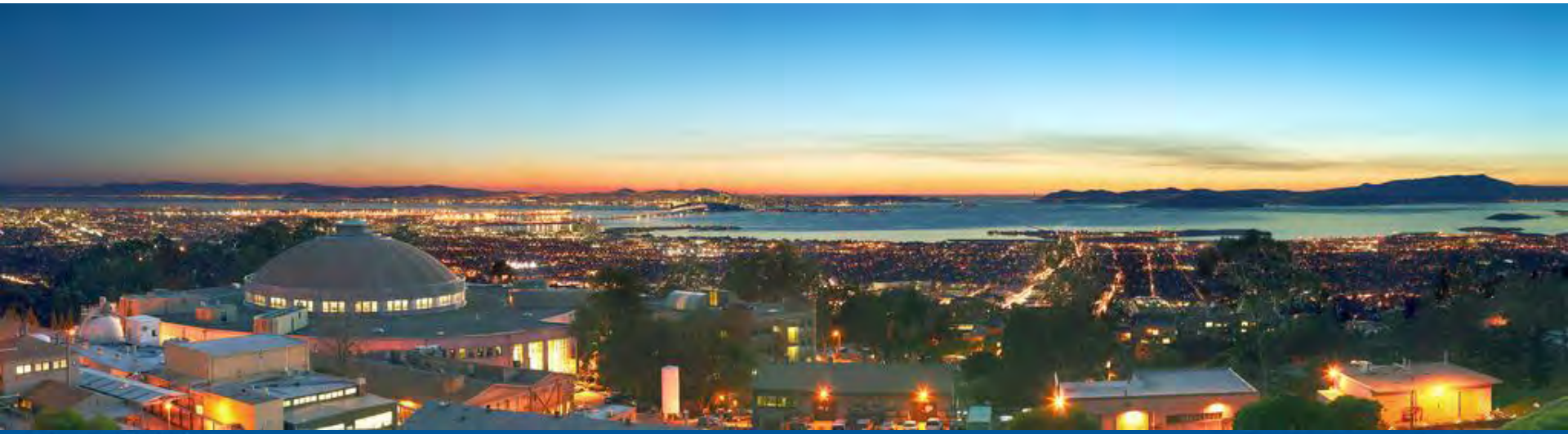
Towards X-ray Microscopy with Wavelength Limited Spatial Resolution: Progress and Applications

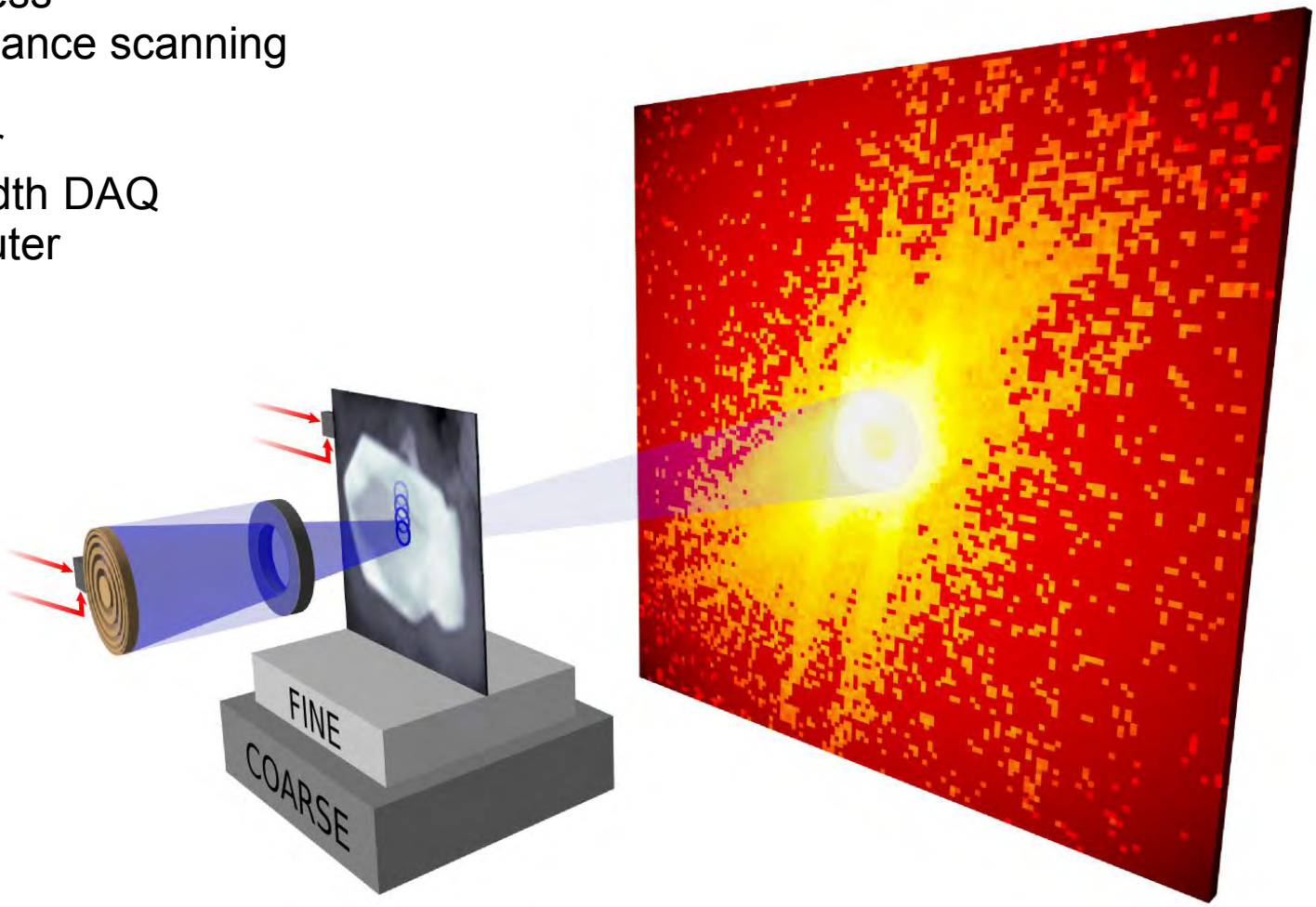
David Shapiro
Advanced Light Source, Lawrence
Berkeley National Lab
dashapiro@lbl.gov



