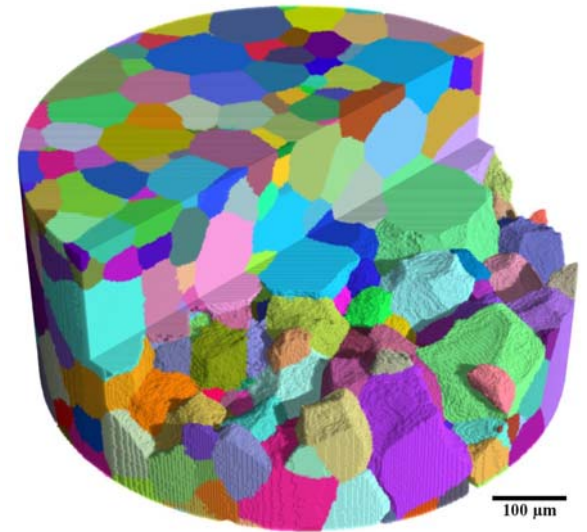


Case for studies of bulk materials at XFEL ?

Henning Friis Poulsen
Risø DTU

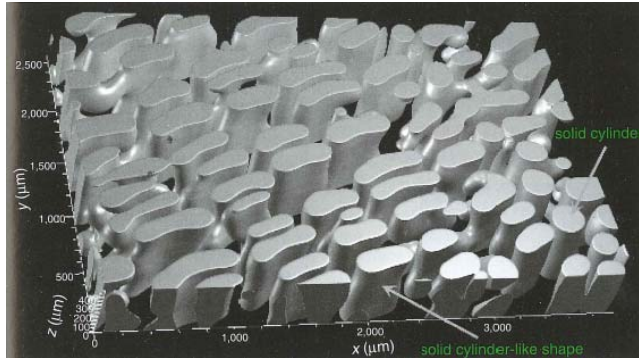
- Ultimate 4D microscope
- X-ray detector with 100 nm resolution
- Alternative algorithm to hybrid-input-output



Materials science in 3D

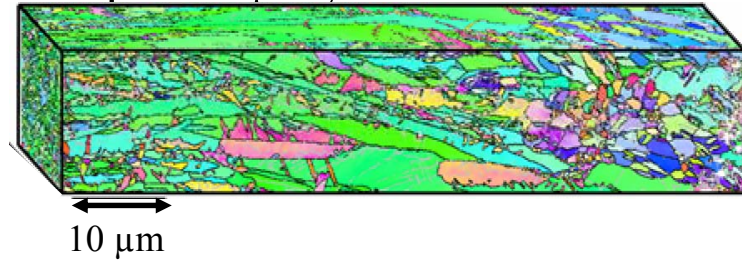
Sectioning + optical microscopy

Sample 1cm, Res: 2 μm



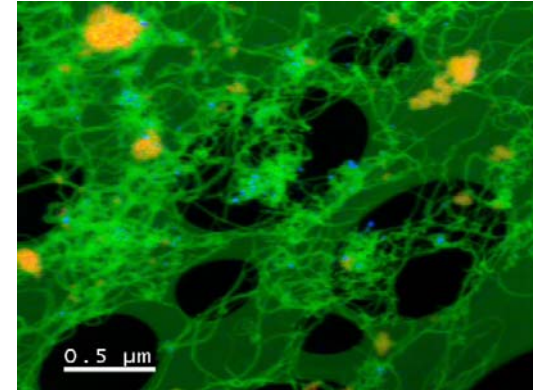
FIB+EBSD:

Sample 20 μm , Res: 30 nm



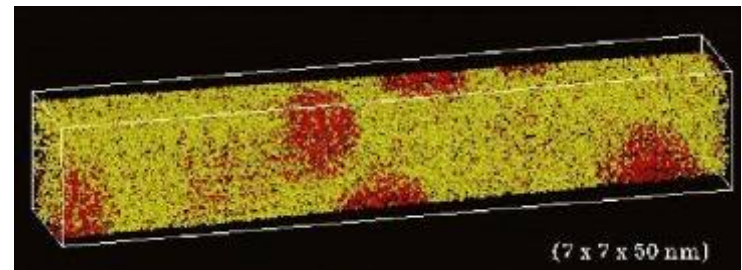
TEM tomography

Sample 500 nm. Res 5 nm

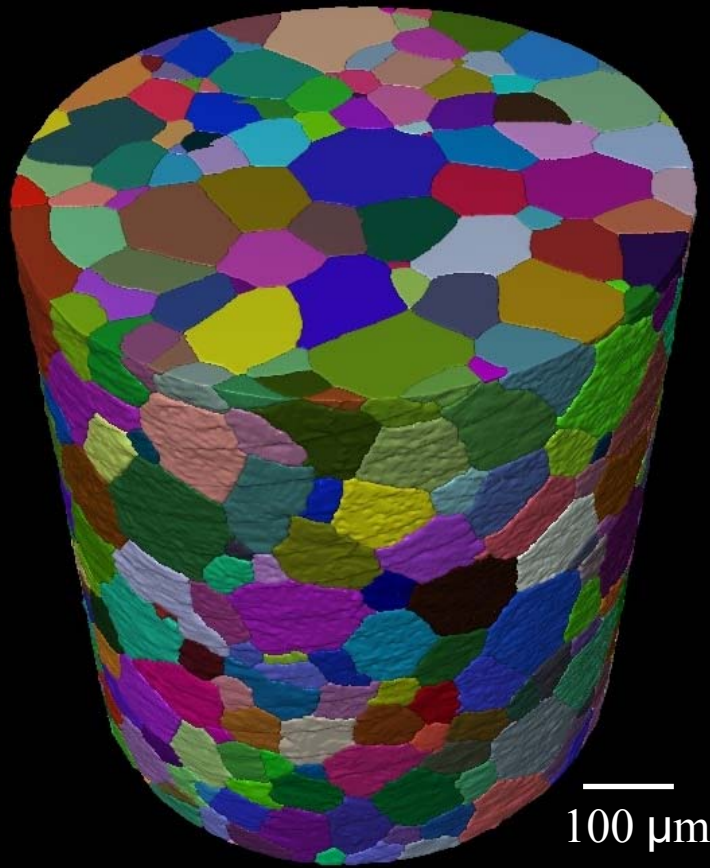


3D Atom Probe

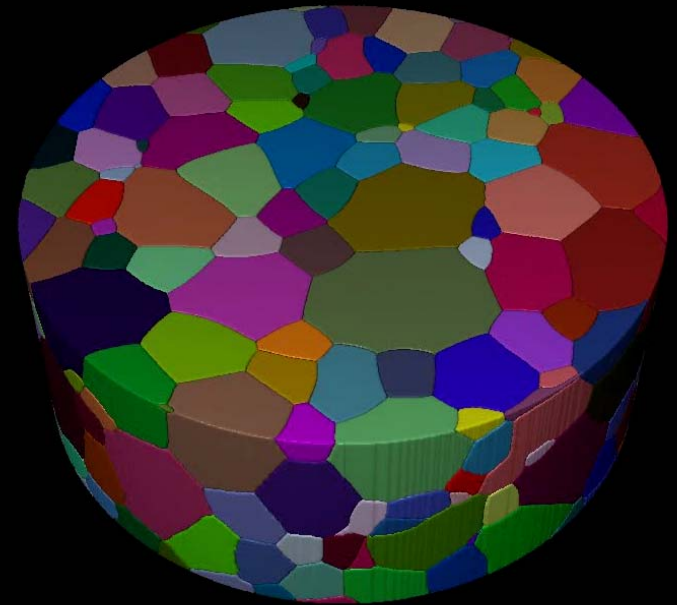
Sample 30 nm. Res 1 \AA



Materials science in 4D



Diffraction contrast tomography



Phase field simulations

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

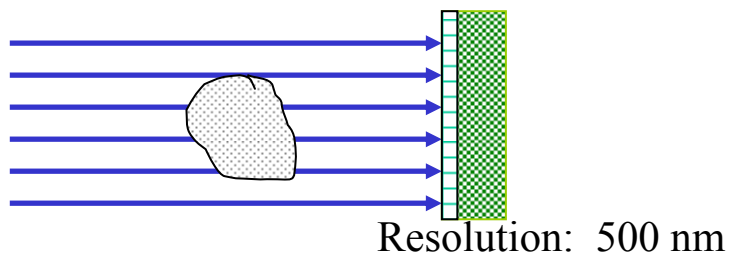
