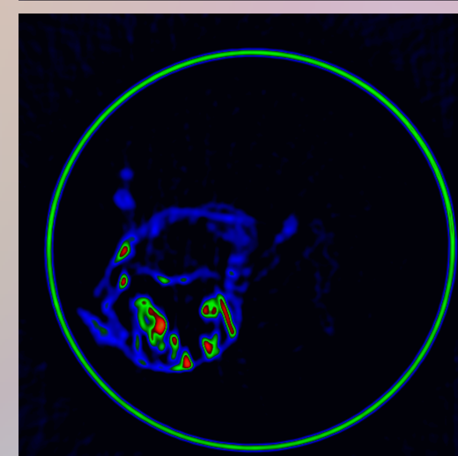
sample: cicada (insect)

measurement time: 20s x 600 (3 hours 20min)

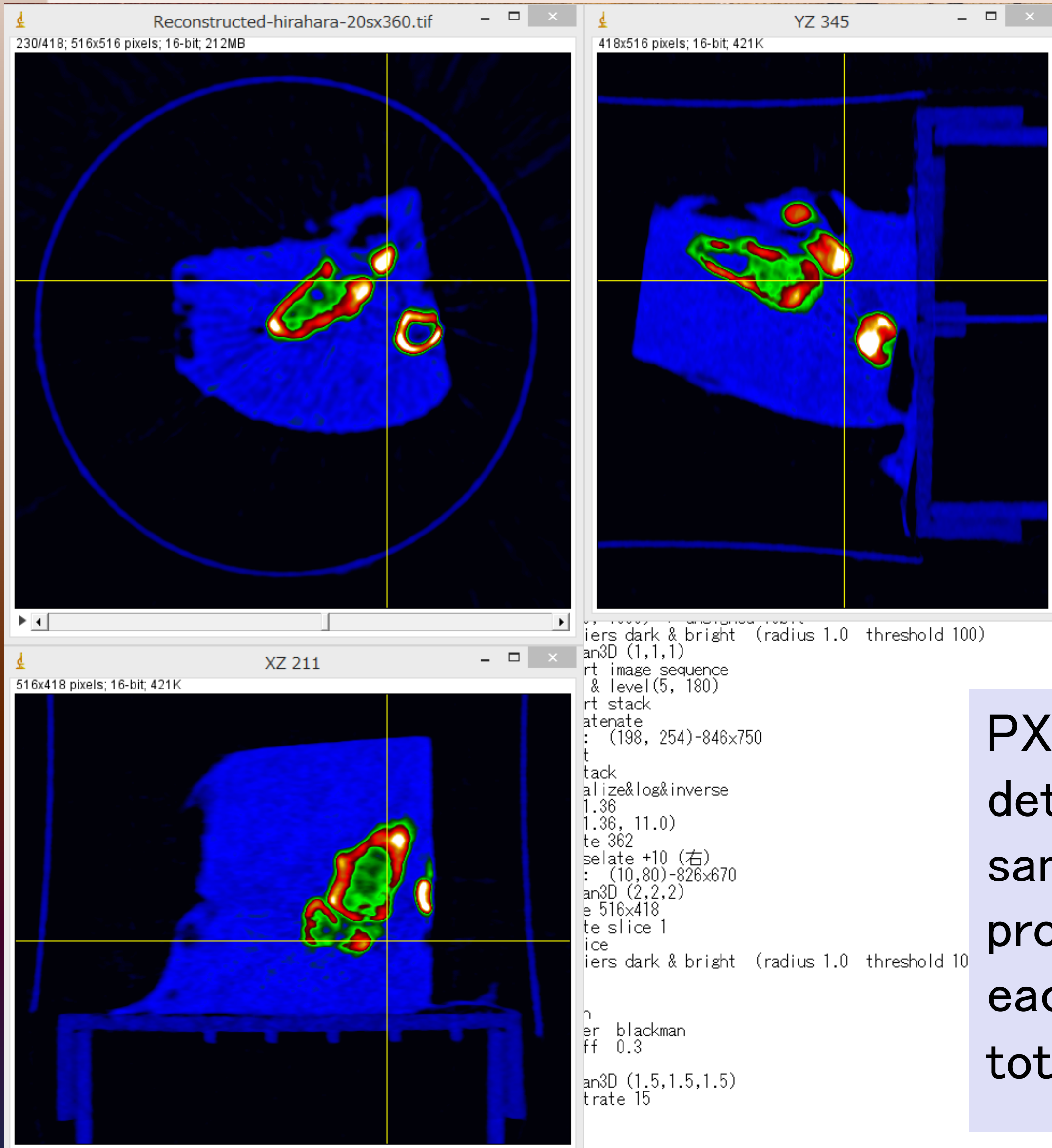
FPD: Shad-o-Box 1280HS (pixel size: 100μm)

