Toward Sequential Image Reconstruction with Large Area Detector in Hard X-ray Diffraction Microscope

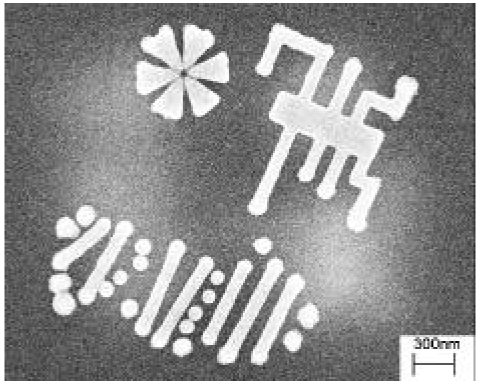
Yoshinori Nishino (SPring-8 / RIKEN)

X-ray Diffraction Microscopy at SPring-8

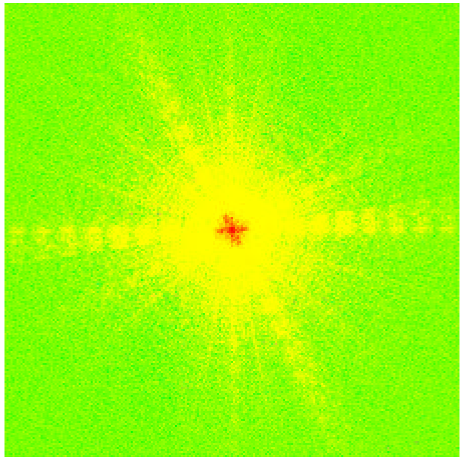
- using hard x-rays for high spatial resolution
  - started in 2001 in collaboration with J. Miao.
  - BL29XUL (1 km long beamline) at SPring-8

2D and 3D Imaging

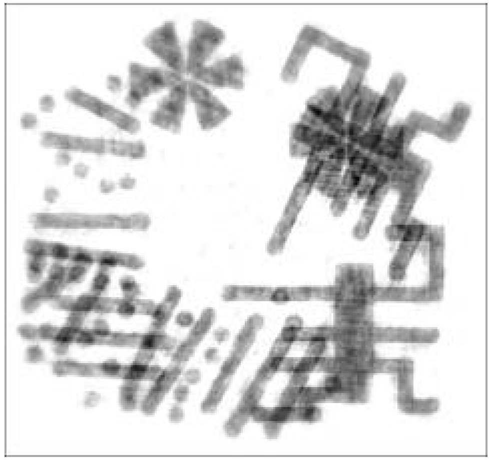
Ni Patterns on surface and
on layer 1 µm depth from surface.
The same pattern rotated 65° to each other.



