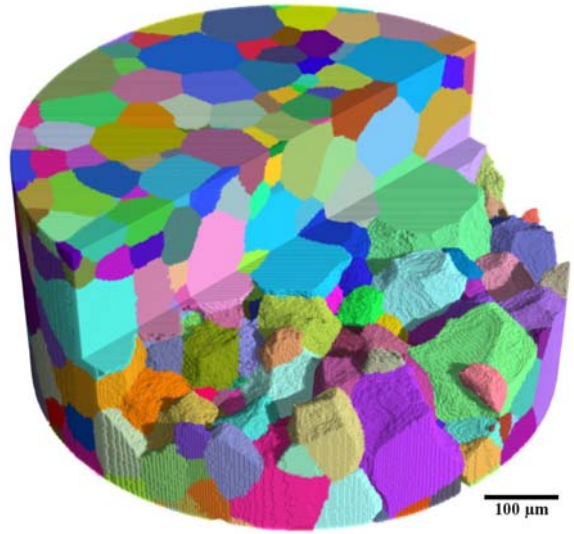
Case for studies of bulk materials at XFEL ?

Henning Friis Poulsen
Risø DTU



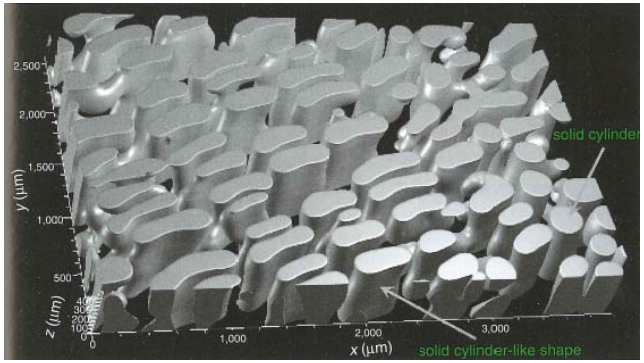
- Ultimate 4D microscope

- X-ray detector with 100 nm resolution
- Alternative algorithm to hybrid-input-output

Materials science in 3D

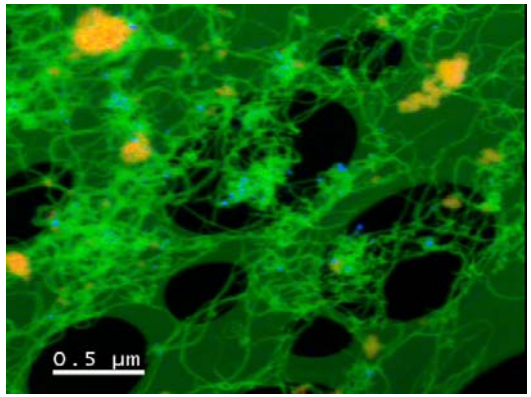
Sectioning + optical microscopy

Sample 1cm, Res: 2 µm



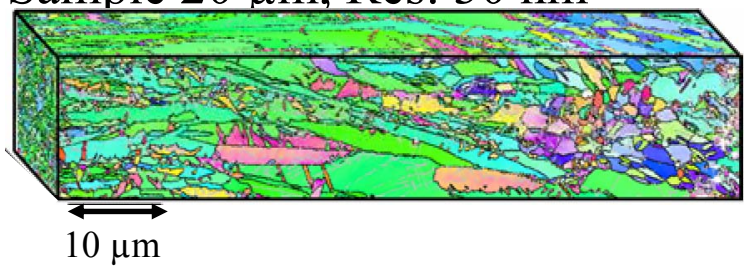
TEM tomography

Sample 500 nm. Res 5 nm



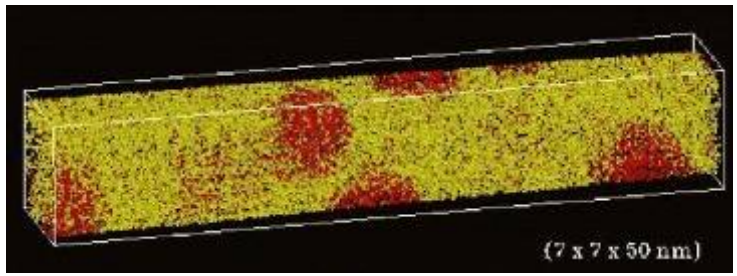
FIB+EBSD:

Sample 20 µm, Res: 30 nm

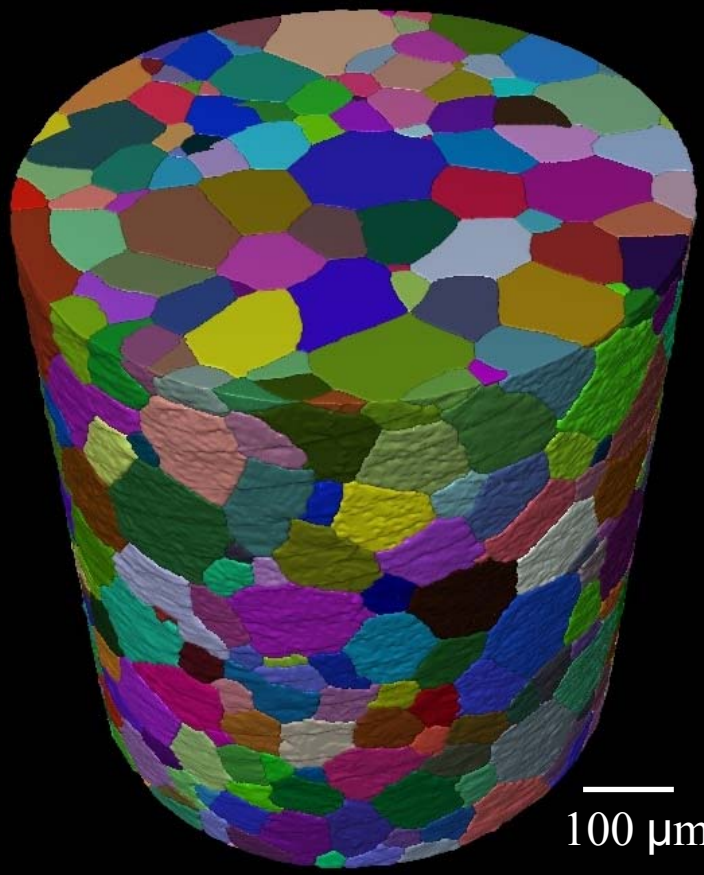


3D Atom Probe

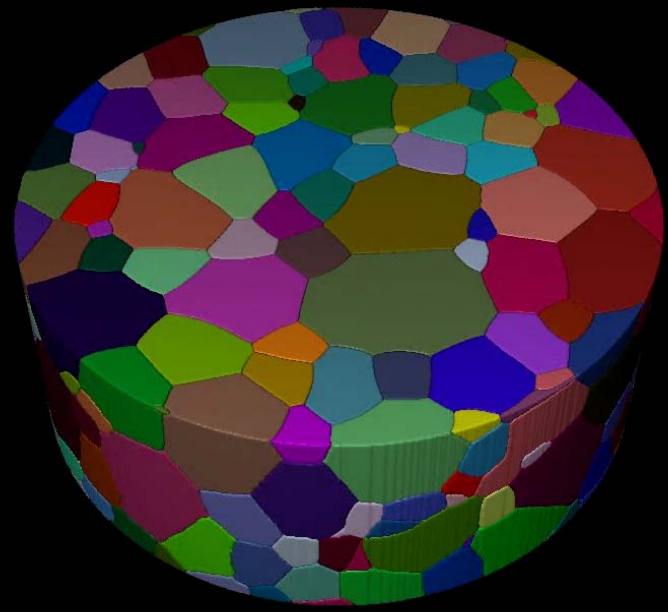
Sample 30 nm. Res 1 Å



Materials science in 4D



Diffraction contrast tomography



Phase field simulations

Risø: E.M. Lauridsen, S. Poulsen, A. Lyckegaard.

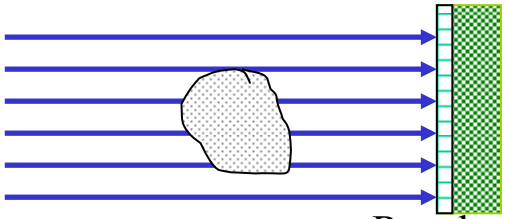
Northwestern: P. Voorhees, I. McKenna

Navy Resarch Lab: R. Fonda

ESRF: W. Ludwig, A. King, S. Rolland

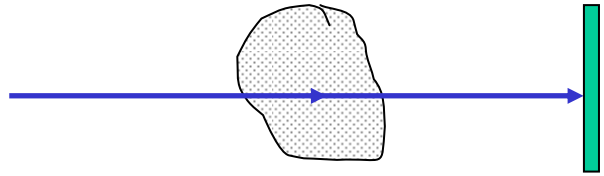
4D going Nano

Parallel beam geometry:



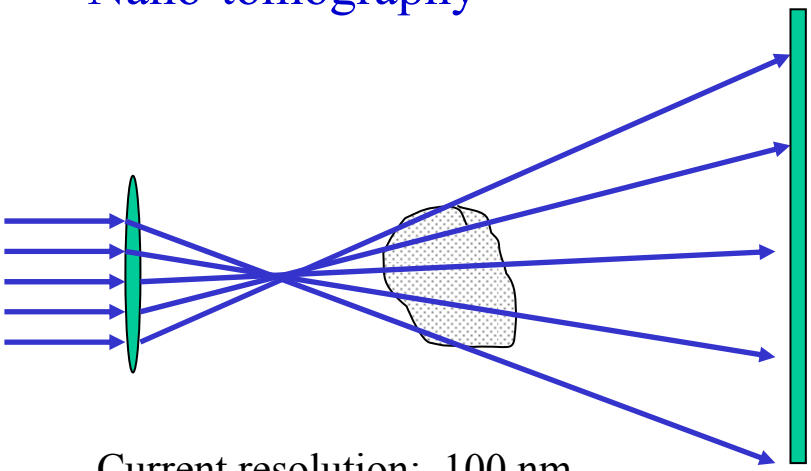
Resolution: 500 nm

Scanning methods



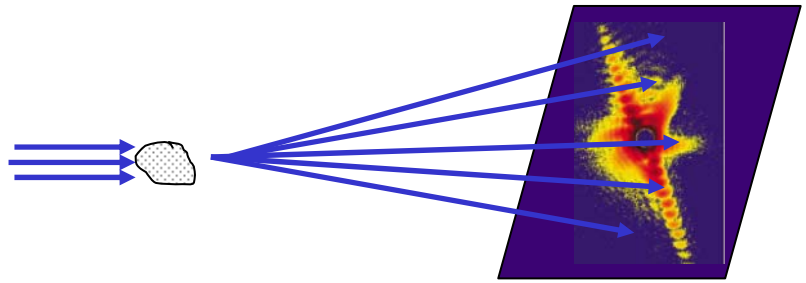
Aim:10 nm (1 nm)

Nano-tomography



Current resolution: 100 nm

Coherent scattering



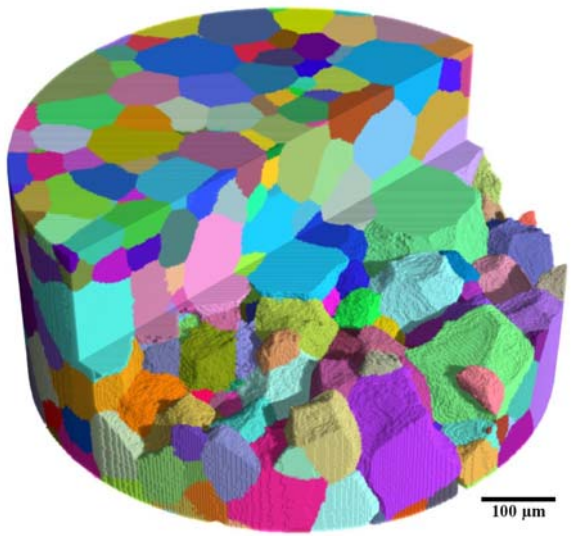
Farfield

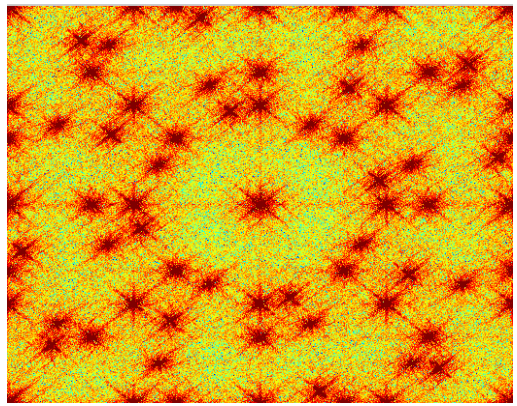
Current resolution: 5 nm

XFEL as ultimate 4D microscope

Penetration: ✓ (third harmonic)
Beam damage. ✓ (third harmonic + largish beam)
Time structure ✓

