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

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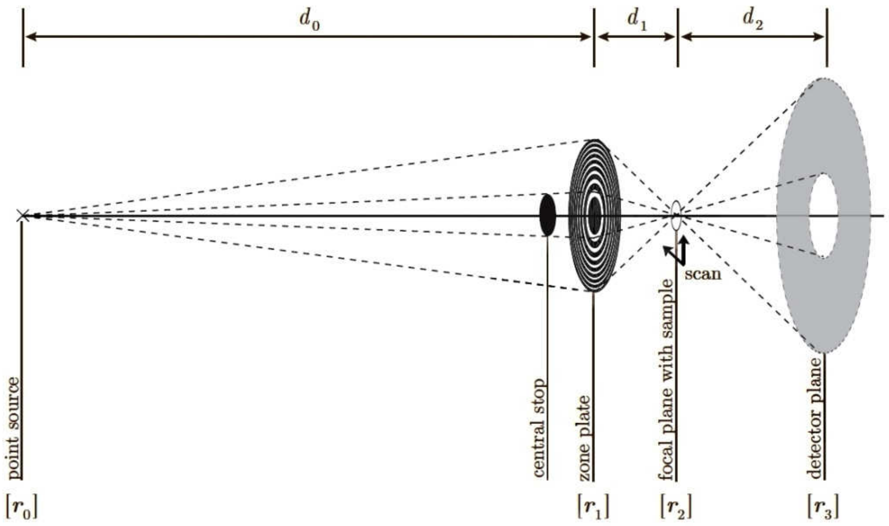
Outline

- 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, $\boldsymbol{\omega_3} = (k/d_2)\boldsymbol{r_3}$

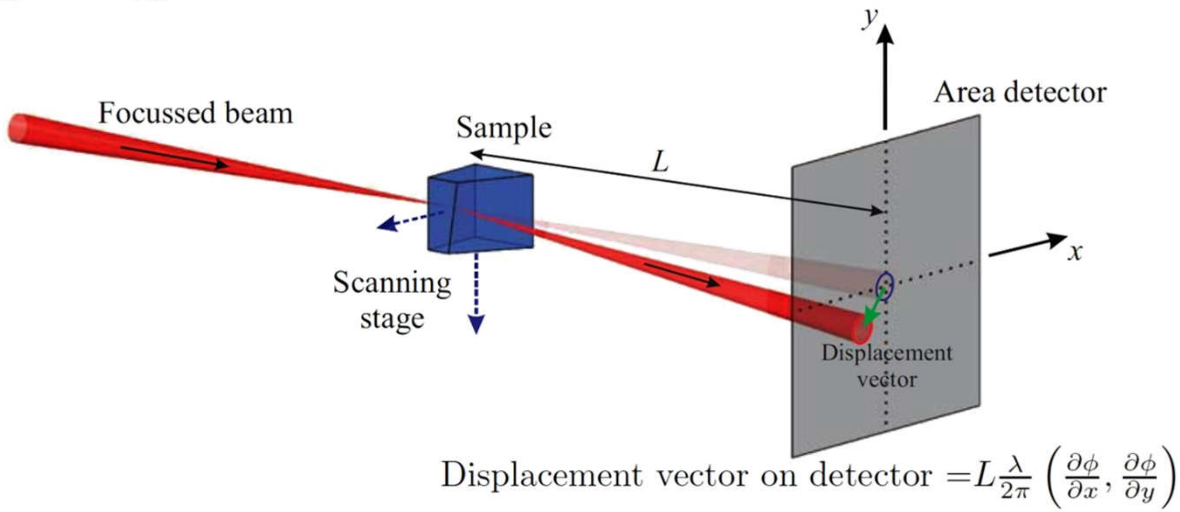
$$\Psi_3(\boldsymbol{\omega_3}; \boldsymbol{R_s}) \propto \mathcal{F}_{\boldsymbol{\omega_3}}\{O(\boldsymbol{r_2})P(\boldsymbol{r_2} - \boldsymbol{R_s})\}$$

$$I_3(\boldsymbol{\omega_3}; \boldsymbol{R_s}) \propto \left|O(\boldsymbol{\omega_3}) \otimes P(\boldsymbol{\omega_3})e^{\mathrm{i}\boldsymbol{R_s}\cdot\boldsymbol{\omega_3}}\right|^2$$