Northwestern: P. Voorhees, I. McKenna

Navy Resarch Lab: R. Fonda

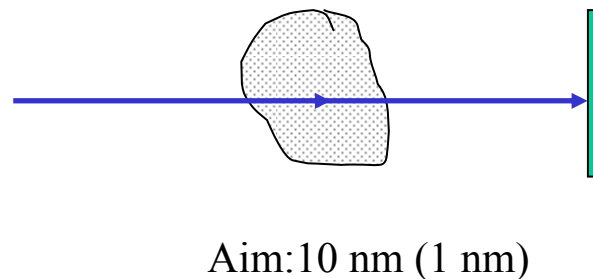
ESRF: W. Ludwig, A. King, S. Rolland

4D going Nano

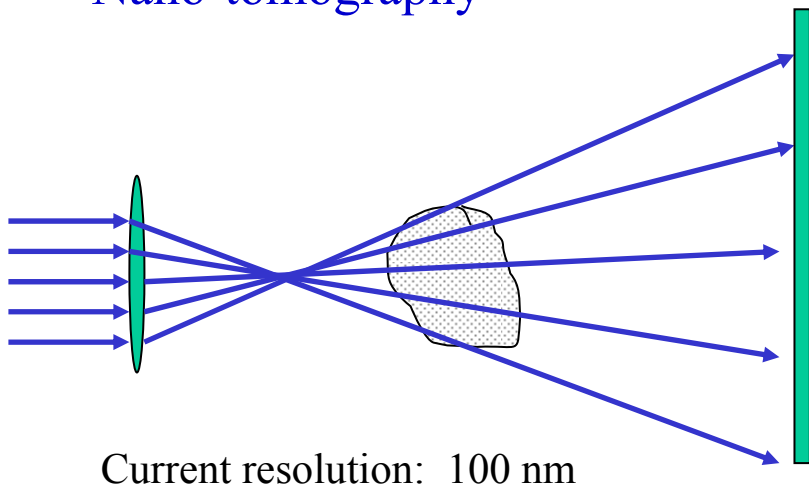
Parallel beam geometry:



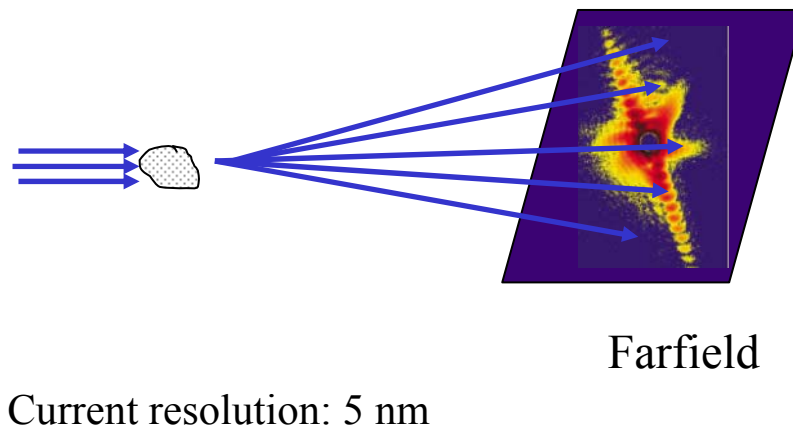
Scanning methods



Nano-tomography



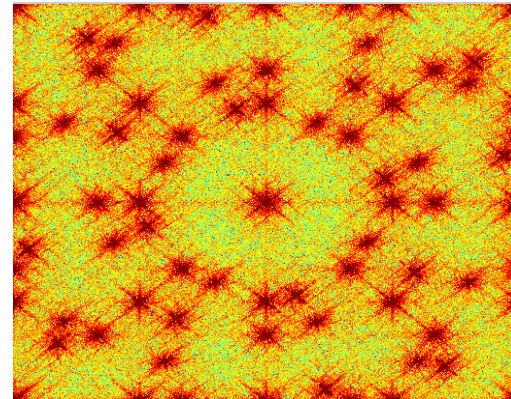
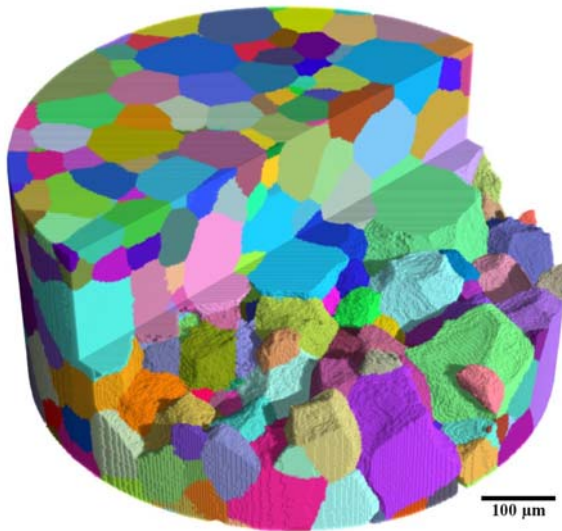
Coherent scattering