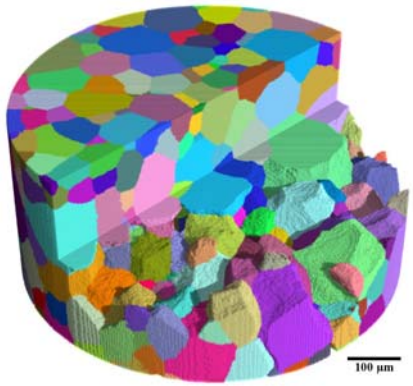
Problem: Complexity





Solution: decrease size of solution space

A priori information



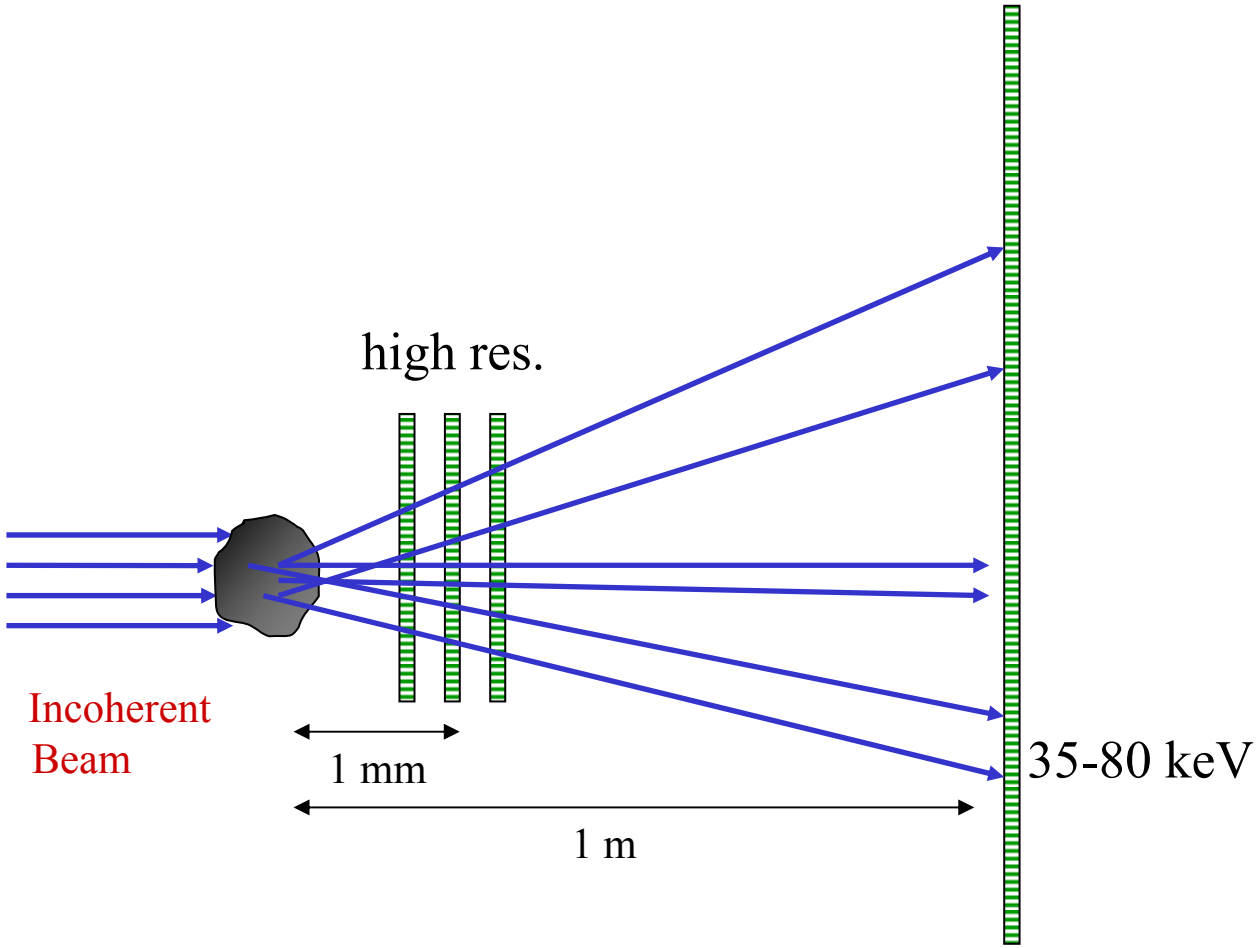
- Discrete objects.
- Space filling
- Smoothness
- Approx. polyhedra