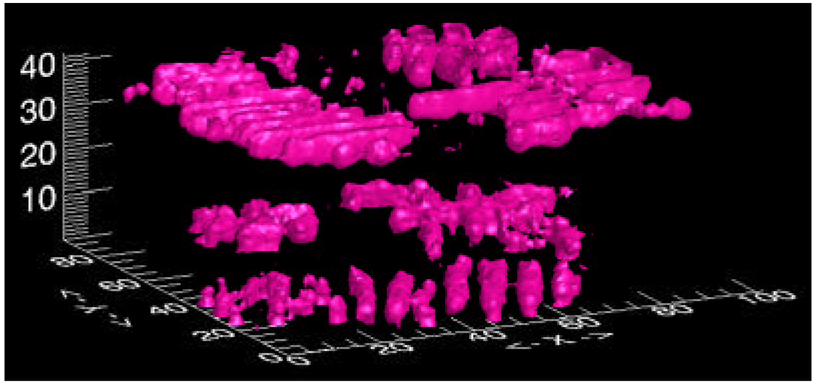
SEM Image



Diffraction Pattern
$\lambda = 2$ Å
SPring-8 BL29XUL



2D Reconstructed Image
single pixel size: 4 nm



3D Reconstructed Image

unit of axes: 25 nm

31 sets of 2D diffraction data:
from –75° to 75° with 5° increment

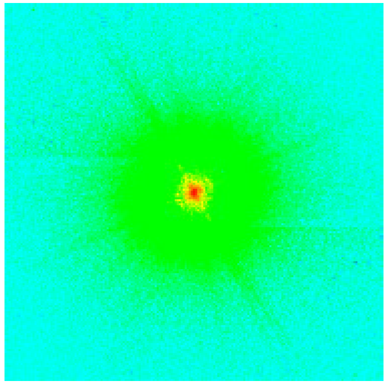
Y. Nishino

J. Miao, T. Ishikawa, B. Johnson, E.H. Anderson,
B. Lay & K.O. Hodgson, PRL **89**, 088303 (2002).

Applications

- Biology

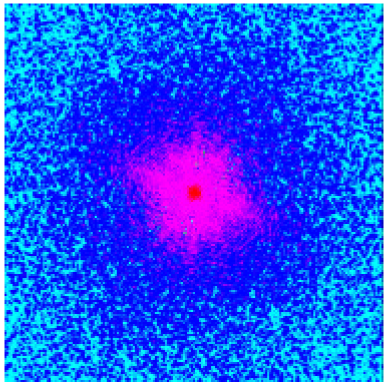
Escherichia Coli labeled with $KMnO_4$

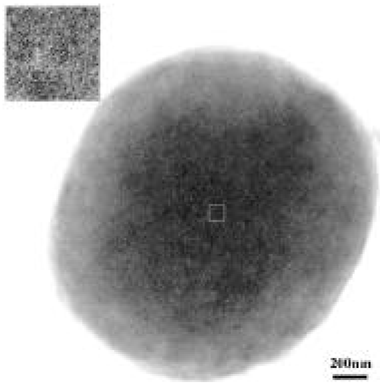


J. Miao, K.O. Hodgson, T. Ishikawa, C.A. Larabell, M.A. LeGros & Y. Nishino, PNAS **100**, 110 (2003).

- Materials Science

Porous Silica with about 2 µm in size





J. Miao, J. E. Amonette, Y. Nishino, T. Ishikawa & K. O. Hodgson, PRB **68**, 012201 (2003).

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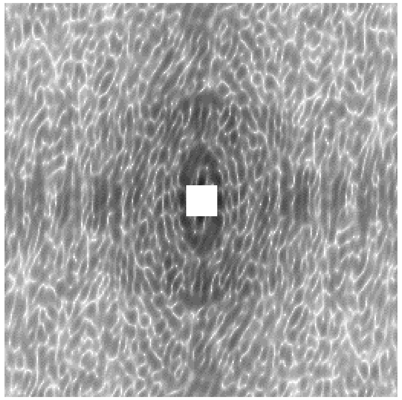
- sequential data analysis by solving the missing central-data problem
  - image reconstruction solely from hard x-ray diffraction data
  - iterative normalization algorithm (modified HIO)
  - missing data-region within centro-speckle
- faster data analysis
  - dynamic reconfigurable processor
- higher spatial resolution with large-area detector
  - in-vacuum imaging plate detector

Missing Central-Data Problem

Missing central-data problem has been preventing us from reconstructing sample image only from diffraction data.

Missing Data

- Exact Forward Pixel
  - Diffraction data can not be measured due to the additional contribution of the transmitted x-rays.
- Near Forward Pixels
  - Parasitic Scatterings from Optical Components
  - Limited Dynamic Rage of Detector

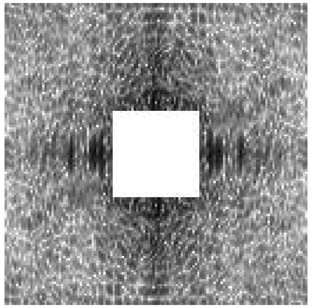


Importance of Missing Data

- Diffraction intensity at exact forward pixel determines the total number of electron in the sample
- Near forward diffraction data determine approximate shape of the sample

Supplemental low resolution experiment has been needed for image reconstruction.