XFEL as ultimate 4D microscope

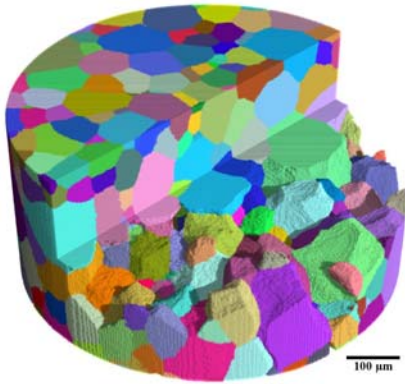
- Penetration: ✓ (third harmonic)
- Beam damage. ✓ (third harmonic + largish beam)
- Time structure ✓

Problem: Complexity



Solution: decrease size of solution space

A priori information



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

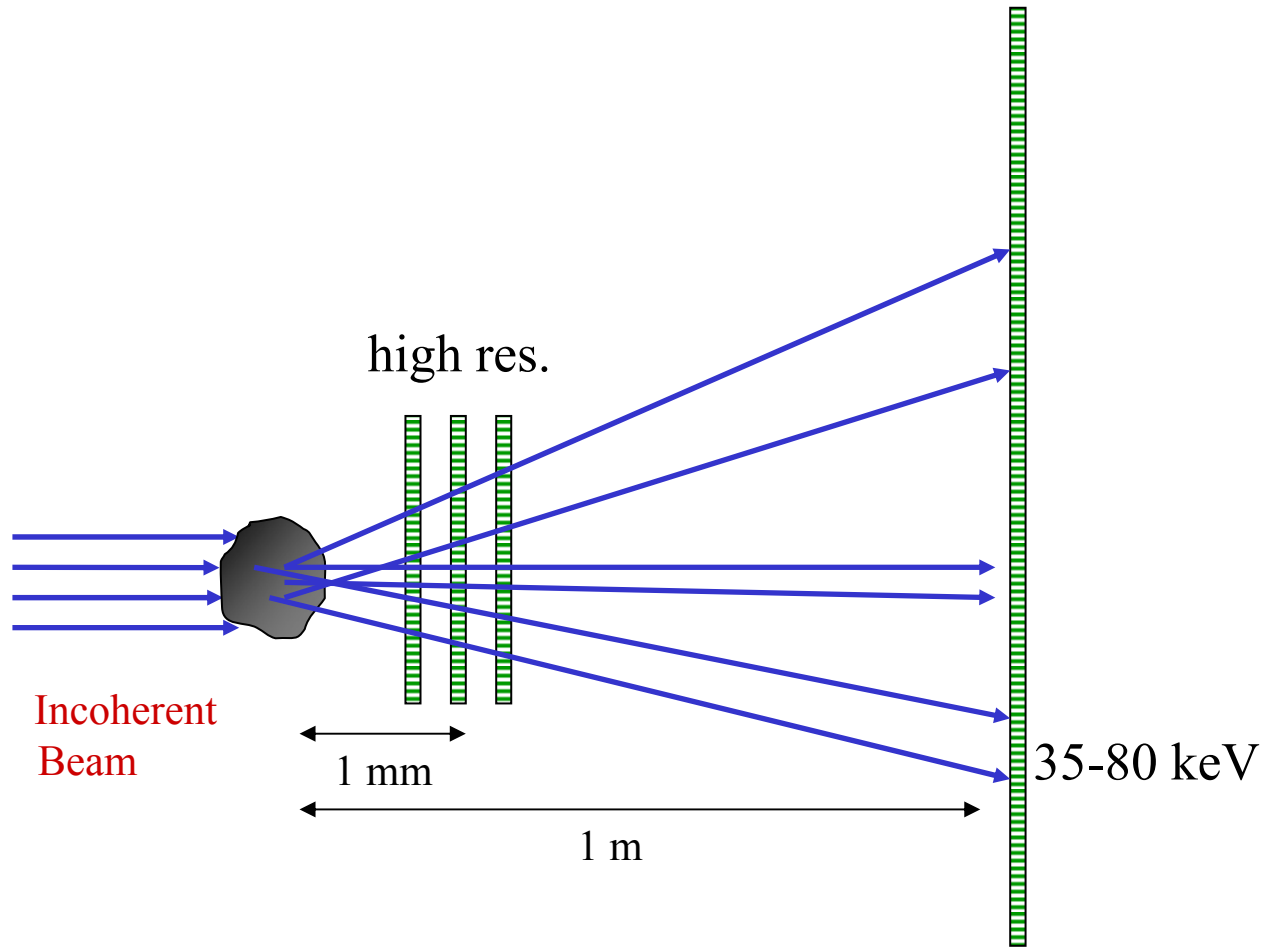
Combine direct space and
Fourier space imaging