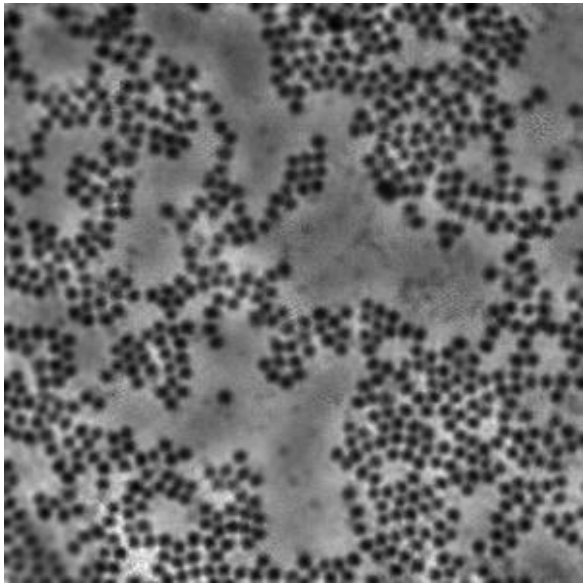
Ptychography: high-NA imaging with low-NA optics

Basic Requirements

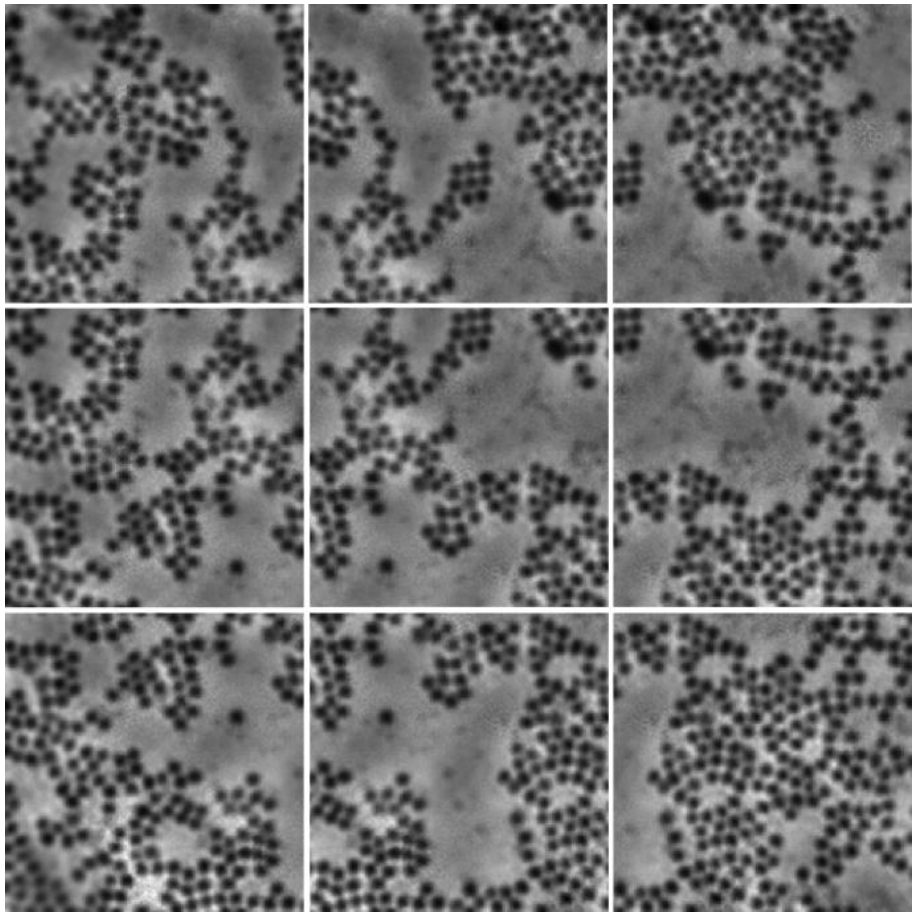
- High brightness
- High performance scanning (fast, stable)
- Fast detector
- High bandwidth DAQ
- Super computer