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

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

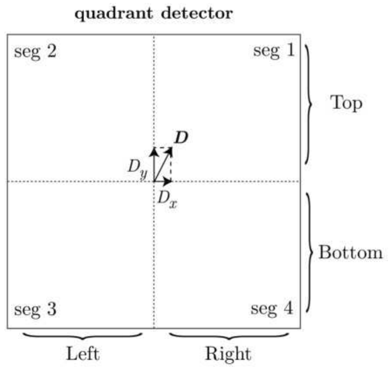
$$\alpha_y = \frac{\lambda}{2\pi}\frac{\partial\phi(x,y)}{\partial y}$$



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

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

Centre of mass approach

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

$$DPC_x = \frac{\sum_{r'} \boldsymbol{x'} \boldsymbol{I_j}(r')}{\sum_{r'} I_j(r')} - x'_{ref}$$

$$DPC_y = \frac{\sum_{r'} \boldsymbol{y'} \boldsymbol{I_j}(r')}{\sum_{r'} I_j(r')} - y'_{ref}$$

$j = 1, \dots, N_{PIE}$

N_{PIE} - total number of diffraction patterns

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

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

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

Simulation - propagators

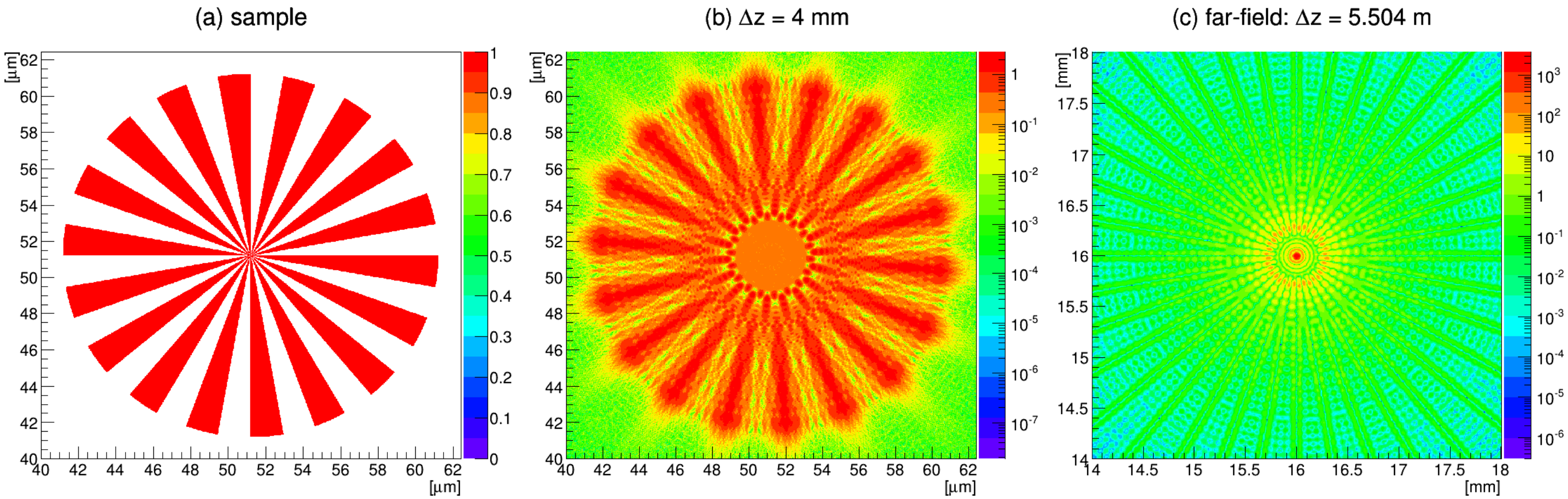
- The convolutional approach (angular spectrum):