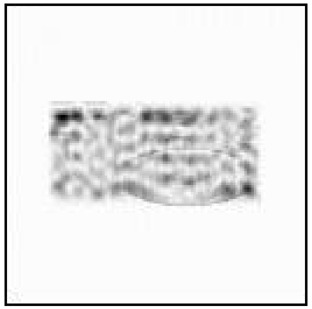
Iterative Normalization



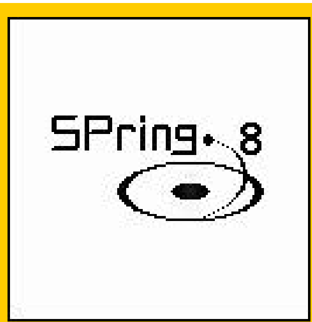
Calculated Diffraction Pattern
(129 x 129 pixels)
with missing central 37 x 37 pixels

Sample Image
(91 x 45pixels)

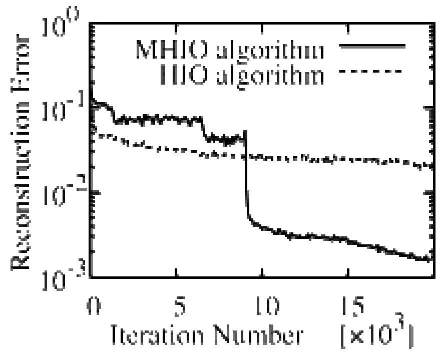
Reconstructed Images
(after 2 x 10^4 iterations)

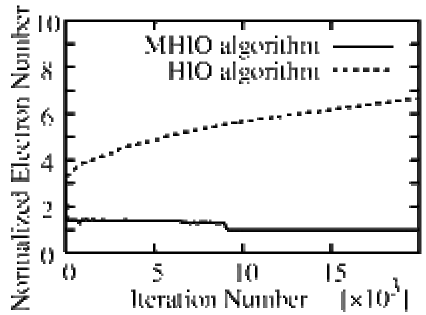


(a) HIO Algorithm



(b) MHIO Algorithm





Y. Nishino

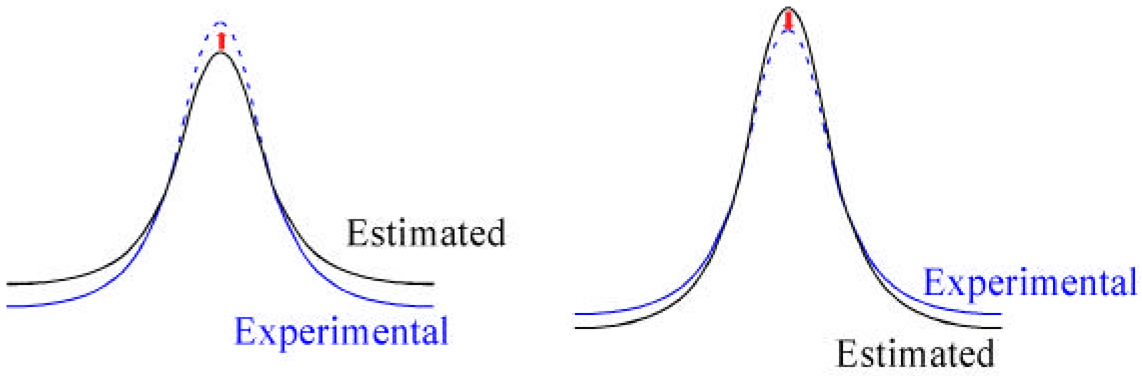
Y. Nishino, J. Miao, and T. Ishikawa, Phys. Rev. B **68**, 220101(R) (2003).

Modified HIO (MHIO) Algorithm

Initial Normalization $g_{\text{norm}}(\boldsymbol{K}) = \dfrac{\max\left(|f(\boldsymbol{K})|\right)_{\boldsymbol{K}\in D}}{\max\left(|g(\boldsymbol{K})|\right)_{\boldsymbol{K}\in D}} g(\boldsymbol{K}), \quad \text{for } \boldsymbol{K} \notin D$ D: diffraction data region

Iterative Normalization $g_{\text{norm}}(\boldsymbol{0}) = mg(\boldsymbol{0}),$ $m = a\left(\dfrac{1}{\text{average}\left(|f(\boldsymbol{K})|/|g(\boldsymbol{K})|\right)_{\boldsymbol{K}\in D}} - 1\right) + 1$

Iterative Normalization of Diffraction Intensities

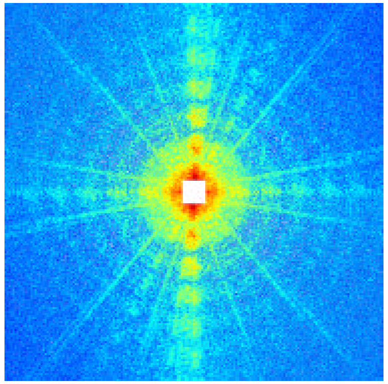


When the estimated diffraction patter is broader/sharper than experimental one, increase/decrease the total number of electron.