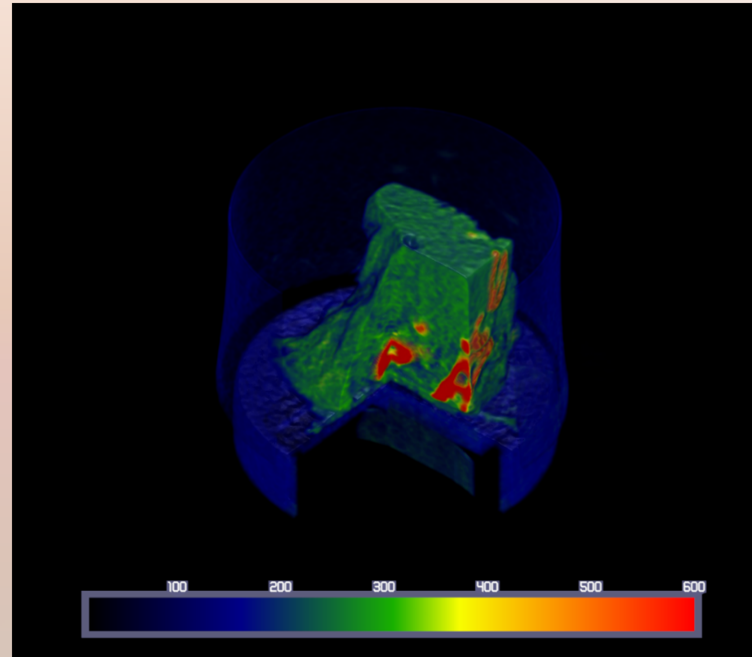






CT image of biological sample





PXR: 25keV
detector: Shad-o-Box 1280HS
sample: tumor of dog forefoot
projection images: 360
each exposure time: 20s
total measurement time: 2 hours

Element detection (Sr)

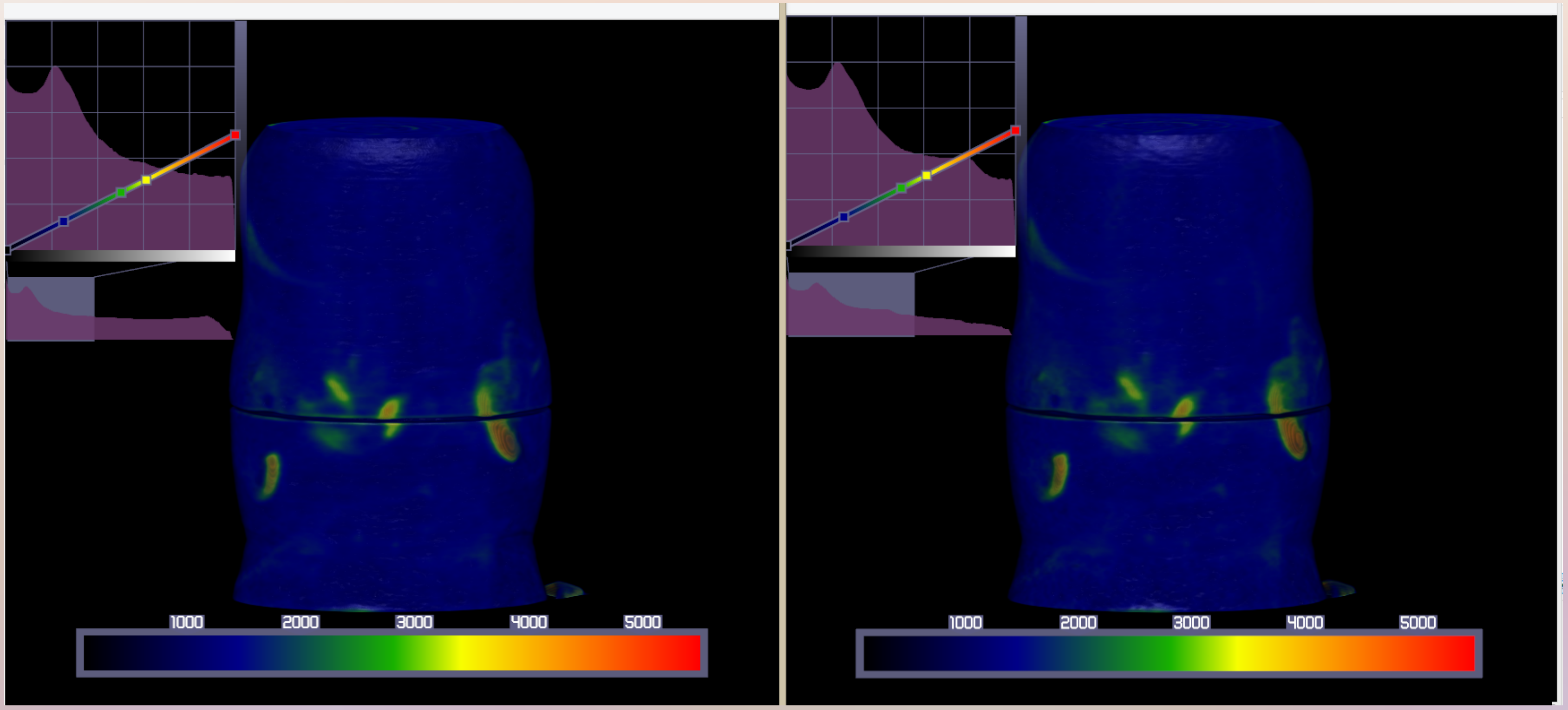
Sample:
matryoshka doll
(3 layers)