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

- Direct application of the Fresnel diffraction formula

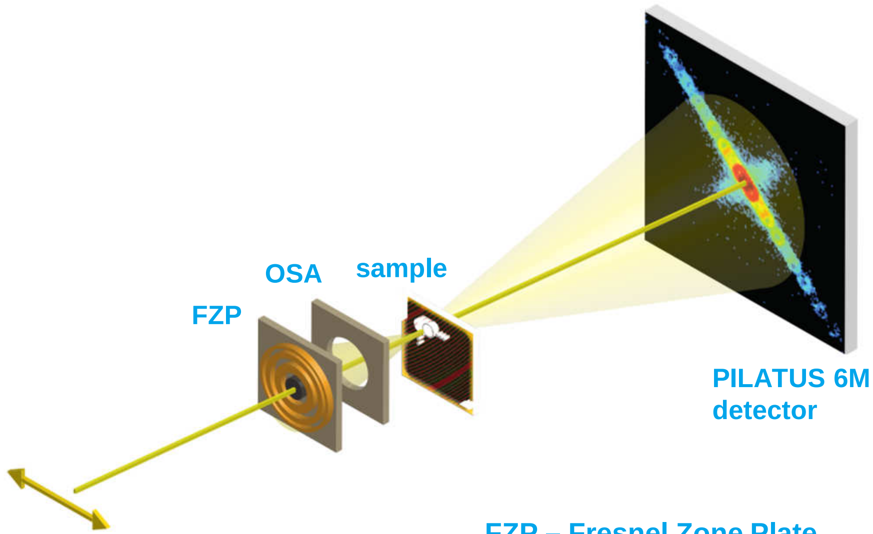
$$E_\omega(x_2,y_2,z_2) = e^{ik\Delta z}P(x_2,y_2)\mathcal{F}[E_\omega(x_1,y_1,z_1)P(x_1,y_1)]$$

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



FZP – Fresnel Zone Plate
OSA – Order Sorting Aperture

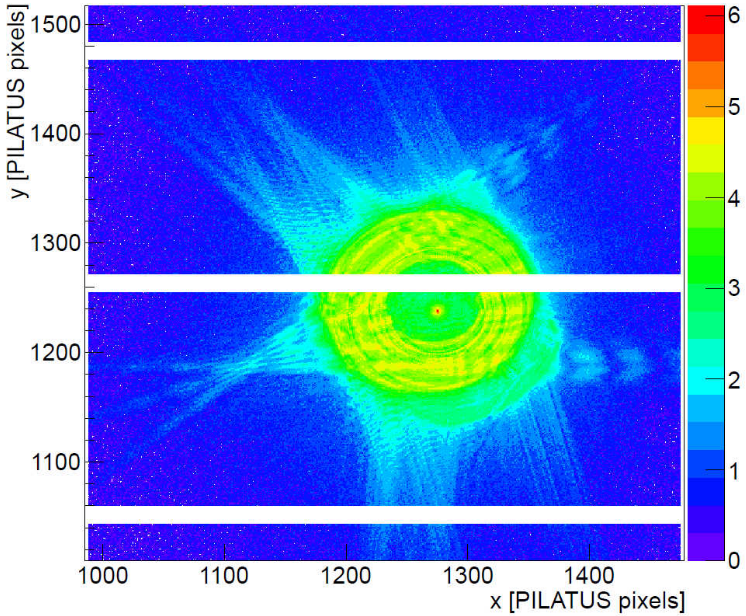
	Siemens star scan
Beam energy	**6.2 keV**
Beam defining pinhole (diameter)	100 µm
Central stop (diameter)	50 µm
Focusing zone plate	Diameter: 100 µm Focal length: 12.5 mm Outermost zone width: 25 nm
Order sorting aperture (diameter)	10 µm
Sample-to-detector distance	**395 cm**