Combine direct space and
Fourier space imaging

Blurred image from direct space
as starting point for
Fourier space reconstruction

Restoration:

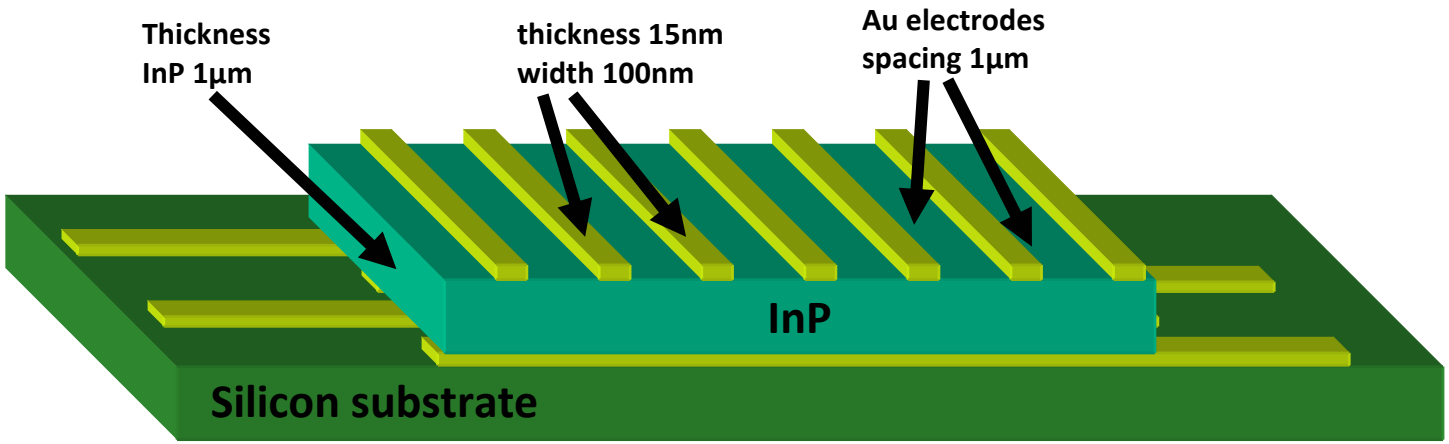
Nanoscope @ ID11, ESRF



G. Vaughan, J. Wright, L. Margulies, U.L. Olsen, S. Schmidt

Nano-detector

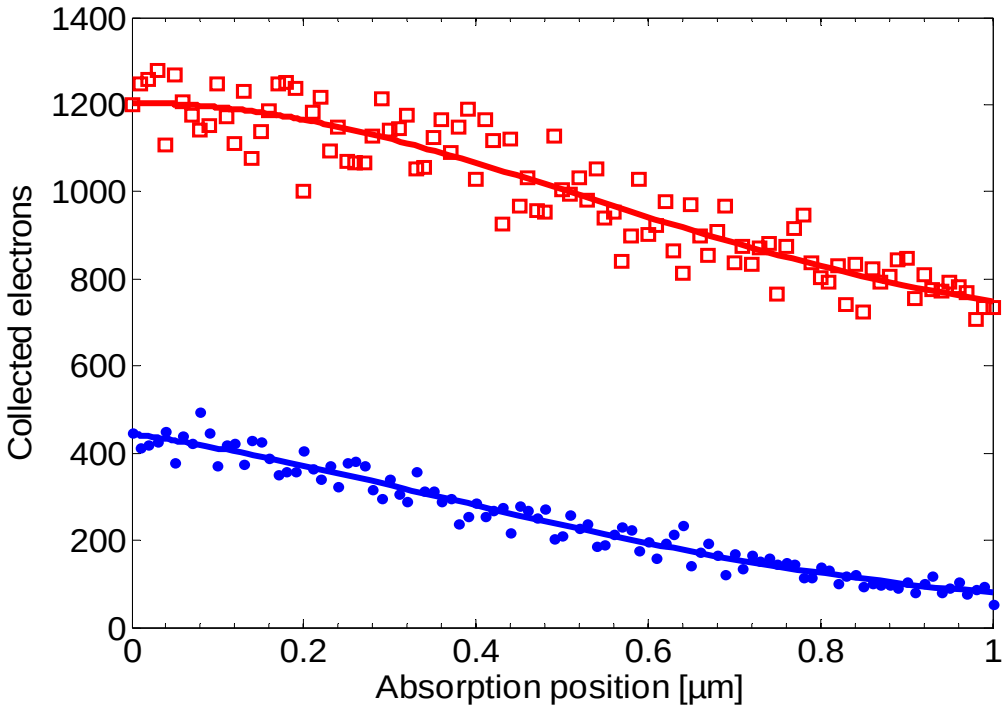
Work by U.L. Olsen, S. Schmidt

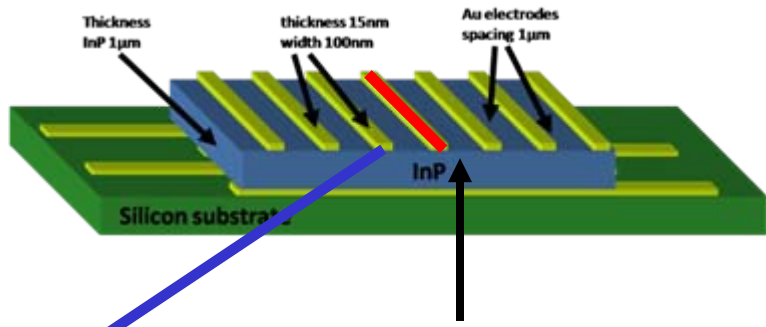