Y. Nishino, J. Miao, and T. Ishikawa, Phys. Rev. B **68**, 220101(R) (2003).

Image Reconstruction only from Diffraction Data

SEM image of sample
Au nanostructured pattern
(2.5 μm × 2.0 μm)

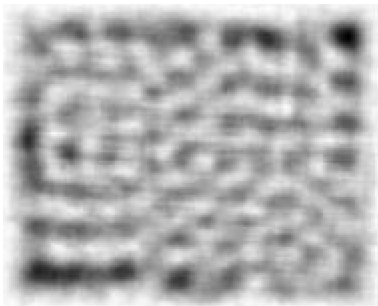


diffraction pattern
(1001 × 1001 pixels) with
missing central 61 × 61 pixels

SPring-8 BL29XUL
λ = 2.13Å

Reconstructed Images

single pixel size: 7 nm × 7 nm



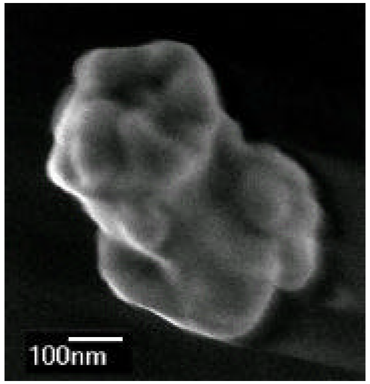
(a) HIO Algorithm

(b) MHIO Algorithm

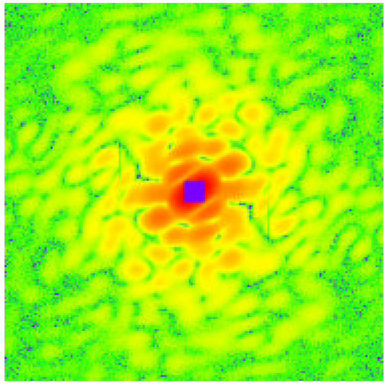
Y. Nishino, J. Miao, and T. Ishikawa, Phys. Rev. B **68**, 220101(R) (2003).

Missing Data Region within Centro-Speckle

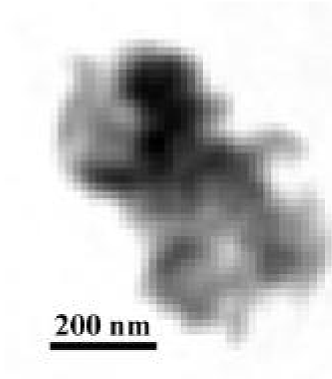
GaN Nanoparticle



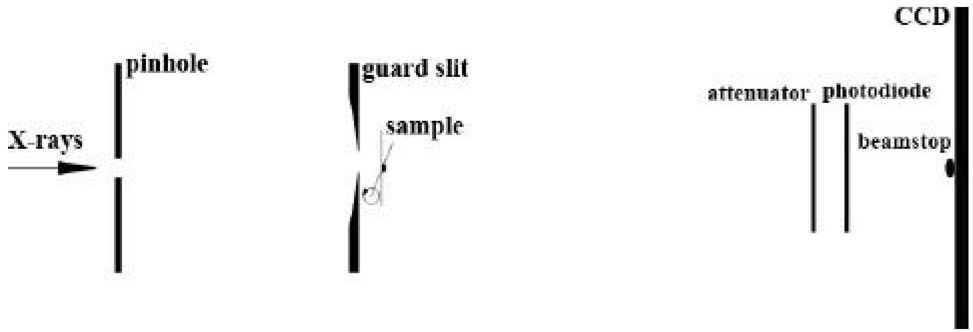
SEM image



X-ray Diffraction Pattern
missing central 29 x 29 pixels



Reconstructed Image
(HIO algorighm)