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

Restoration:

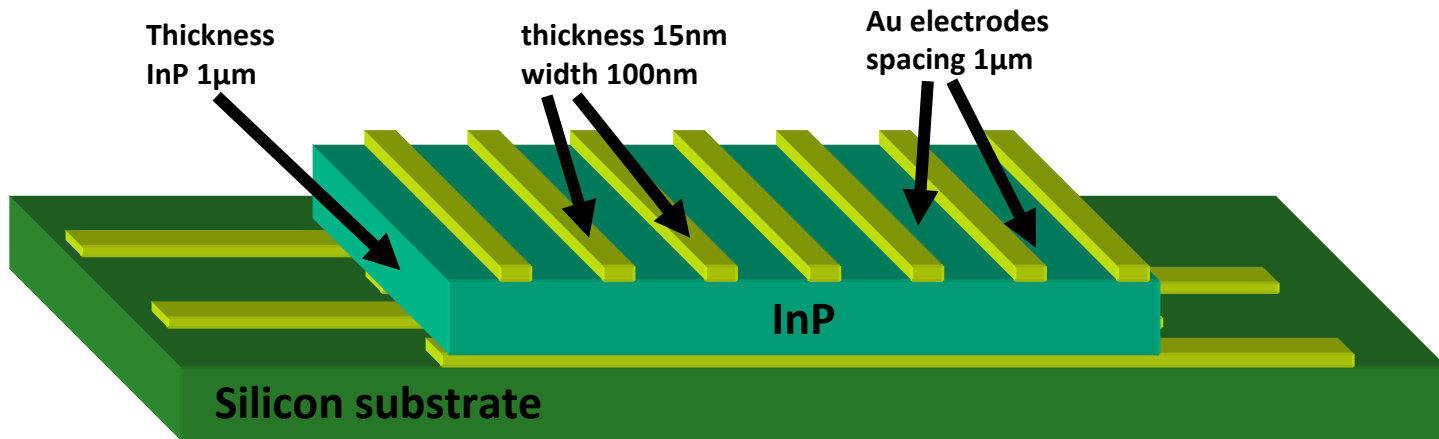


Nanoscope @ ID11, ESRF



Nano-detector

Work by U.L. Olsen, S. Schmidt

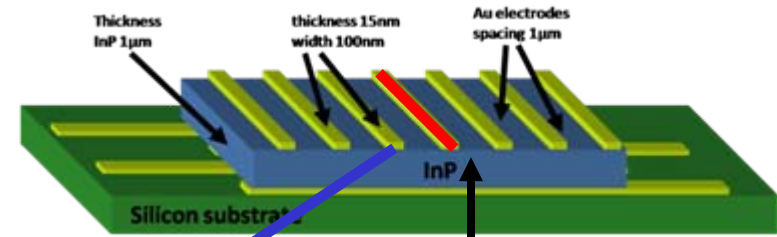
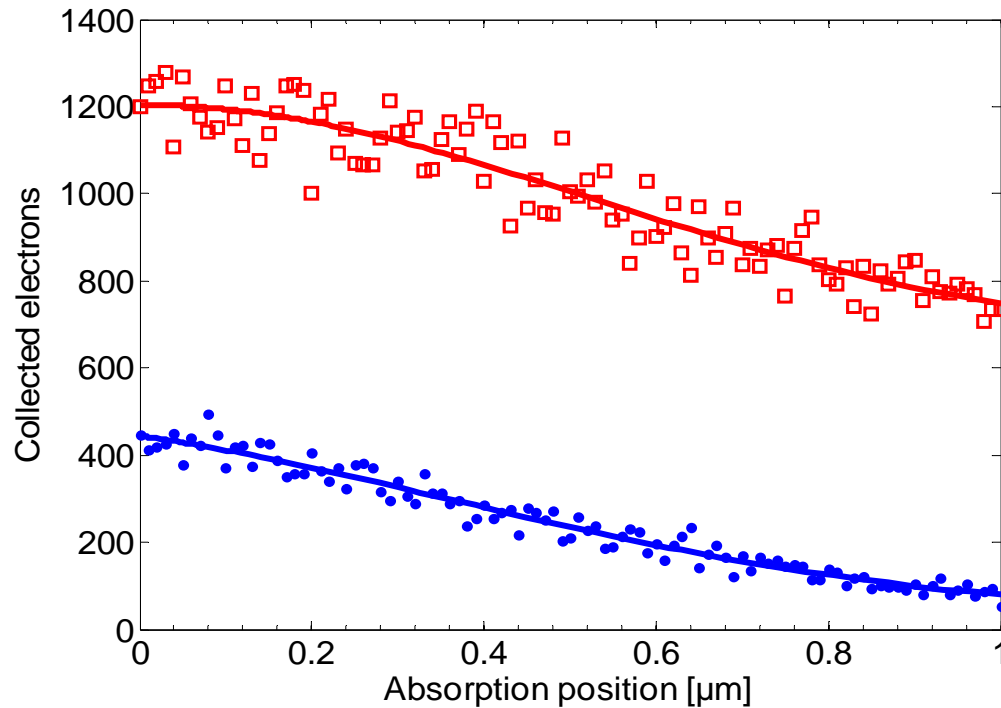