- 10 – 200 keV
- Single photon counting
- Spatial resolution: 100 nm
- Flux: 10^9 at synchrotron
- Efficiency: 3% at 35 keV

3D by stacking

Simulated Performance





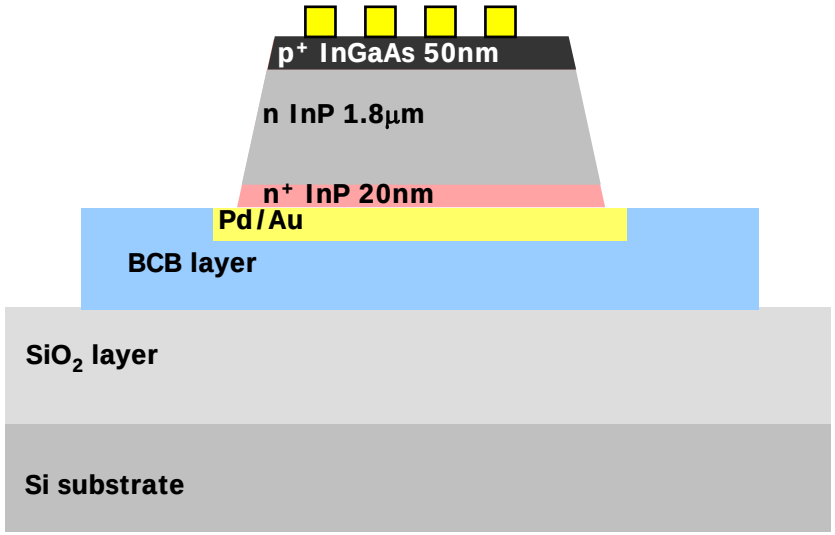
absorption position

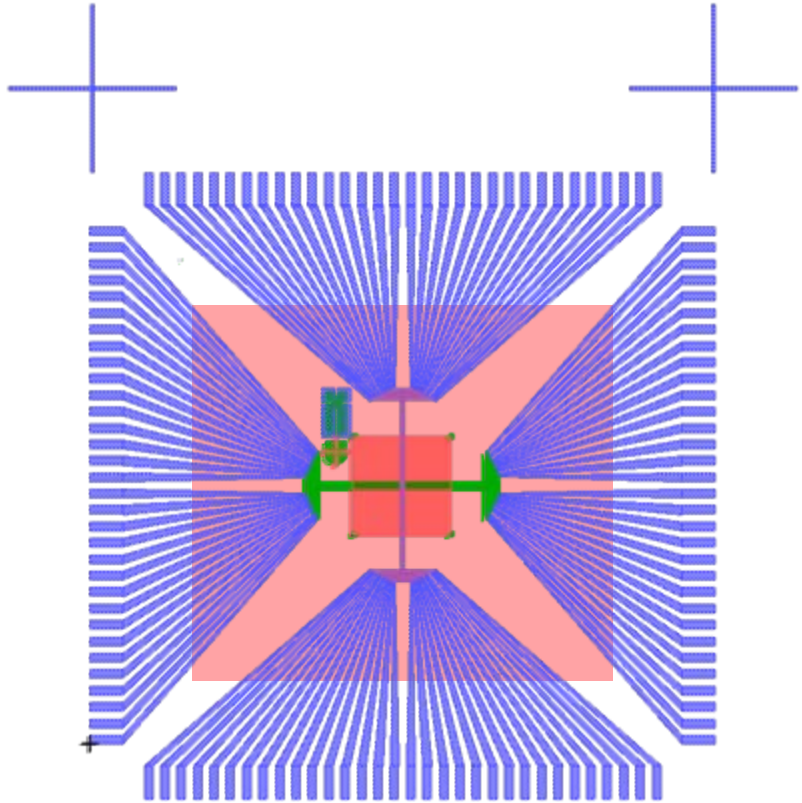
- 10keV photon - 2500 e/h pairs
- 150 –e typical electronic noise
- Absorption in middle of sensor

