Scanning X-ray microscopy with a single photon counting 2D detector

Karolina Stachnik

Faculty of Physics and Applied Computer Science,
AGH University of Science and Technology, Kraków

XLVIII Zakopane School of Physics

Zakopane, 21 May 2013
Outline

- Imaging with Scanning Transmission X-ray Microscopy
  - STXM - scanning image formation
  - Determining the Differential Phase Contrast
- Simulation tool for X-ray imaging
- Measurement
  - Experimental setup
  - Data analysis
- Simulated data analysis
- Concepts of ptychography
- Conclusion
**Scanning image formation**

> **Intensity** of the wavefield in the detector plane, $\omega_3 = (k/d_2)r_3$

$$
\Psi_3(\omega_3; R_s) \propto \mathcal{F}_{\omega_3}\{O(r_2)P(r_2 - R_s)\}
$$

$$
I_3(\omega_3; R_s) \propto |O(\omega_3) \otimes P(\omega_3)e^{iR_s \cdot \omega_3}|^2
$$

> The **angular deviation** as a function of the coordinates $(x, y)$

$$
\alpha_x = \frac{\lambda}{2\pi} \frac{\partial \phi(x, y)}{\partial x}
$$

$$
\alpha_y = \frac{\lambda}{2\pi} \frac{\partial \phi(x, y)}{\partial y}
$$

Ch. Holzner, *Hard X-ray Phase Contrast Microscopy – Techniques and Applications*

MccMorrow D., *Elements of Modern X-ray Physics, Wiley, 2011*
Differential Phase Contrast

Quadrant detector approach

- The arbitrary deflection \( D \) (related to intensity distribution shift).
- DPC signals for the each scan point
  \[
  DPC_x = \frac{I_R - I_L}{I_{total}} \\
  DPC_y = \frac{I_B - I_T}{I_{total}}
  \]
- Reference point: the direct beam position

Centre of mass approach

- The real space coordinates of the detector \( r' = (x', y') \)
- The recorded intensity distribution \( I_j \) for the \( j \)-th scan point
- Reference point: the direct beam position at \( (x'_{ref}, y'_{ref}) \)

\[
DPC_x = \frac{\sum_{r'} x' I_j(r')}{\sum_{r'} I_j(r')} - x'_{ref}
\]
\[
DPC_y = \frac{\sum_{r'} y' I_j(r')}{\sum_{r'} I_j(r')} - y'_{ref}
\]

\( j = 1, \ldots, N_{PIE} \)

\( N_{PIE} \) - total number of diffraction patterns

Ch. Holzner, *Hard X-ray Phase Contrast Microscopy – Techniques and Applications*
Simulation tool for X-ray imaging

> Purpose:

- test of parameters of experiment
- evaluation of measured data

> Implemented in C++ with support of the ROOT Data Analysis Framework

> Flexibility: opportunity to build setup according to requirements of experiment

- Complex and real 2D arrays
  - Standard operations
  - FFT implementation

- Complex Wavefield 2D
  - Physical parameters
  - Near-field and far-field propagators
  - I/O
  - Data analysis (e.g. DPC)

- Optical elements
  - Fresnel zone plate
  - Pinhole (e.g. order sorting aperture)
  - Central stop
  - Test sample: Siemens star
Simulation - propagators

> The convolutional approach (angular spectrum):

\[ E_\omega(x_2, y_2, z_2) = e^{ik\Delta z} \mathcal{F}^{-1}\left[e\left(-\frac{i\Delta z}{2k}(k_x^2+k_y^2)\right)\mathcal{F}[E_\omega(x_1, y_1, z_1)]\right] \]

> Direct application of the Fresnel diffraction formula

\[ E_\omega(x_2, y_2, z_2) = e^{ik\Delta z}P(x_2, y_2)\mathcal{F}\left[ E_\omega(x_1, y_1, z_1)P(x_1, y_1)\right] \]

where \( P(x_2, y_2) = \exp\left(\frac{ik}{2\Delta z}(x_i^2 + y_i^2)\right) \).
Experimental setup

Experiment conducted at beamline P11 of PETRA III, Deutsches Elektronen-Synchrotron in Hamburg, Germany