J. Miao, Y. Nishino, Y. Kohmura,
B. Johnson, C. Song, S.H. Risbud &
T. Ishikawa, submitted (2005)

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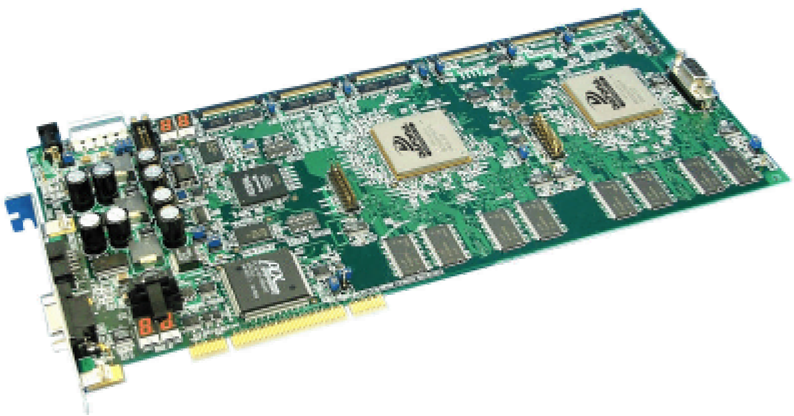
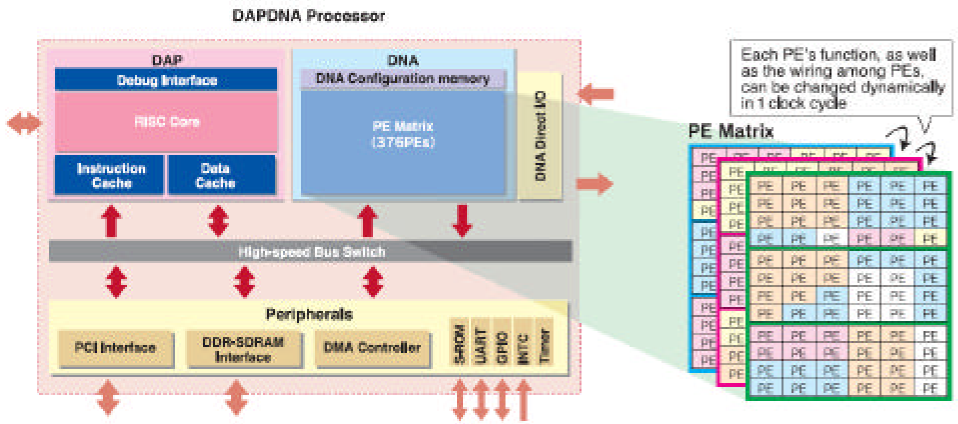
Dynamic Reconfigurable Processor

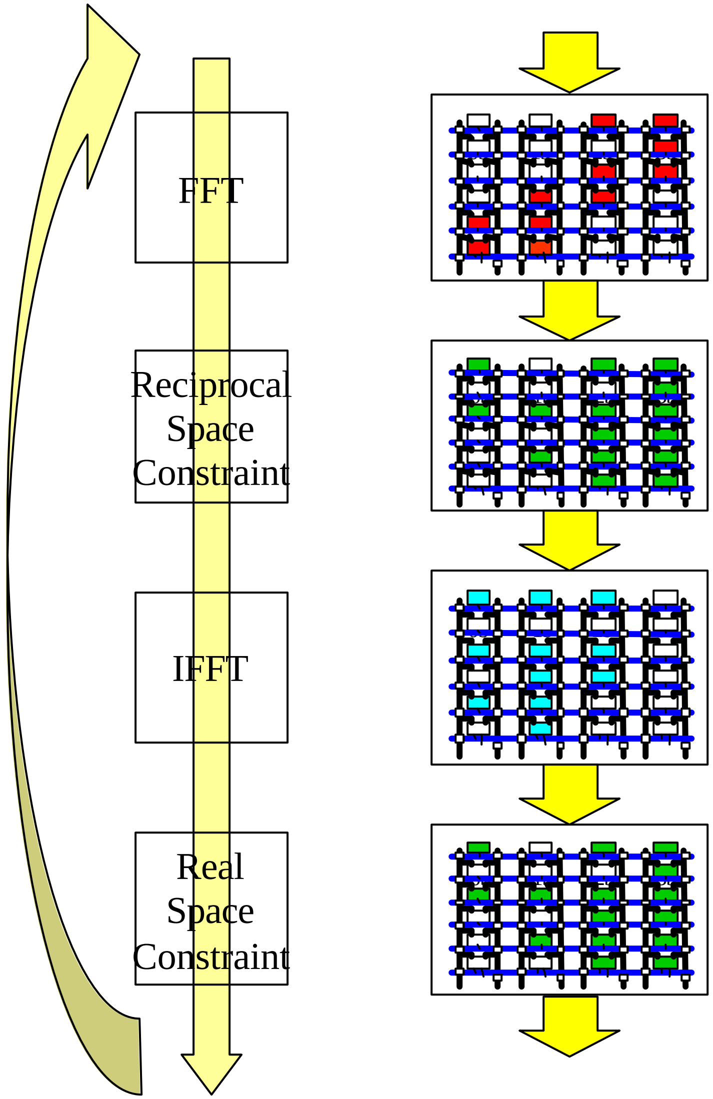
- von Neumann architecture . most computers
  - Ø general purpose hardware
  - Ø application specific software
- ASIC (Application Specific Integrated Circuit)
- FPGA (Field Programmable Gate Array)
  - static reconfigurable
- Dynamic Reconfigurable Processor