- 10 – 200 keV
- Single photon counting
- Spatial resolution: 100 nm
- Flux: 10^9 at synchrotron
- Efficiency: 3% at 35 keV

3D by stacking



Simulated Performance



absorption
position

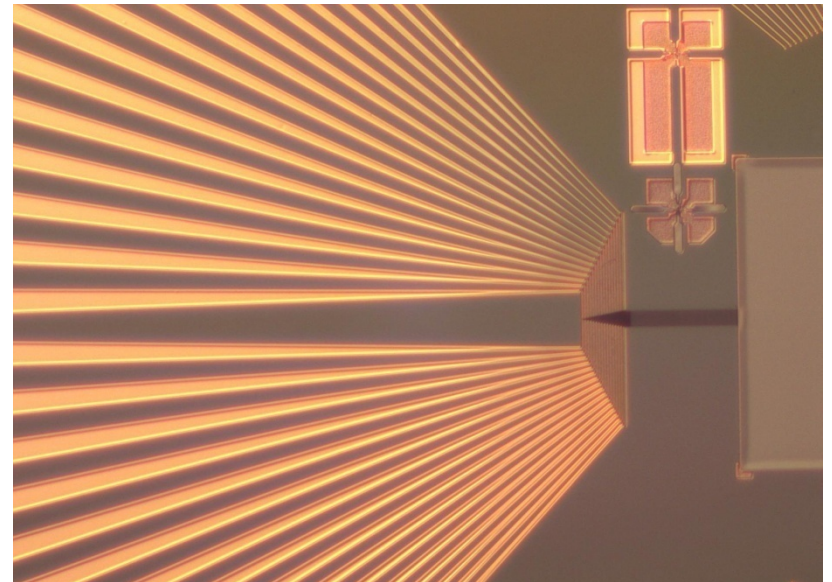
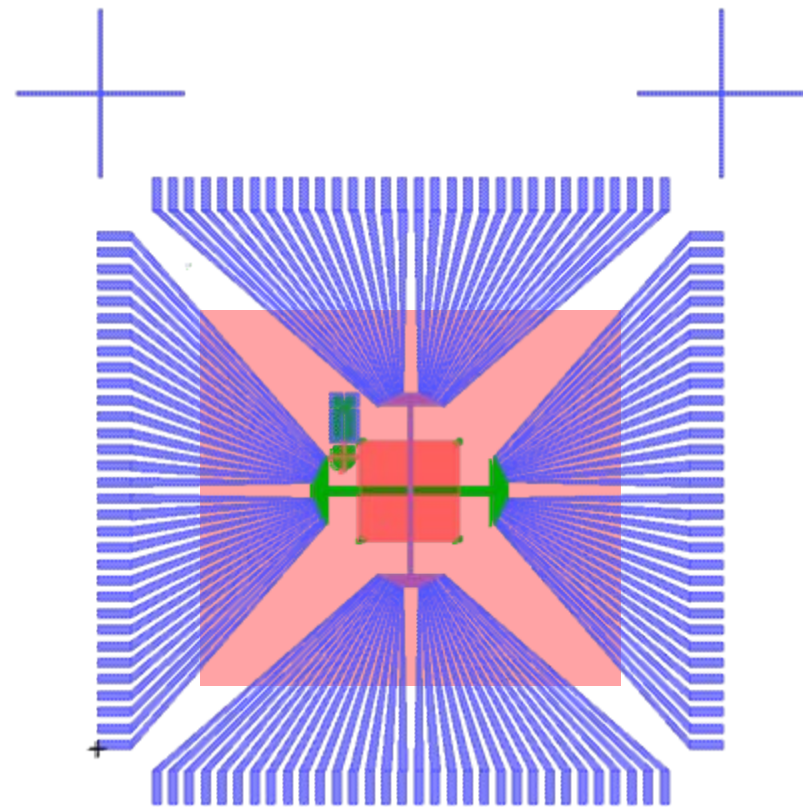
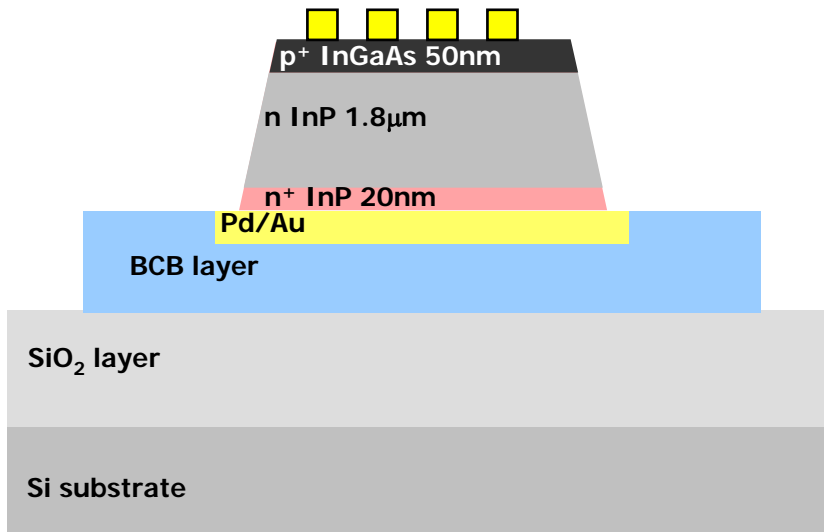
- 10 keV photon - 2500 e/h pairs
- 150 $-e$ typical electronic noise
- Absorption in middle of sensor