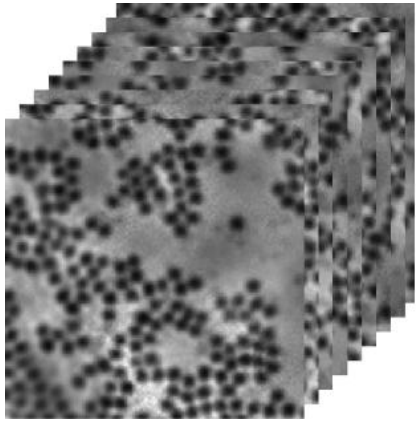


Ptychography makes use of redundant data

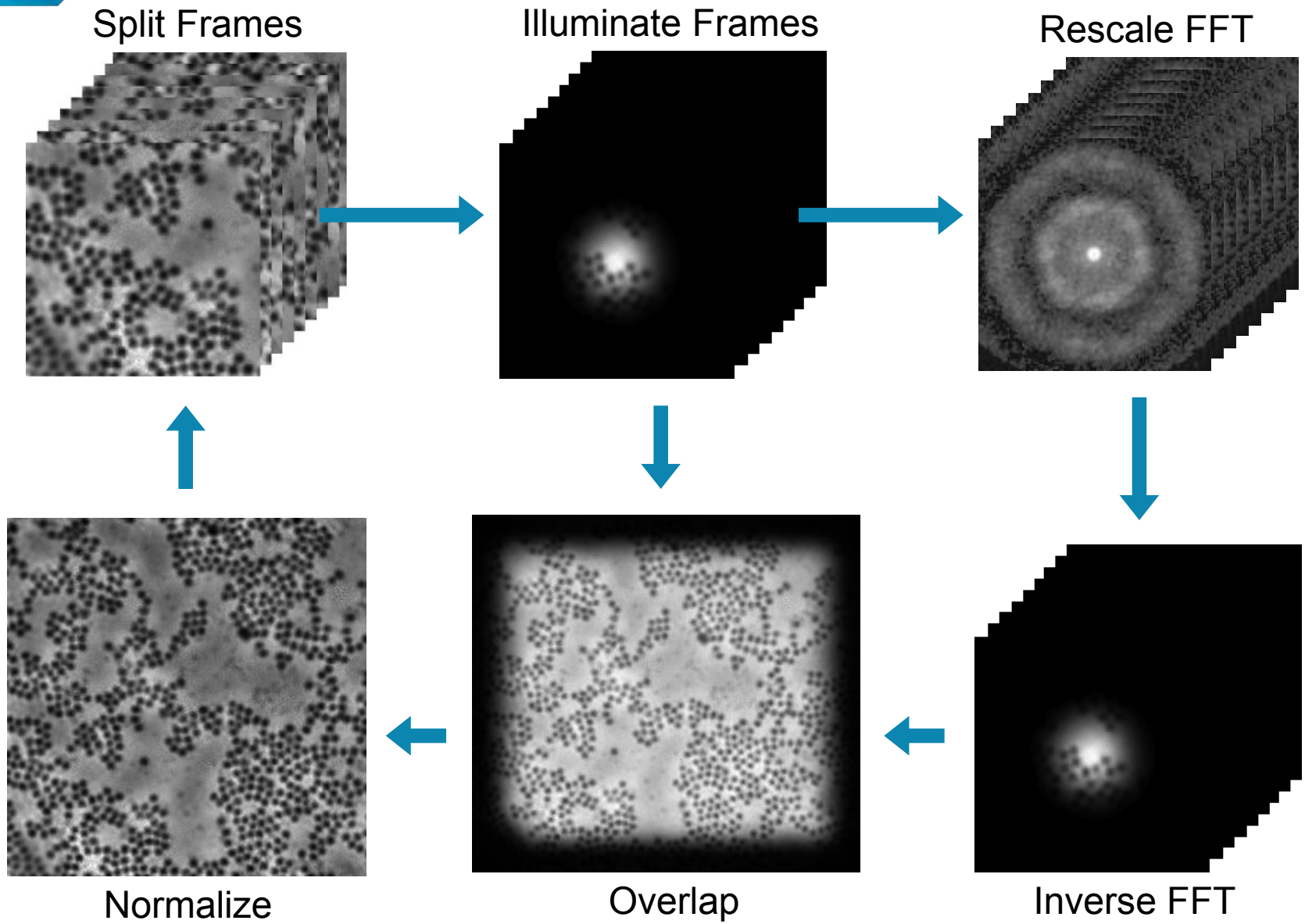


Object is split into frames with known centers
Each frame is illuminated separately
Neighbors overlap





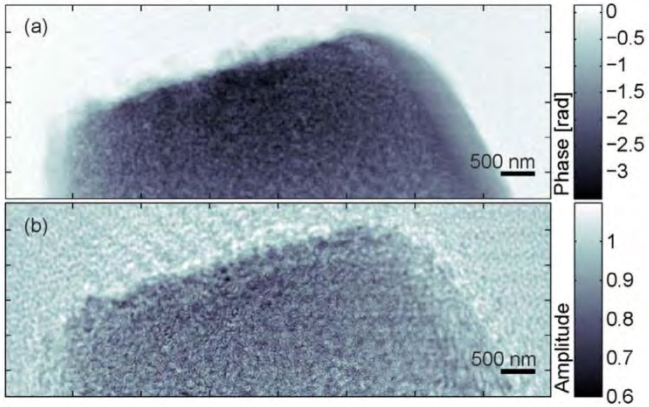
The Basic Iteration



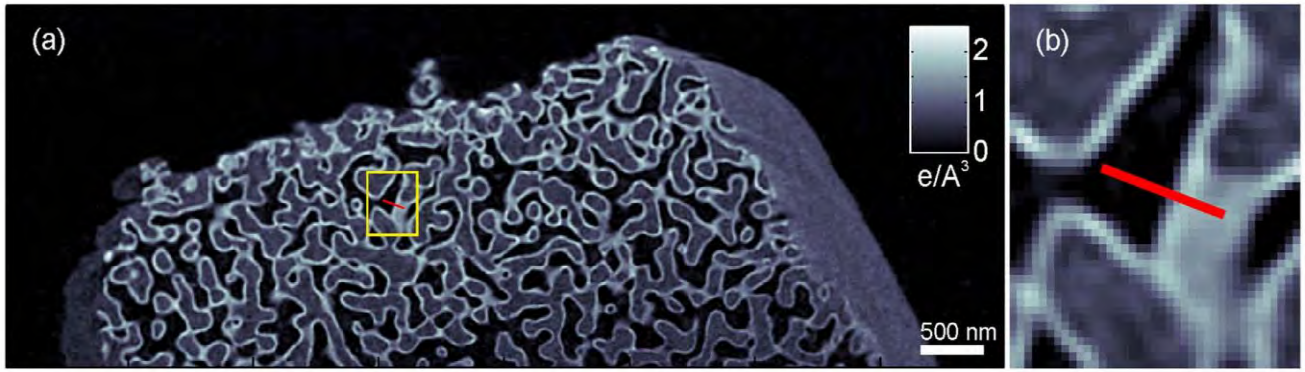
Swiss Light Source: ptycho-Tomography at cSAXS

Table 1 | Estimated resolution of the tomograms reconstructed with different numbers of projections and expected resolution according to Nyquist angular sampling. The FSC analysis was based on the half-bit criterion and was performed by processing two independent tomograms with double angular spacing

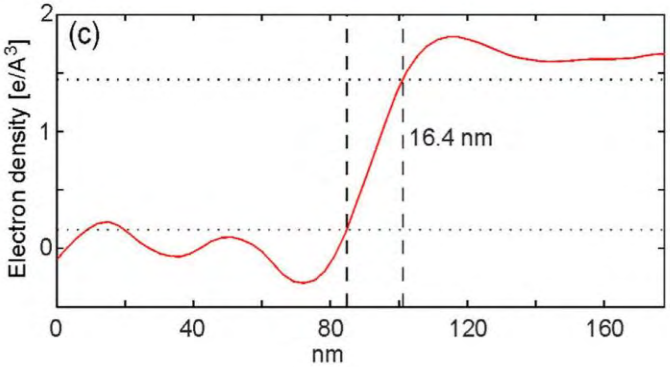
Number of projections	Isotropic 3D resolution [nm]	Expected resolution [nm]
180	58.5	50
360	30.0	25
720	15.9	12.5