DAPDNA-EB4 (PCI card)
IP FLEX inc.

Image Reconstruction with Dynamic Reconfigurable Processor



reconfiguration in one clock
~ 6 ns with 166 MHz clock frequency

FFT / IFFT
~ 13 times faster
than 3.60 GHz Pentium 4 Processor

It takes 87 sec for 1000 iterations of
1024 x 1024 pixel image reconstruction

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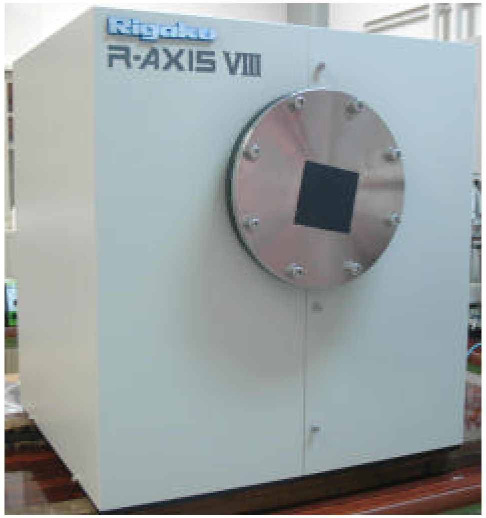
In-Vacuum Imaging Plate Detector



R-AXIS VIII (Rigaku Inc.)