112 nm
FWHM

Proof-of-principle

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



Challenges with hybrid-input-output for polycrystals

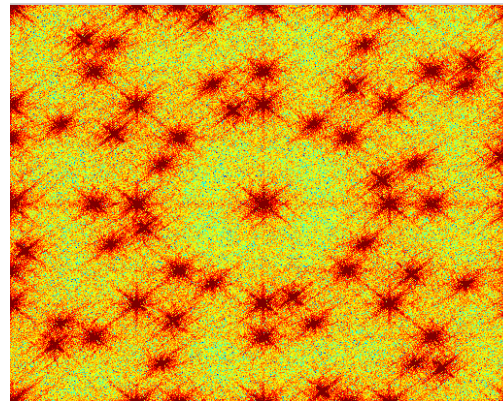


A. Alpers

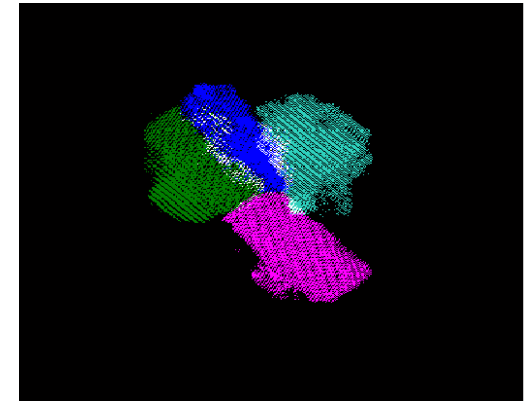
Phantom



Fourier Transform



Iterative input-output



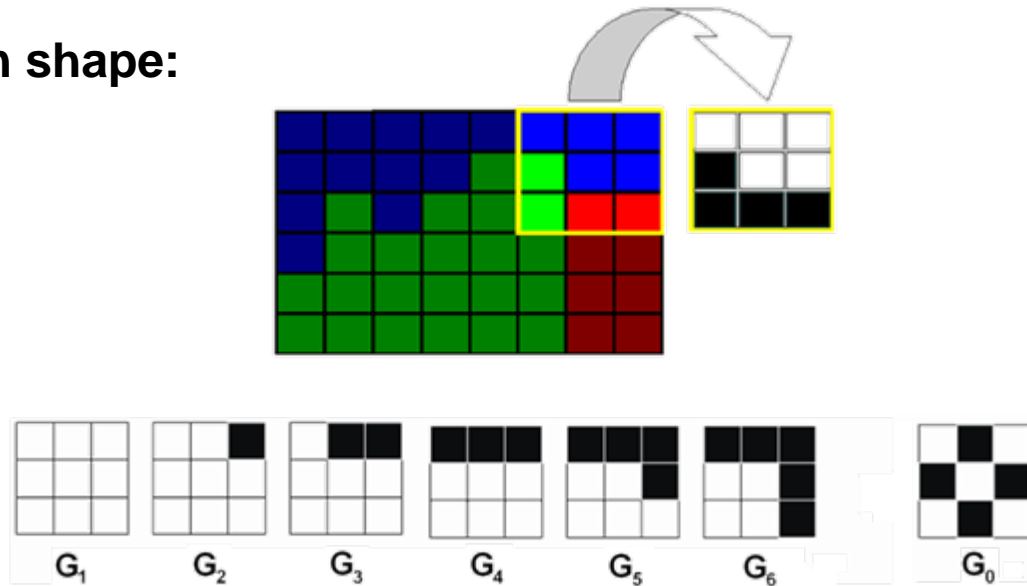
Problem: overlap of the FTs of the individual shape functions
(e.g., symmetry important for phase retrieval)

Monte Carlo approach

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