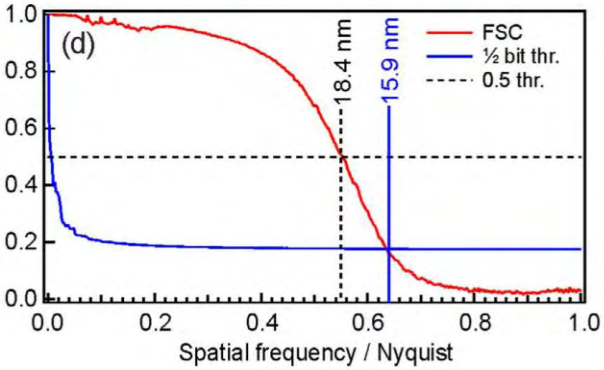


X-ray ptychographic computed tomography at 16 nm isotropic 3D resolution
M. Holler, et al
SCIENTIFIC REPORTS | 4 : 3857



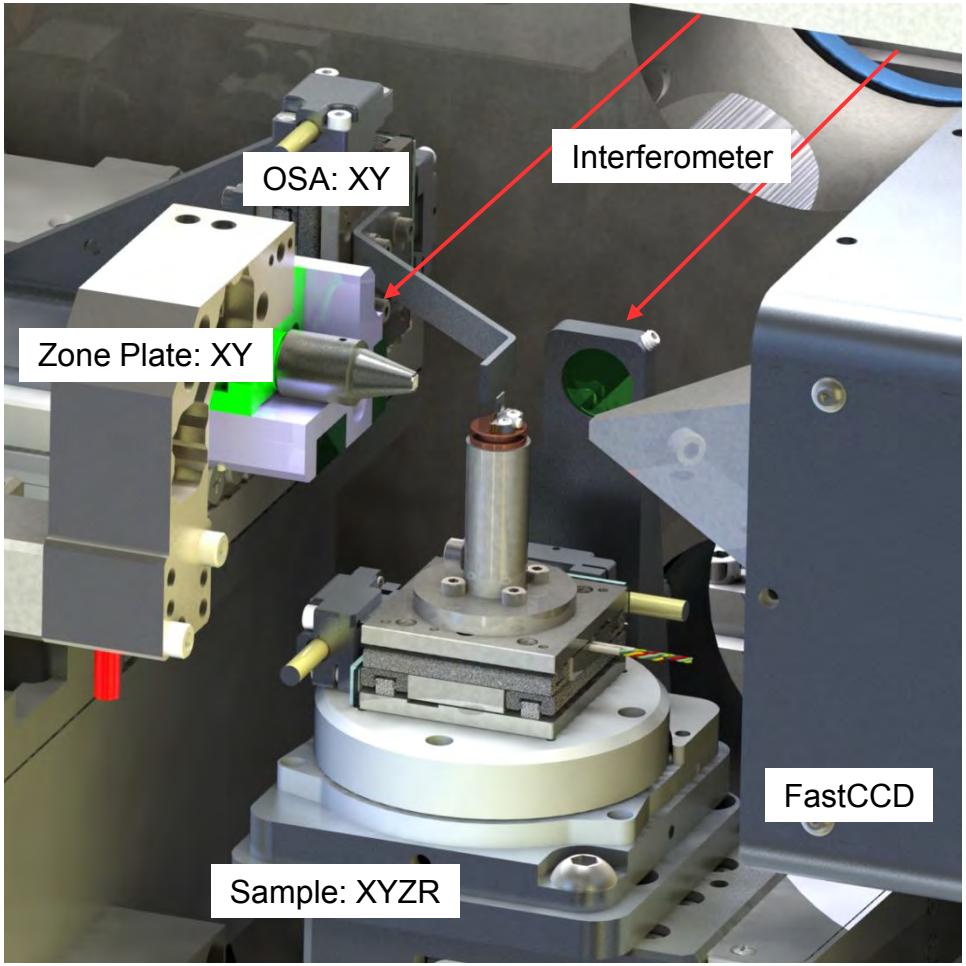
6.2 keV, 50 s/μm^2,
7nm pixel, 10-11 nm
2D resolution
12 nm RMS stability
3 Day Measurement!