material: wood
diameter: 34mm
height: 55mm

polyethylene pellets containing $SrTiO_3$ (STO) (white pigment)

density: 1.0 g/cm^3
Sr: 4.8 wt %

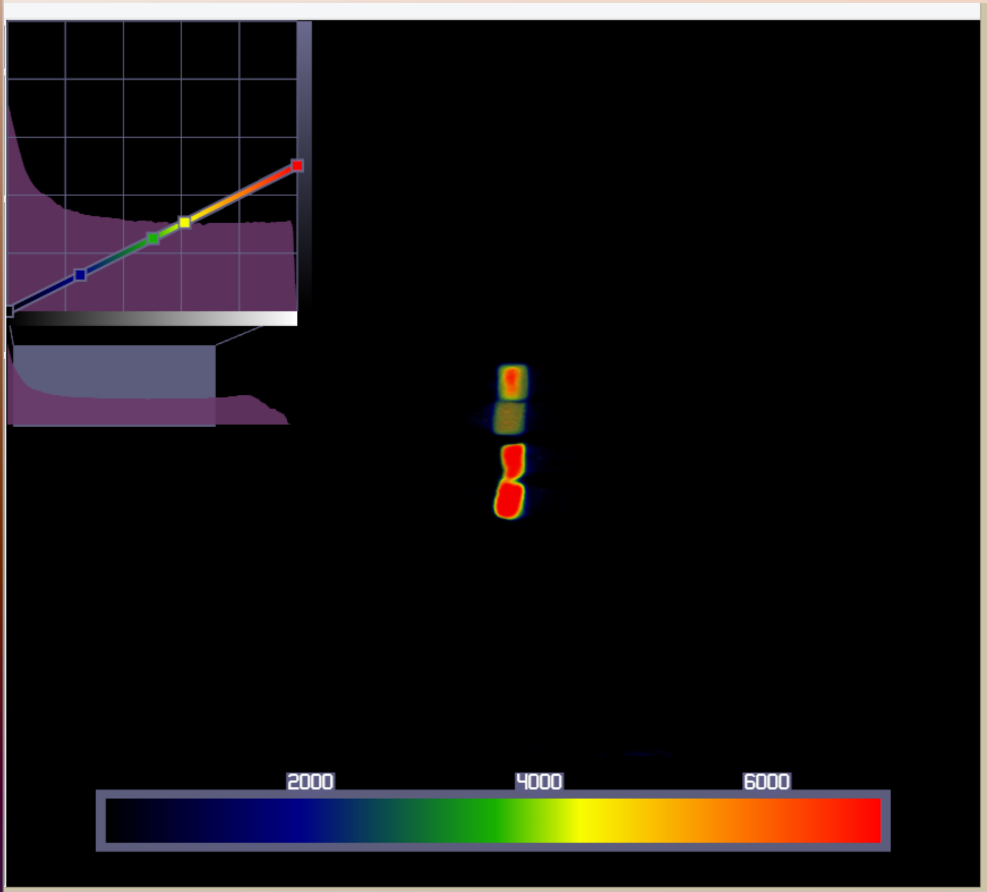
Effect of K-shell absorption edge



16.7 keV　　　　　15.5 keV

Sr K-shell absorption edge: 16.1 keV
each measurement time: 1 hr (360 projections)
Both image contrasts are normalized at the wooden region.