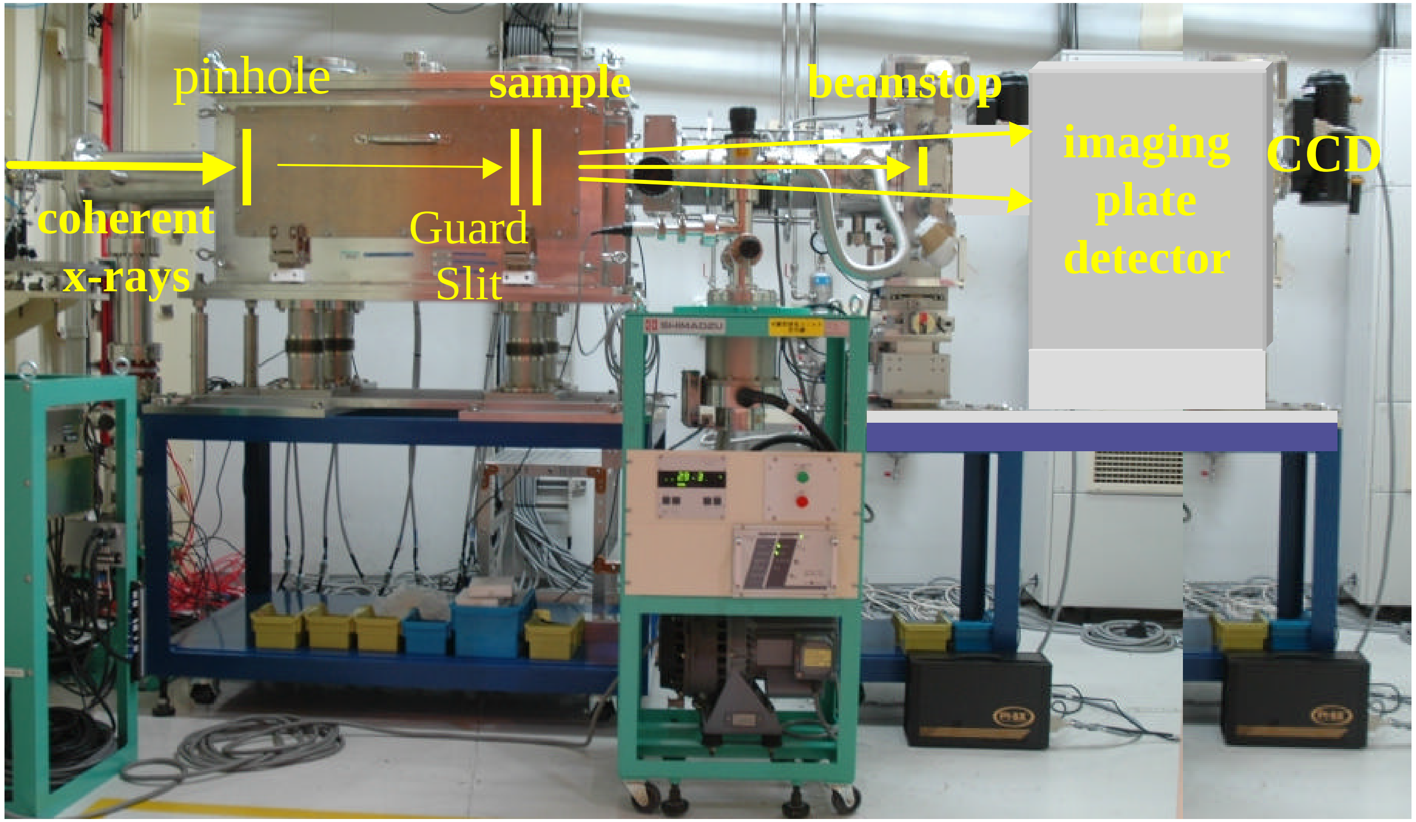
Imaging Plate (in Vacuum)
Reader and Eraser (in Air)

two sets

taking data while reading & erasing the other

	R-AXIS VIII	PI-LCX CCD
Total Area	125 mm square	26 mm x 26.8 mm
Pixel Size	25 μm square	20 μm square
Total Pixel	5000 x 5000	1300 x 1340
Dinamic Range	10^4-10^5	10^2 (direct illumination w/o phosphor)

Planned Experimental Setup



(composite picture)

Issues to be Considered with Higher Spatial Resolution

- Projection Approximation $\quad$ sample thickness $. \quad \dfrac{(\text{resolution})^2}{l}$

  Curvature of Ewald Sphere

- Anisotropic Atomic Scattering Factor & Debye-Waller Factor

- Polarization Factor $\quad P = \sin^2\Phi + \cos^2\Theta\cos^2\Phi$

  weak Φ dependence for small Θ
  for Θ = 0.1, P ˜ 0.99 ? decrease of diffraction intensity by 1 %

- Temporal Coherence

$$\frac{\Delta E}{E} \;.\; \sqrt{\frac{2\times\text{oversampling ratio}}{\text{pixel number of detector}}}$$

Collaborators

SPring-8 (RIKEN Harima Institute)

Yoshiki Kohmura, Yukio Takahashi, Tetsuya Ishikawa (project leader)

Poster: P29

Imaging Plate Detector

Masaki Yamamoto

RIGAKU (http://www.rigaku.co.jp/)

RIKEN Wako Institute

Dynamic Reconfigurable Processor

Kuniaki Koike, Toshikazu Ebisuzaki

IP FLEX Inc. (http://www.ipflex.com/)

UCLA

Jianwei Miao, Changyoung Song

Poster: P49

Summary

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