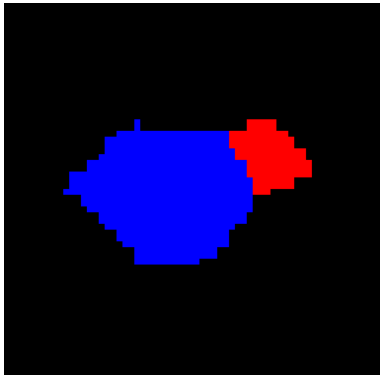
A-priori information term (e.g. shape) Projection term

Gibbs priors on shape:

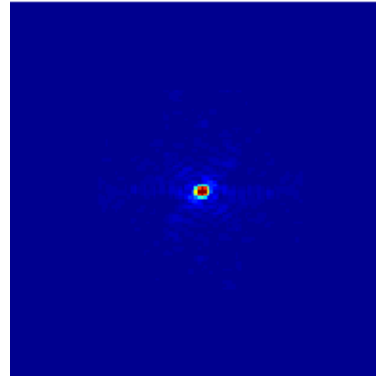


Extreme case: complete overlap

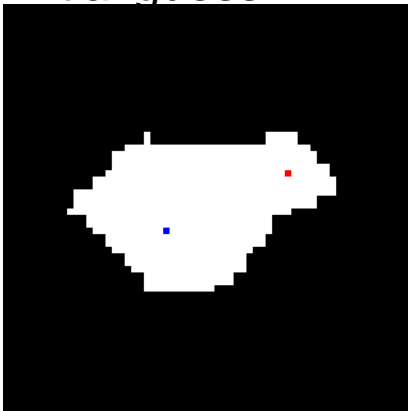
Phantom



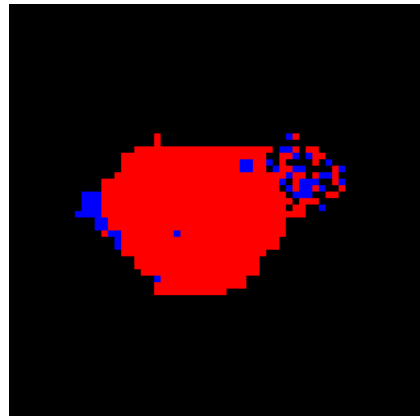
Fourier Transform



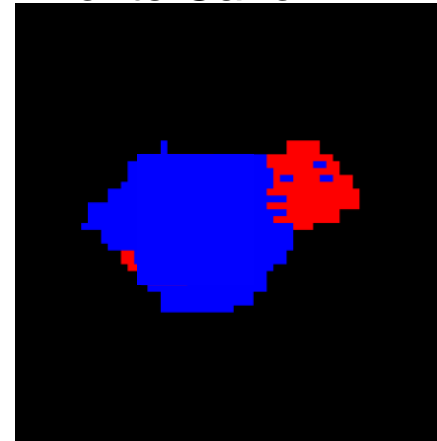
Initial guess



HIO



Monte Carlo



Specifications for bulk materials

- Option for third harmonics
 - In situ processing
 - Focus on algorithms
-
- Coupling with direct space imaging