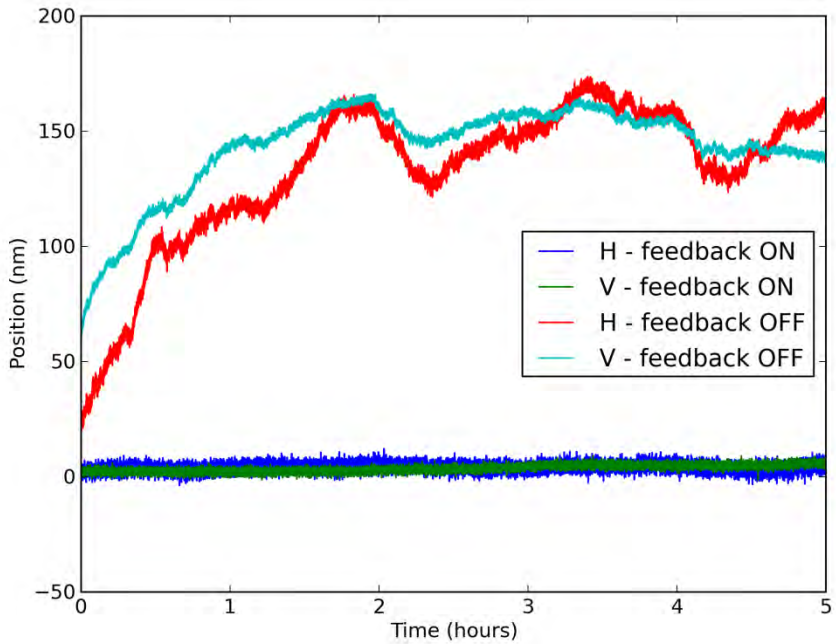


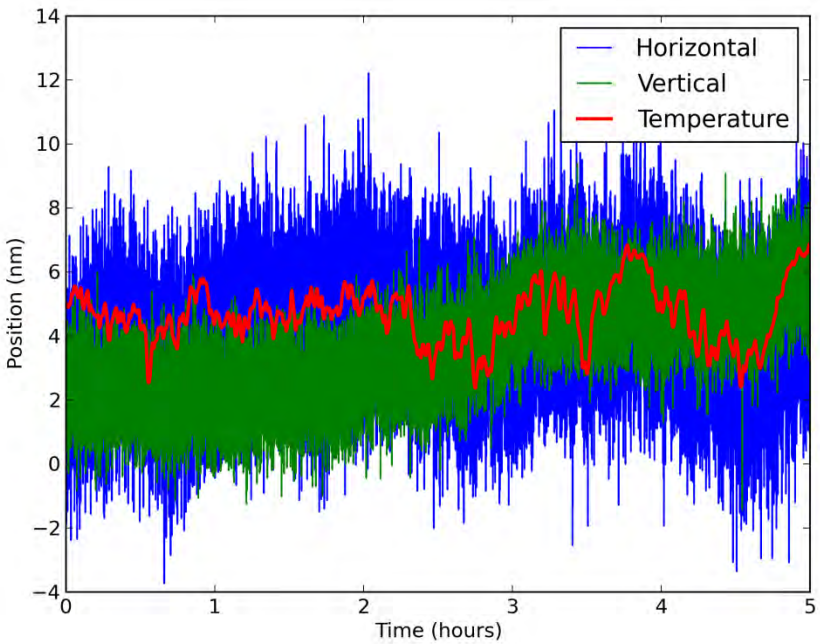
“Nanosurveyor”: A Ptychographic Microscope @ ALS BL9.0.1

- 750 eV
- 7 s / μm^2 measurement time
- 5-10 nm pixel, 10-20 nm resolution
- 2 nm RMS stability
- 250 nm zone plate
- 13.6 mm focal length, 100 μm depth of field



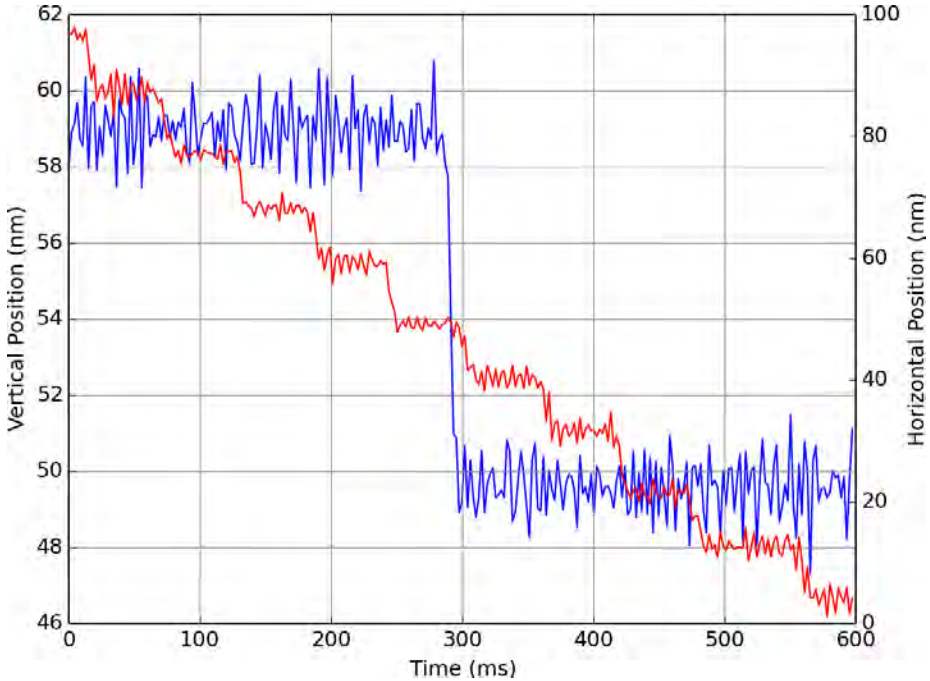
“Nanosurveyor”: Ultra-stable scanning mechanism