<table>
<thead>
<tr>
<th></th>
<th>Siemens star scan</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beam energy</td>
<td>6.2 keV</td>
</tr>
<tr>
<td>Beam defining pinhole (diameter)</td>
<td>100 µm</td>
</tr>
<tr>
<td>Central stop (diameter)</td>
<td>50 µm</td>
</tr>
</tbody>
</table>
| Focusing zone plate   | Diameter: 100 µm  
Focal length: 12.5 mm  
Outermost zone width: 25 nm |
| Order sorting aperture (diameter) | 10 µm                        |
| Sample-to-detector distance | 395 cm                      |
Intensity control
Detector PILATUS 6M

RESULTS
Intensity control

Single view from PILATUS 6M detector (zoomed)

Number of modules: 5 x 12
Format: 2463 x 2527 pixels
Pixel size: 172 x 172 µm²

Intensity distribution for single projection from the scan of the Siemens star.

10 new bad pixels detected.

Simulated diffraction pattern for scan of a Siemens star
Scan of Siemens star
Diameter: 20 µm

RESULTS - EXPERIMENT
DPC quadrant detector

Number of positions: **80 x 80**

Step size: **250 nm**

**ROI** (size of the virtual quadrant detector):
- **512 x 512 pixels** (top)
- **2350 x 2350 pixels** (bottom)
DPC – centre of mass approach

Number of positions: 80 x 80
Step size: 250 nm
ROI: all valid pixels of the detector

DPC quadrant detector approach in black
DPC centre of mass approach in red
Horizontal profile: along line $y = 5.25 \ \mu m$
Vertical profile: along line $x = 1.25 \ \mu m$
Scan of Siemens star
Diameter: 20 µm

RESULTS - SIMULATION
### Simulation parameters

<table>
<thead>
<tr>
<th>Siemens star scan</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Beam energy</strong></td>
</tr>
<tr>
<td><strong>Beam defining pinhole (diameter)</strong></td>
</tr>
<tr>
<td><strong>Central stop (diameter)</strong></td>
</tr>
<tr>
<td><strong>Focusing zone plate</strong></td>
</tr>
<tr>
<td><strong>Order sorting aperture (diameter)</strong></td>
</tr>
<tr>
<td><strong>Sample-to-detector distance</strong></td>
</tr>
</tbody>
</table>

**Image:**
- Simulation results showing transmission patterns with various parameters.
Differential Phase Contrast Analysis

Number of positions: \(81 \times 81\)
Step size: 250 nm
ROI: all pixels of the detector

DPC quadrant detector approach in black
DPC centre of mass approach in red

Horizontal profile: along line \(y = 3 \, \mu m\)
Vertical profile: along line \(x = 3 \, \mu m\)
Ptychographical Coherent Diffractive Imaging (pCDI)

> **Ptychography** (from the Greek "πτνξ" meaning "to fold")

> Firstly proposed by Hoppe and Hegerl in 1970s for electron microscopy

> The convolution property of the far-field diffraction pattern:
  - Diffraction orders are convoluted ("folded") with the far-field of the illumination

> X-ray ptychography: combination of coherent diffractive imaging and STXM

> Diffraction patterns recorded from a series of **overlapping beam positions**

M. Dierolf et al., *Ptychography and lensless X-ray imaging*

> **Prerequisite**: localized and highly coherent illumination

> **Parameters**:
  - Data: real-valued intensity
  - Positions of illumination function

> **Overlap** of about 70% - increase of image resolution in reconstruction process

> Iterative phase retrieval: e.g. extended Ptychographical Iterative Engine

O. Bunk et al., Ultramicroscopy 108 (2008) 481-487

Conclusion

- STXM often used when optimal conditions for CDI cannot be achieved.
- **Pixel array detector** allows for **two** implementations of **DPC**.
- **No** substantial **loss** of information when choosing **smaller ROI** in DPC quadrant approach.
- **DPC centre of mass** approach tends to achieve **higher contrast** for experimental data.
- **Lower quality** of the Siemens star scan is not yet fully understood.
- **Simulation** – useful tool for **comparison** with **real data**.
Acknowledgements

> Dr. Alke Meents, HASYLAB, DESY, Hamburg

> Dr. hab. Mariusz Przybycień, AGH UST, Kraków

> Dr. Klaus Giewekemeyer, European XFEL, Hamburg

> Dr. Janusz Lekki, Institute of Nuclear Physics, PAS, Kraków

> Dr. Zbigniew Stachura, Institute of Nuclear Physics, PAS, Kraków
Thank you for your attention!