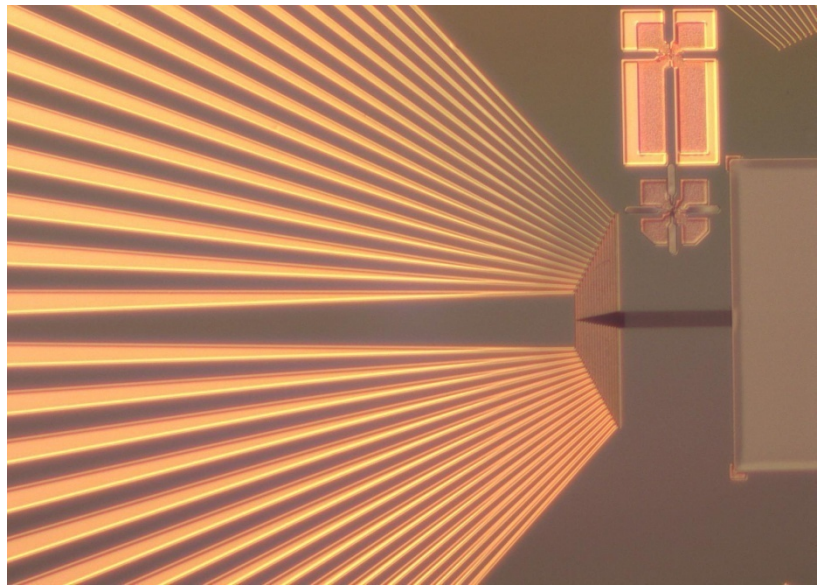
112 nm FWHM

Proof-of-principle

Collaboration with DTU, Denmark:
L. Ottaviano, K. Yvind





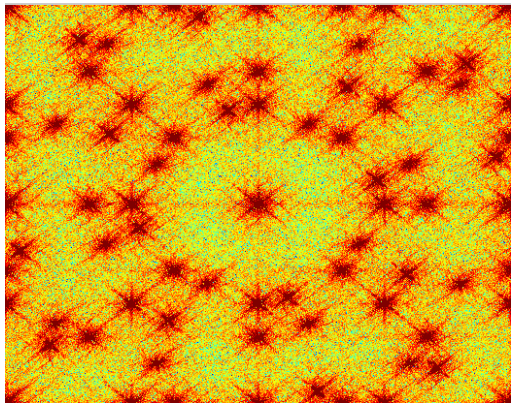


Challenges with hybrid-input-output for polycrystals

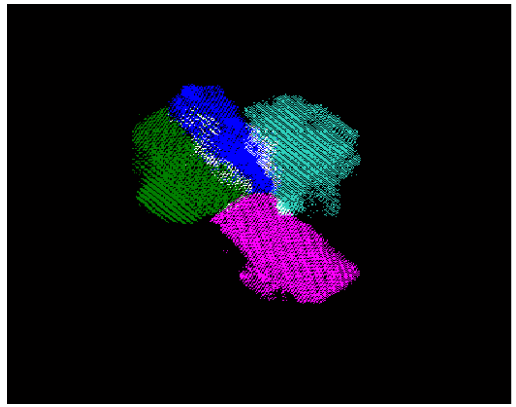
A. Alpers

Phantom

Fourier Transform



Iterative input-output



Problem: overlap of the FTs of the individual shape functions (e.g., symmetry important for phase retrieval)