Intensity control

Detector PILATUS 6M

RESULTS

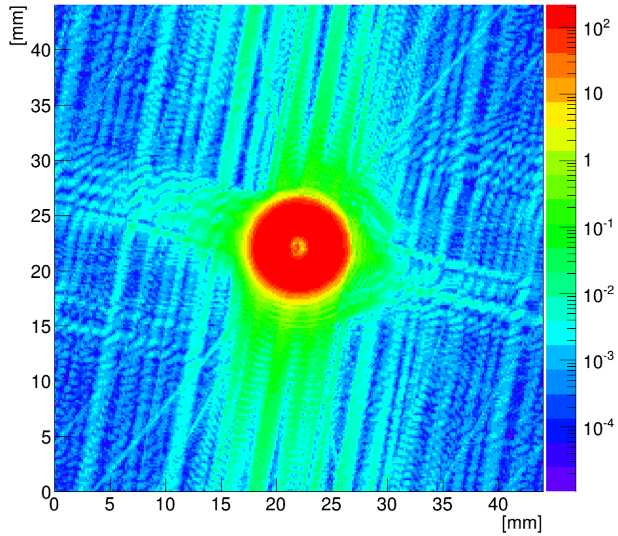
Intensity control



Single view from PILATUS 6M detector (zoomed)

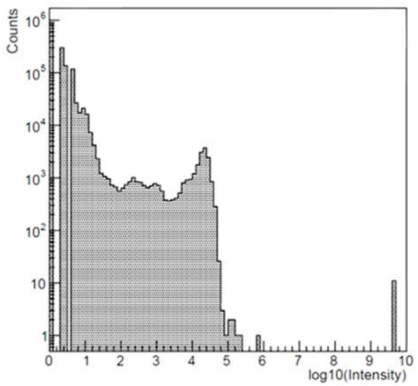
Number of modules: 5 x 12
Format: 2463 x 2527 pixels
Pixel size: 172 x 172 μm^2

Simulated diffraction pattern for scan of a Siemens star



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

10 new bad pixels detected.

