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.

Diffraction Pattern
λ = 2 Å
SPring-8 BL29XUL

SEM Image

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

Applications

• Biology
  Escherichia Coli labeled with KMnO$_4$


• Materials Science
  Porous Silica with about 2 µm in size

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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 Range 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

Sample Image
(91 x 45 pixels)

Reconstructed Images
(after 2 x 10^4 iterations)

(a) HIO Algorithm
(b) MHIO Algorithm

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

Modified HIO (MHIO) Algorithm

Initial Normalization

\[ g_{\text{norm}}(K) = \frac{\max_{K \in D} \|f(K)\|}{\max_{K \in D} \|g(K)\|} \cdot g(K), \quad \text{for } K \notin D \]

\[ D: \text{diffraction data region} \]

Iterative Normalization

\[ g_{\text{norm}}(\theta) = mg(\theta), \quad m = \alpha \left( \frac{1}{\text{average} \left( \|f(K)\|/\|g(K)\|_{K \in D} \right)} - 1 \right) + 1 \]

Iterative Normalization of Diffraction Intensities

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


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Image Reconstruction only from Diffraction Data

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

Reconstructed Images
single pixel size: 7 nm x 7 nm

(a) HIO Algorithm
(b) MHIO Algorithm

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

SPring-8 BL29XUL
λ = 2.13Å

Missing Data Region within Centro-Speckle

GaN Nanoparticle

SEM image

X-ray Diffraction Pattern
missing central 29 x 29 pixels

Reconstructed Image
(HIO algorighm)


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Dynamic Reconfigurable Processor

- von Neumann architecture, most computers
  - general purpose hardware
  - 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.

Y. Nishino  coherence05 (June 15-17, 2005)
Image Reconstruction with Dynamic Reconfigurable Processor

- FFT
- Reciprocal Space Constraint
- IFFT
- Real Space Constraint

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

<table>
<thead>
<tr>
<th>R-AXIS VIII</th>
<th>PI-LCX CCD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Area</td>
<td>125 mm square</td>
</tr>
<tr>
<td>Pixel Size</td>
<td>25 μm square</td>
</tr>
<tr>
<td>Total Pixel</td>
<td>5000 × 5000</td>
</tr>
<tr>
<td>Dynamic Range</td>
<td>$10^4$-10$^5$</td>
</tr>
</tbody>
</table>
Planned Experimental Setup

(coComposite picture)
Issues to be Considered with Higher Spatial Resolution

- **Projection Approximation**
  
  \[
  \Phi \theta + \Phi = 2 \cos^2 \cos \theta \sin \theta 
  \]
  
  Curvature of Ewald Sphere

- **Anisotropic Atomic Scattering Factor & Debye-Waller Factor**

- **Polarization Factor**
  
  \[ P = \sin^2 \Phi + \cos^2 \Theta \cos^2 \Phi \]

  weak \( \Phi \) dependence for small \( \Theta \)

  for \( \Theta = 0.1 \), \( P \approx 0.99 \) ? decrease of diffraction intensity by 1 %

- **Temporal Coherence**

  \[
  \frac{\Delta E}{E} \approx \sqrt{\frac{2 \times \text{oversampling ratio}}{\text{pixel number of detector}}} 
  \]

Y. Nishino

coherence05 (June 15-17, 2005)
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
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Summary

- Using hard x-rays for high spatial resolution
  - Started in 2001 in collaboration with J. Miao.
  - BL29XUL (1 km long beamline) at SPring-8
- Sequential data analysis by solving the missing central-data problem
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- Faster data analysis
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