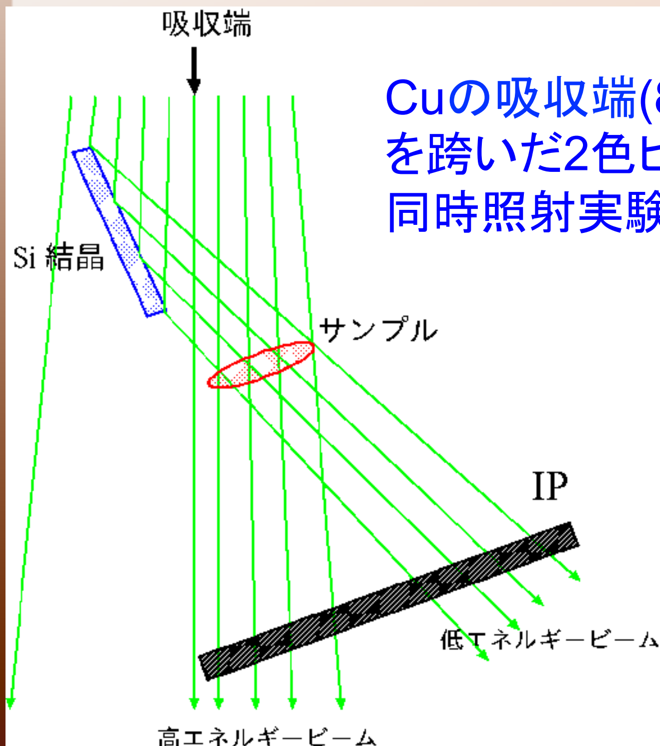
K-edge subtraction (KES) method



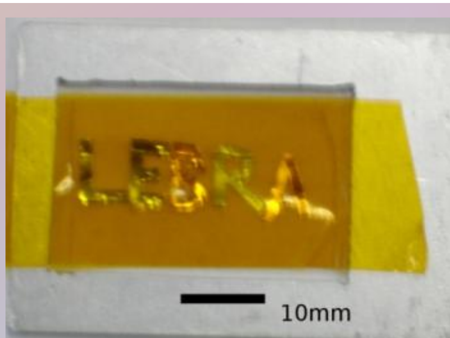
The 3D distribution of Sr element is obtained as difference between the tomographic images of 16.7keV and 15.5keV.

In this case, the datasets of CT were separately acquired. This method, therefore, is referred to as temporal K-edge subtraction (KES).