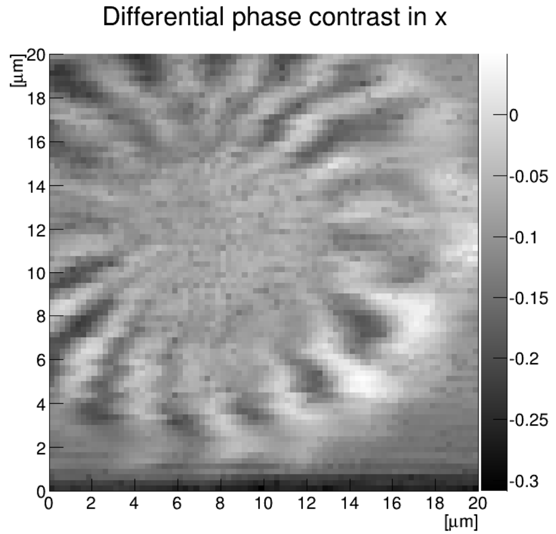


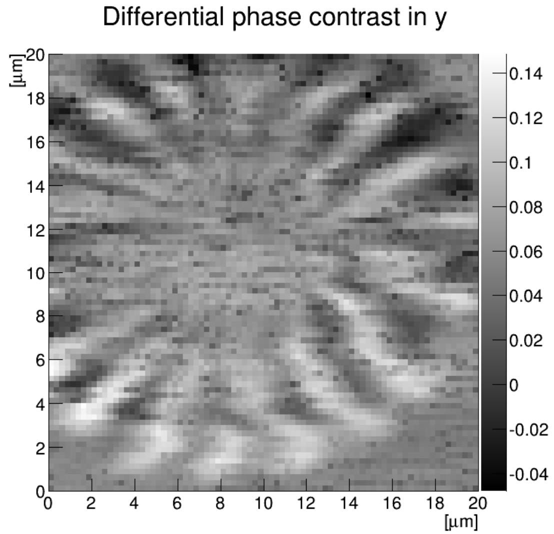
Scan of Siemens star

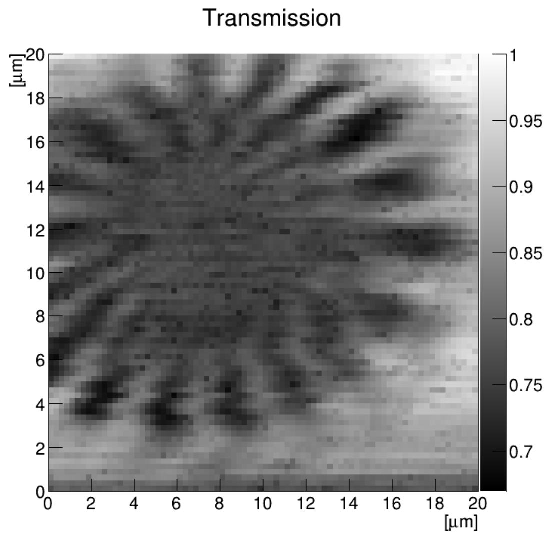
Diameter: 20 μm

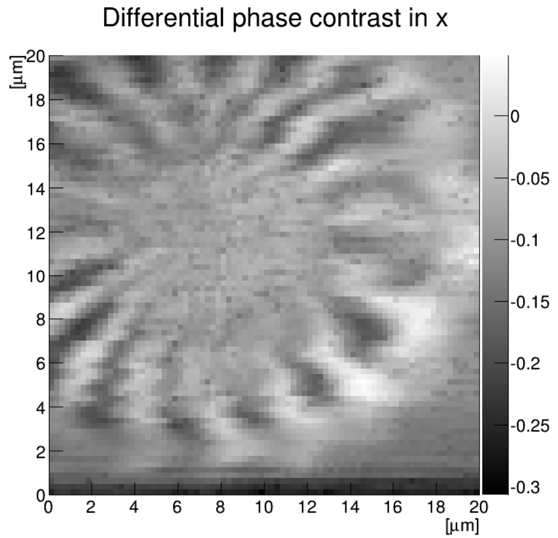
RESULTS - EXPERIMENT

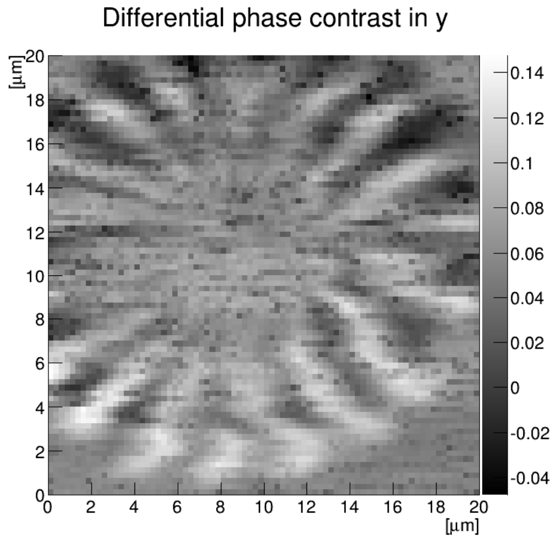
DPC quadrant detector











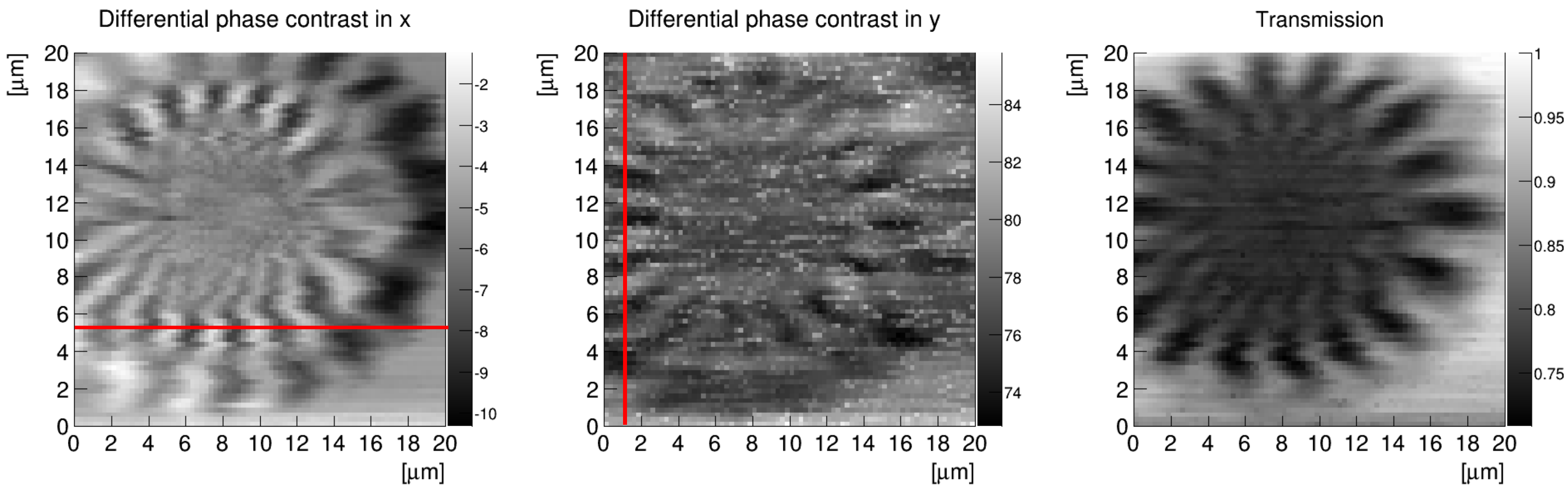