Work with G. Herman, CUNY

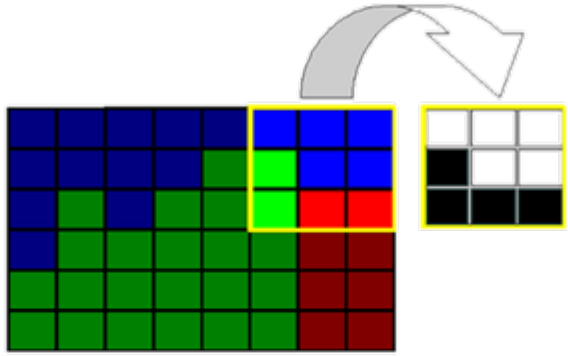
Monte Carlo approach

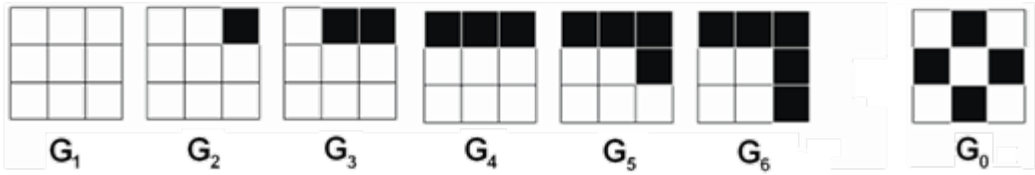
Objective function: $H(f) + \alpha \left\| P(f) - P_0 \right\|_1$

A-priori information term (e.g. shape)

Projection term

Gibbs priors on shape:

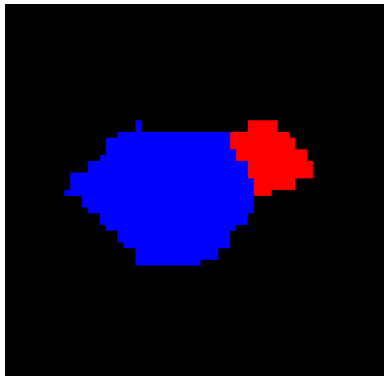




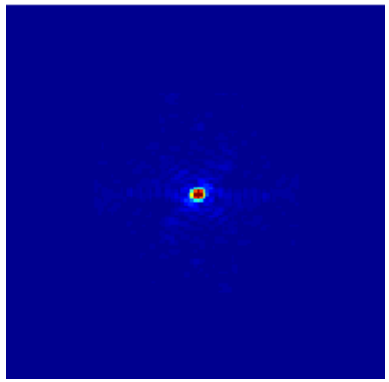
A. Alpers *et al.* *J. Appl. Cryst*. **39** (2006), 582-588.

Extreme case: complete overlap

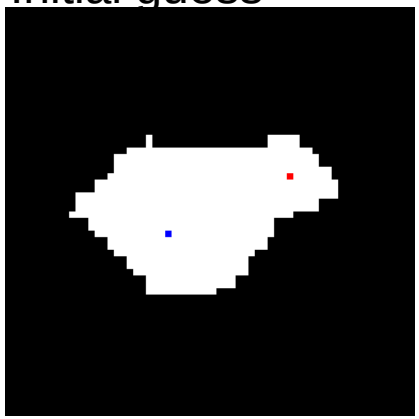
Phantom



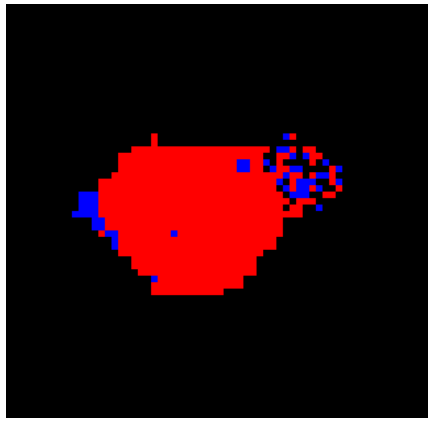
Fourier Transform



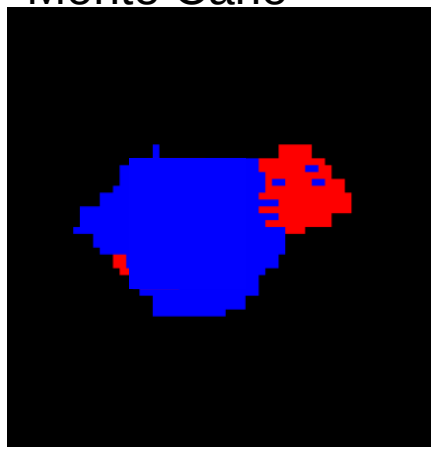
Initial guess



HIO



Monte Carlo



Specifications for bulk materials

- Option for third harmonics

- In situ processing
- Focus on algorithms

- Coupling with direct space imaging