2色同時撮像による元素イメージング



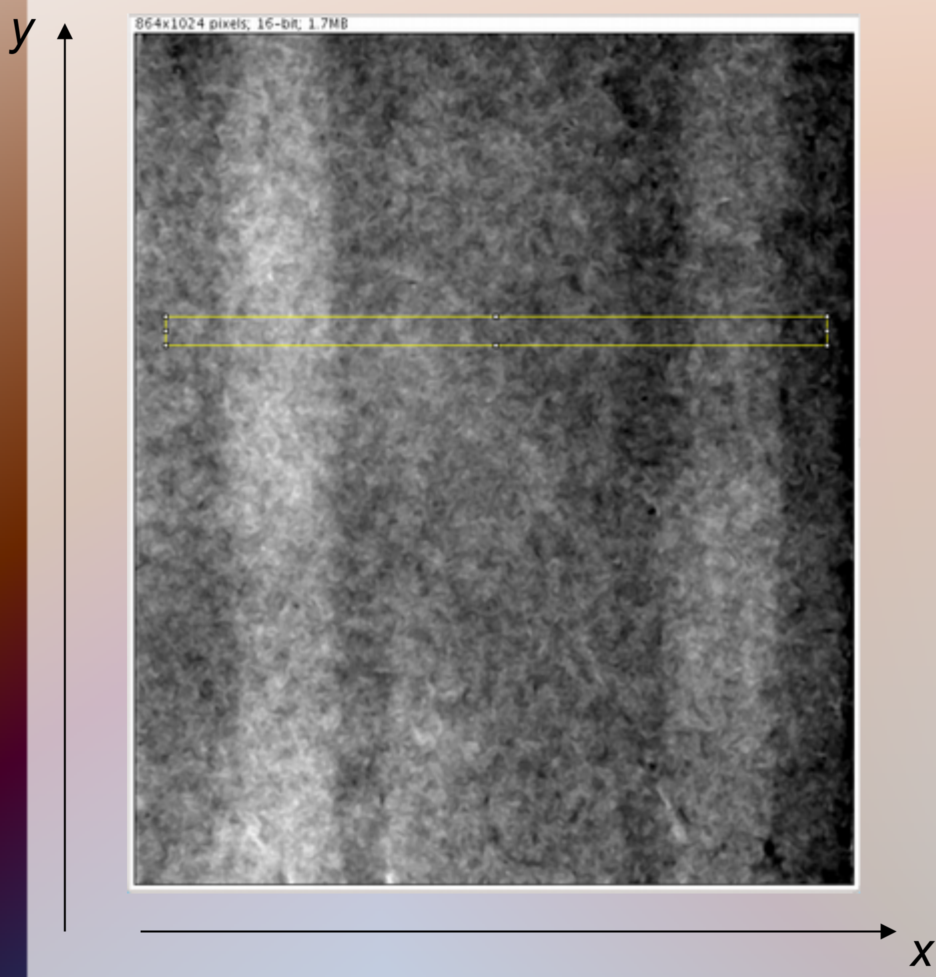
Cuの吸収端(8.98keV)
を跨いだ2色ビーム
同時照射実験



L : Ni (20μm)
E : Ni-Cu (10μm)
B, A : Cu (20μm)
R : Zn (25μm)

元素(Cu)検出を実証

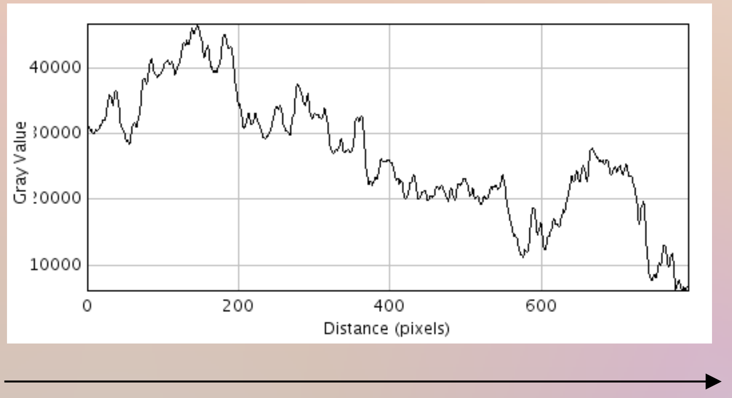
absorption-contrast image



complex refraction index:

$n(x,y) = 1 - \delta(x,y) + i\,\beta(x,y)$

$\delta, \beta \propto \rho$: density



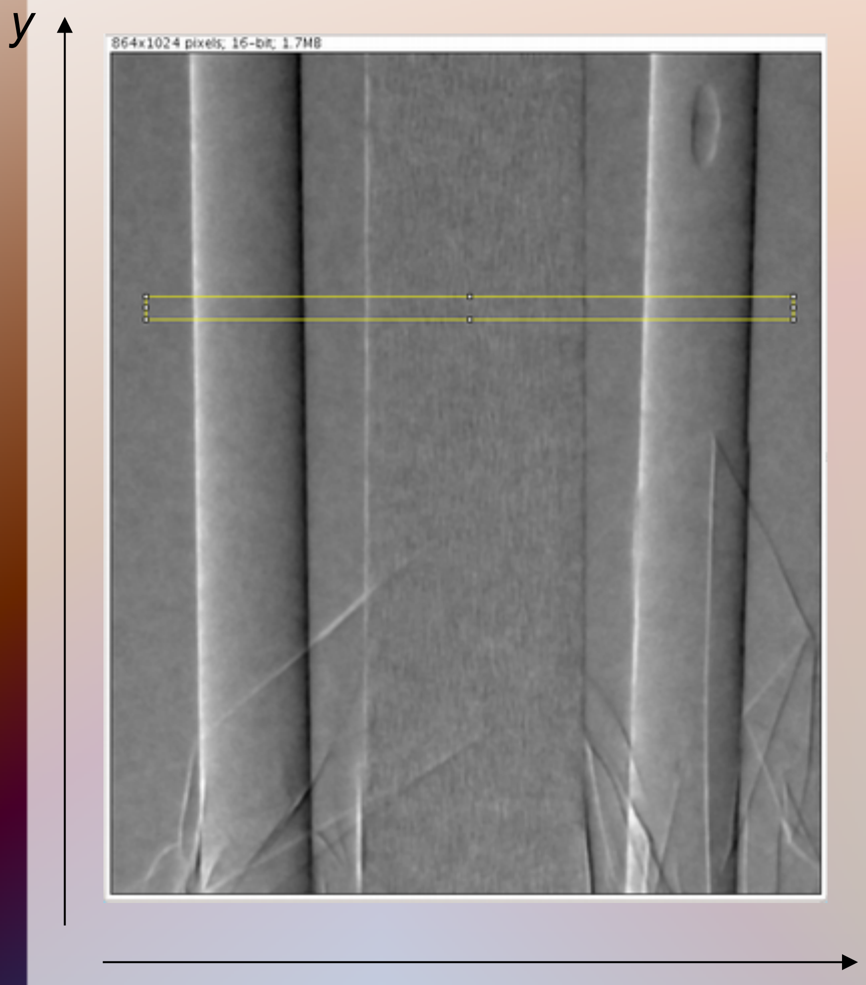
Integral with respect to θ

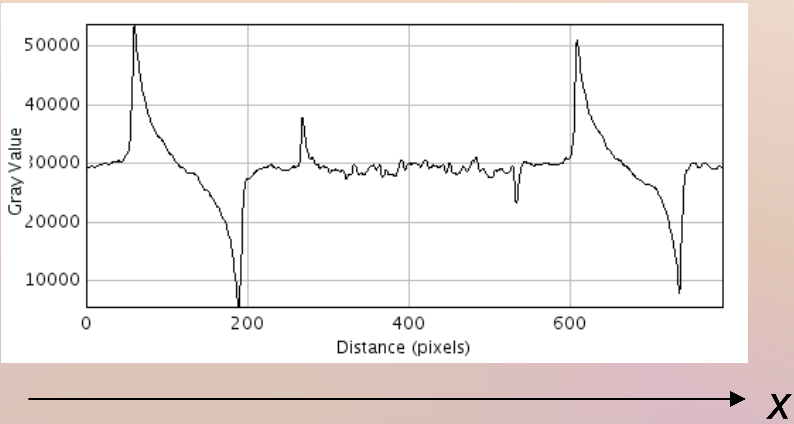
$I_{abs} = \sum I(x,y,\theta)$

$\ln(I_{abs}(x,y)/I_0) \propto \beta(x,y)$

$\propto \rho(x,y)$

phase-gradient image



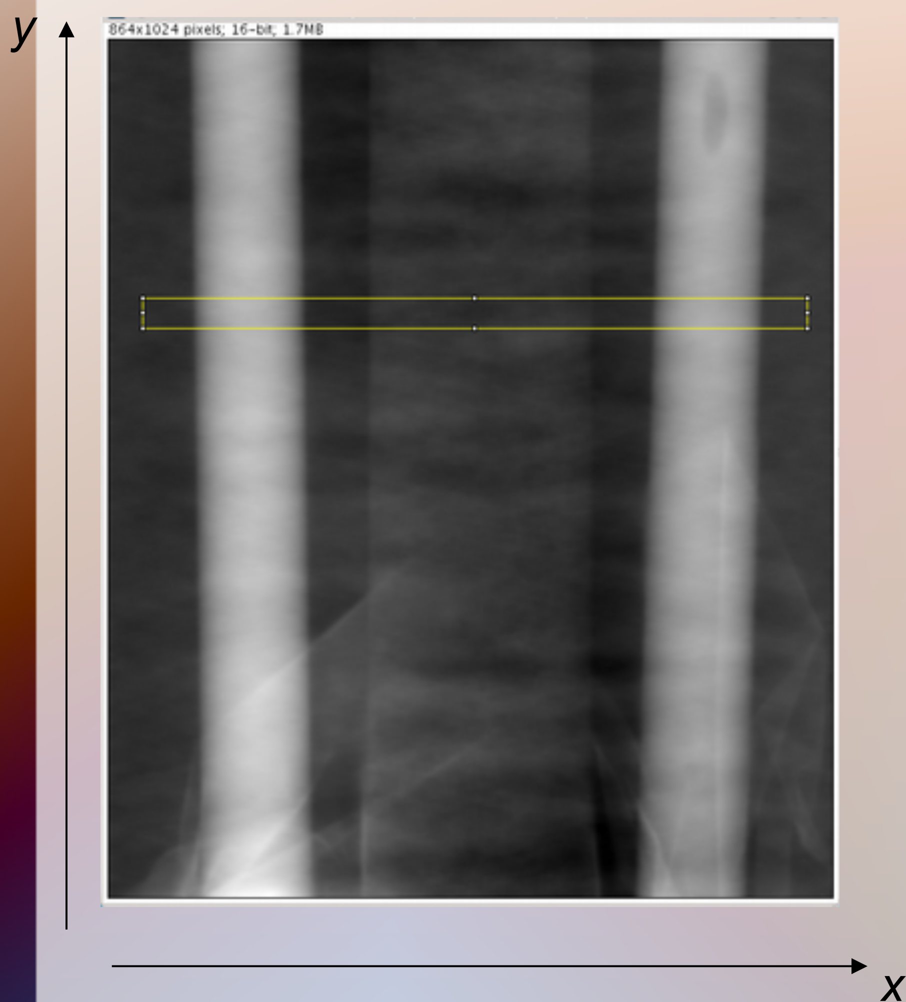