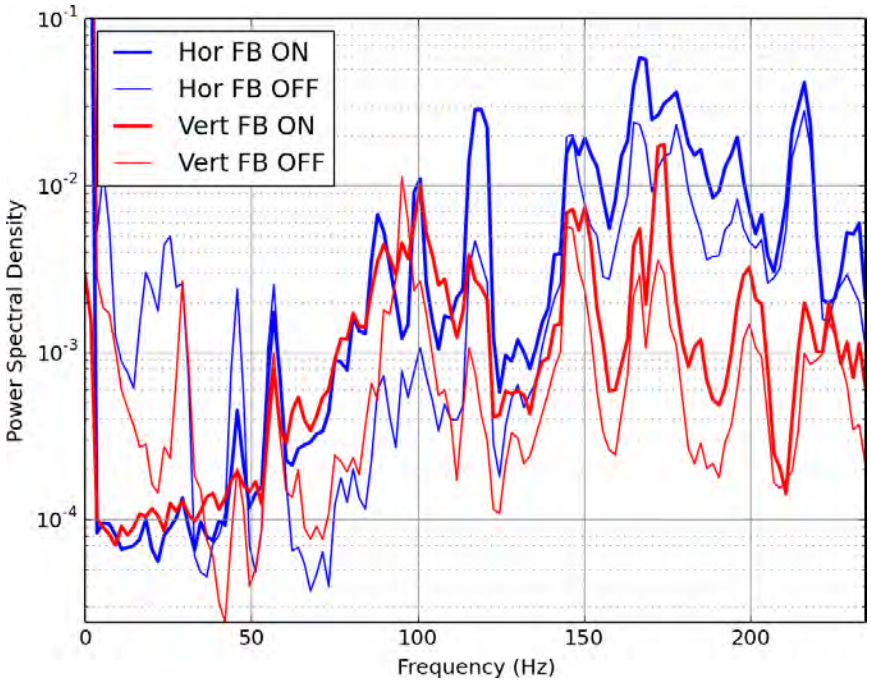




< 2nm RMS vibrations with feedback
0.2 degree temperature variation over 5 hours (at IFM)