Number of positions: **80 x 80**

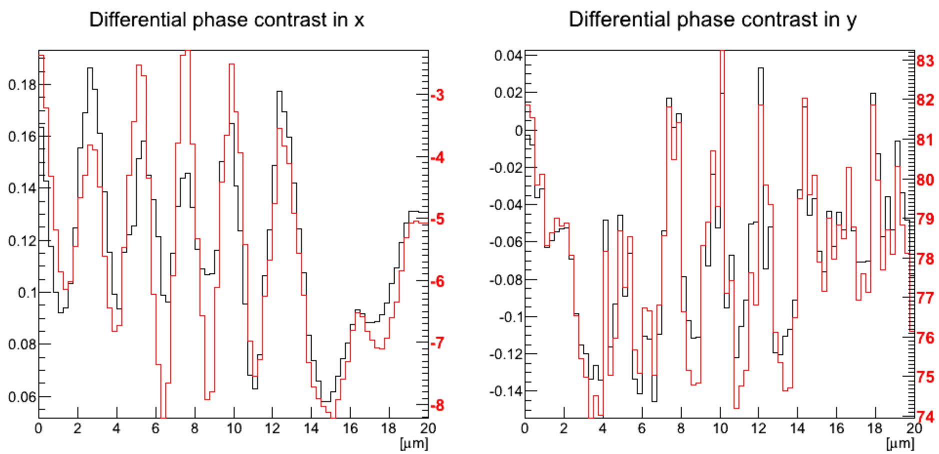
Step size: **250 nm**

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

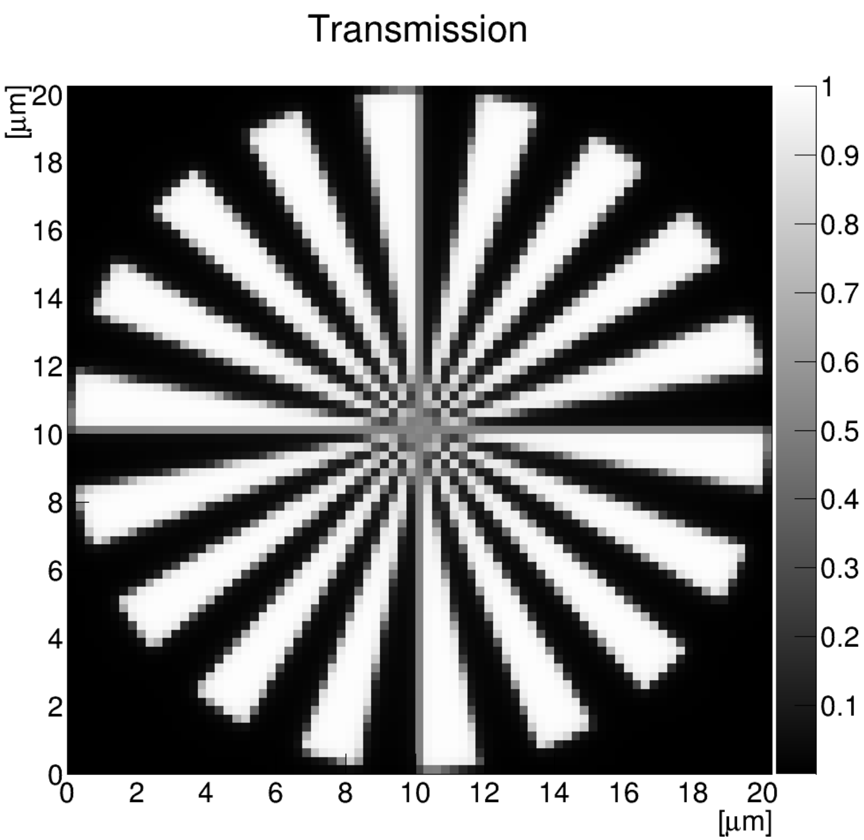
DPC quadrant detector approach in **black**
DPC centre of mass approach in **red**
Horizontal profile: along line $y = 5.25\ \mu m$
Vertical profile: along line $x = 1.25\ \mu m$