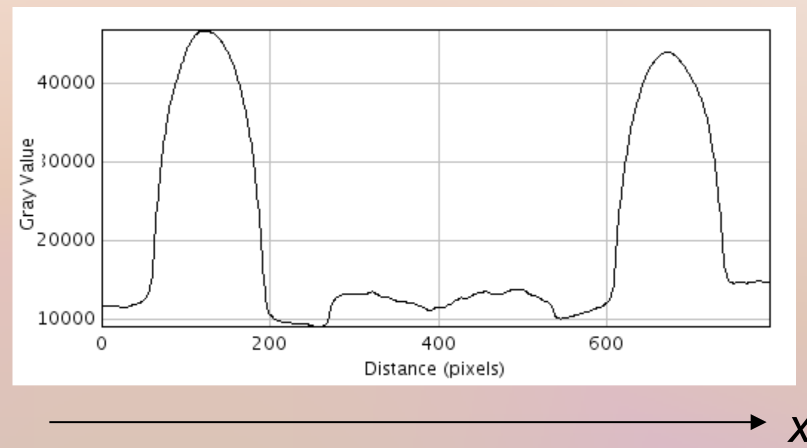
phase-gradient
(refraction-contrast) map

$$\sum \theta \, I(x,y,\theta) / \sum I(x,y,\theta)$$

$$\propto \quad \partial \delta(x,y) / \partial x$$

phase image



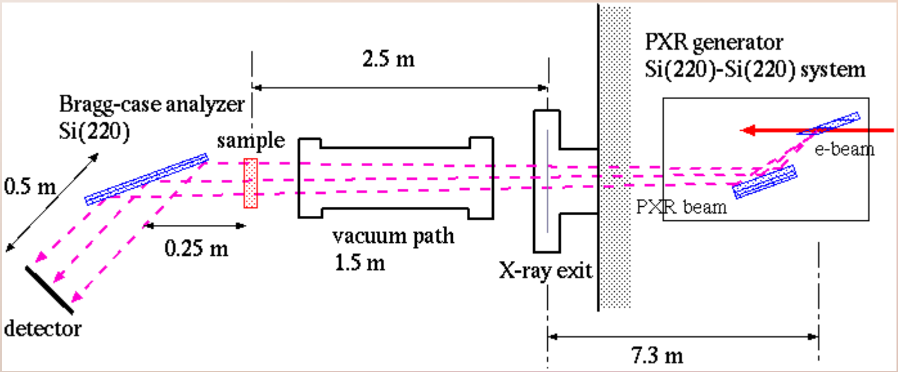


phase map

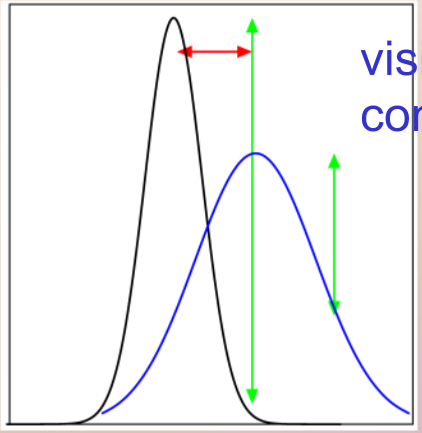
$$\delta(x,y) = \int \partial\delta(x,y) \,/\partial x \; \mathrm{d}x$$