Scan of Siemens star

Diameter: 20 μm

RESULTS - SIMULATION

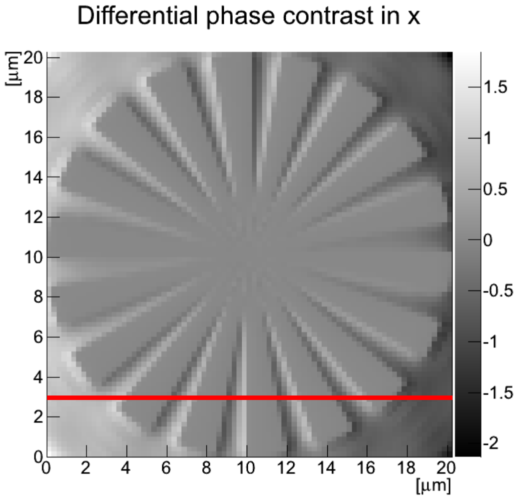
Simulation parameters

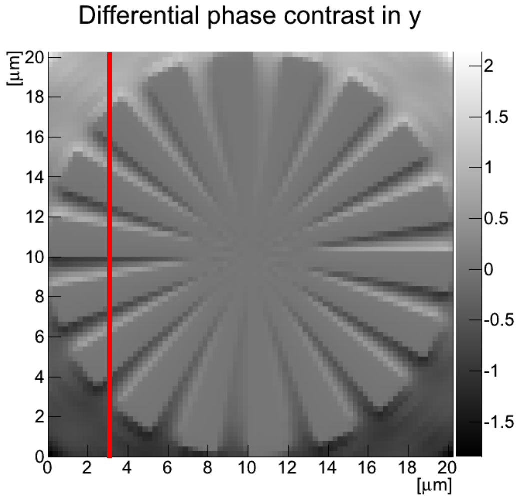


	Siemens star scan
Beam energy	**6.2 keV**
Beam defining pinhole (diameter)	50 µm
Central stop (diameter)	10 µm
Focusing zone plate	Diameter: 50 µm Focal length: 31.25 mm Outermost zone width: 125 nm
Order sorting aperture (diameter)	10 µm
Sample-to-detector distance	**550.4 cm**

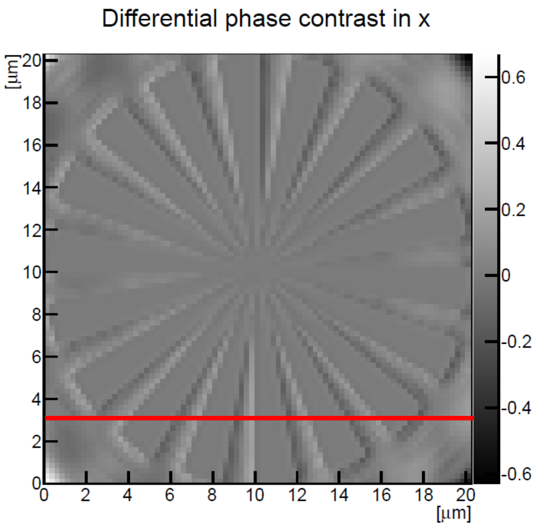
Differential Phase Contrast Analysis

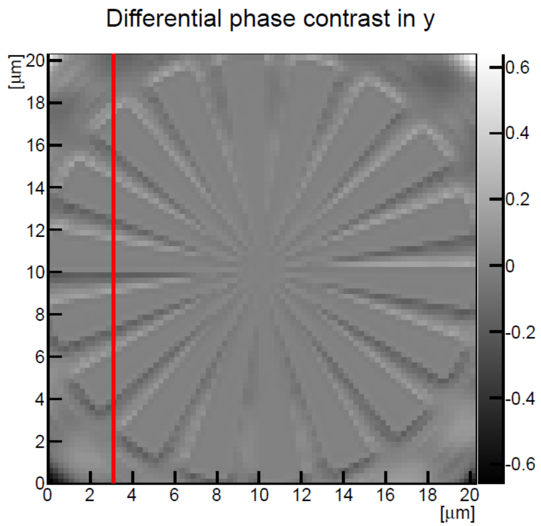
Centre of mass approach



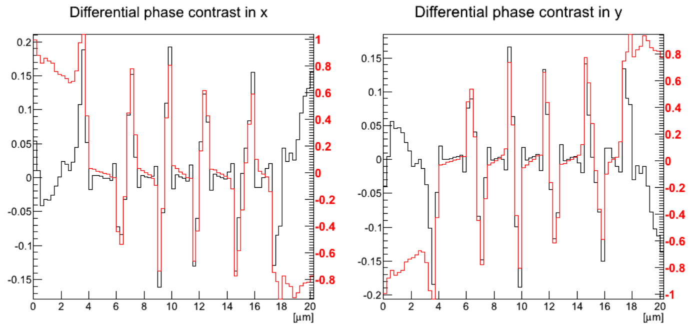


Quadrant detector approach





Number of positions: **81 x 81**
Step size: **250 nm**
ROI: all pixels of the detector

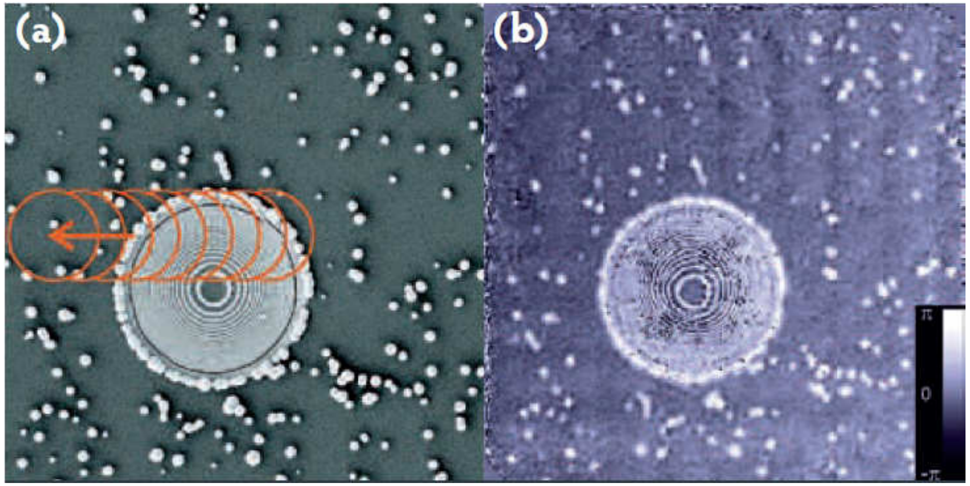


DPC quadrant detector approach in **black**
DPC centre of mass approach in **red**

Horizontal profile: along line $y = 3$ µm
Vertical profile: along line $x = 3$ µm

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*

- **Prerequsite**: 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
A. M. Maiden, J. M. Rodenburg, Ultramicroscopy 109 (2009) 1256

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**.

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Thank you for your attention!