$$\propto \; \rho(x,y)$$

diffraction-enhanced imaging

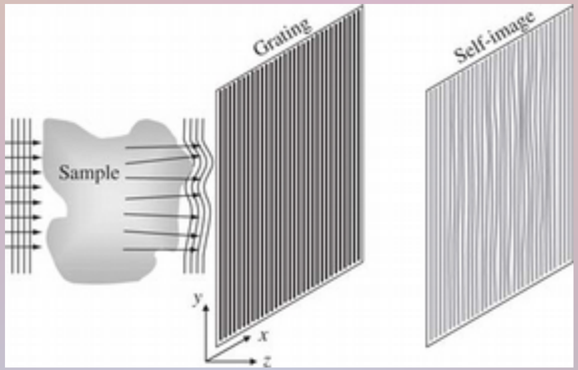


phase contrast



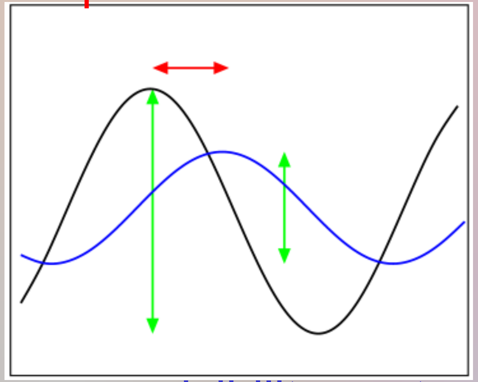
visibility contrast

Talbot interferometer imaging



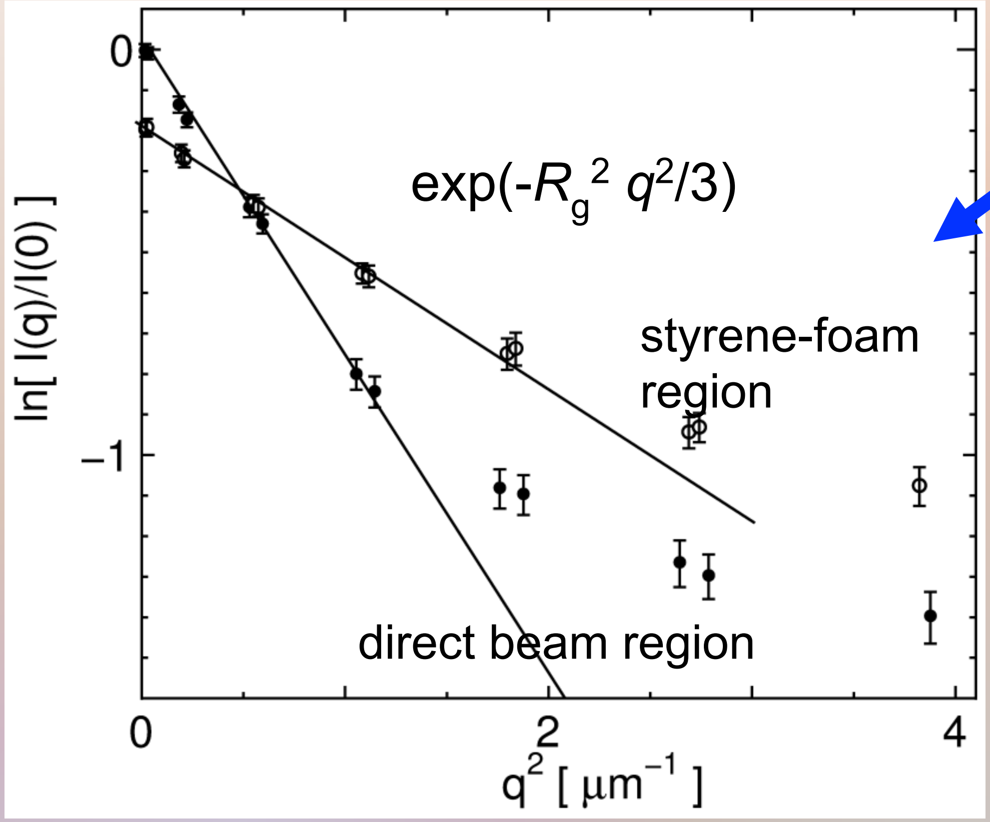
A. Momose et al.: JJAP 42 (2003) L866.

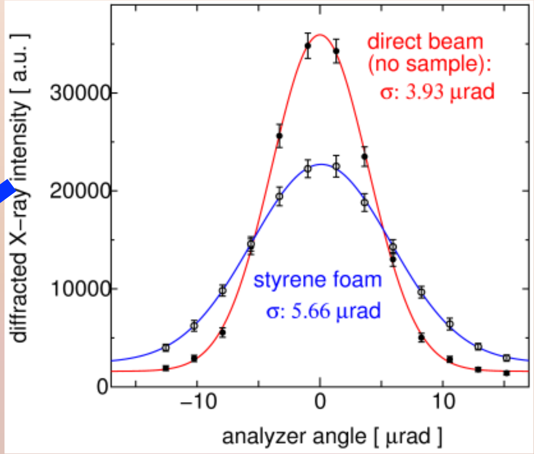
phase contrast



visibility contrast

Guinier plot





inertial radius
$R_g \sim 1\mu\text{m}$
< pixel size (24 μm)

$$q = (\ 4\pi / \lambda\ )\ \sin(\theta/2)$$

For more exact estimation, the sample thickness has to be optimized.