“Nanosurveyor”: Ultra-stable scanning mechanism

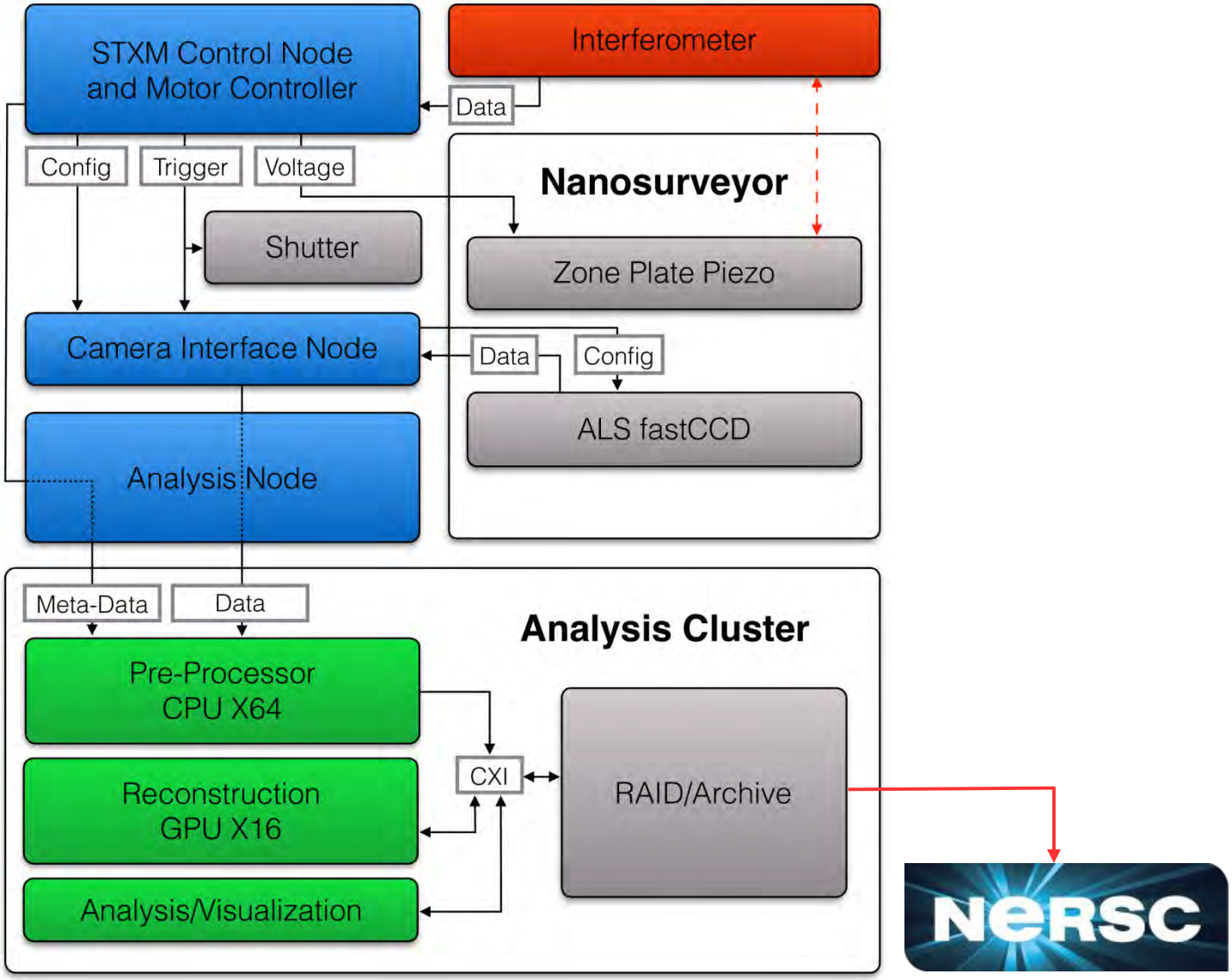




10 nm steps easily resolved
<10 ms move time (up to 100 nm)
Feedback shifts power from low to high frequency

"Nanosurveyor": high performance work flow

- Dedicated 10G network to remote cluster
- ESnet to NERSC
- 400 MB/s

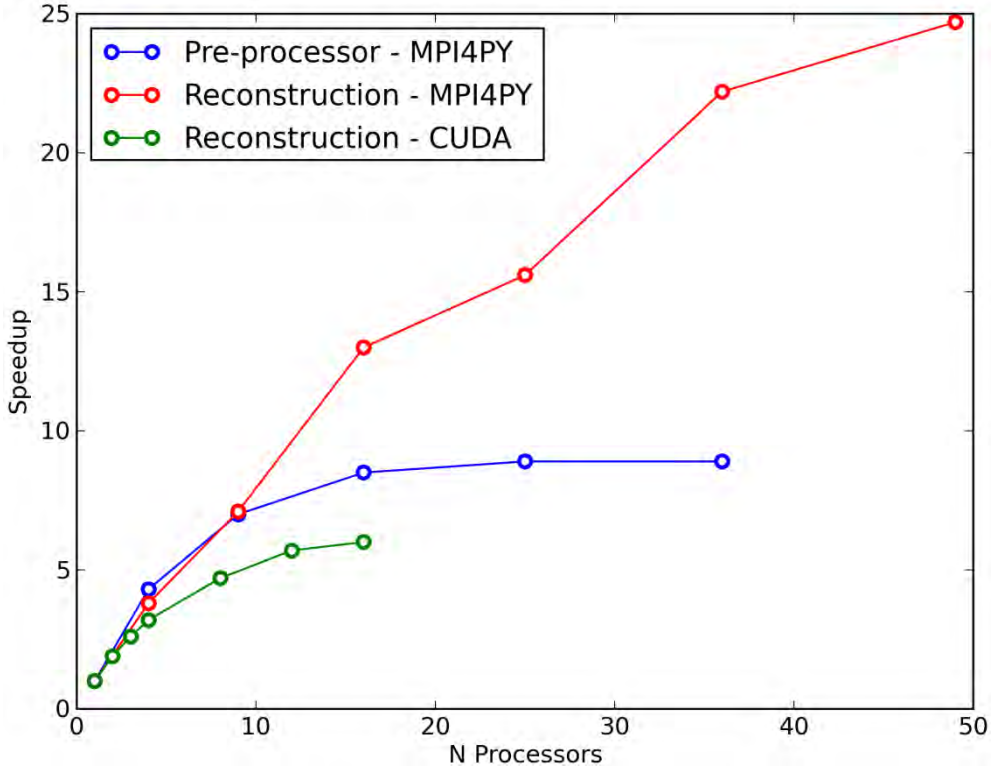


“Nanosurveyor”: high throughput data acquisition/analysis

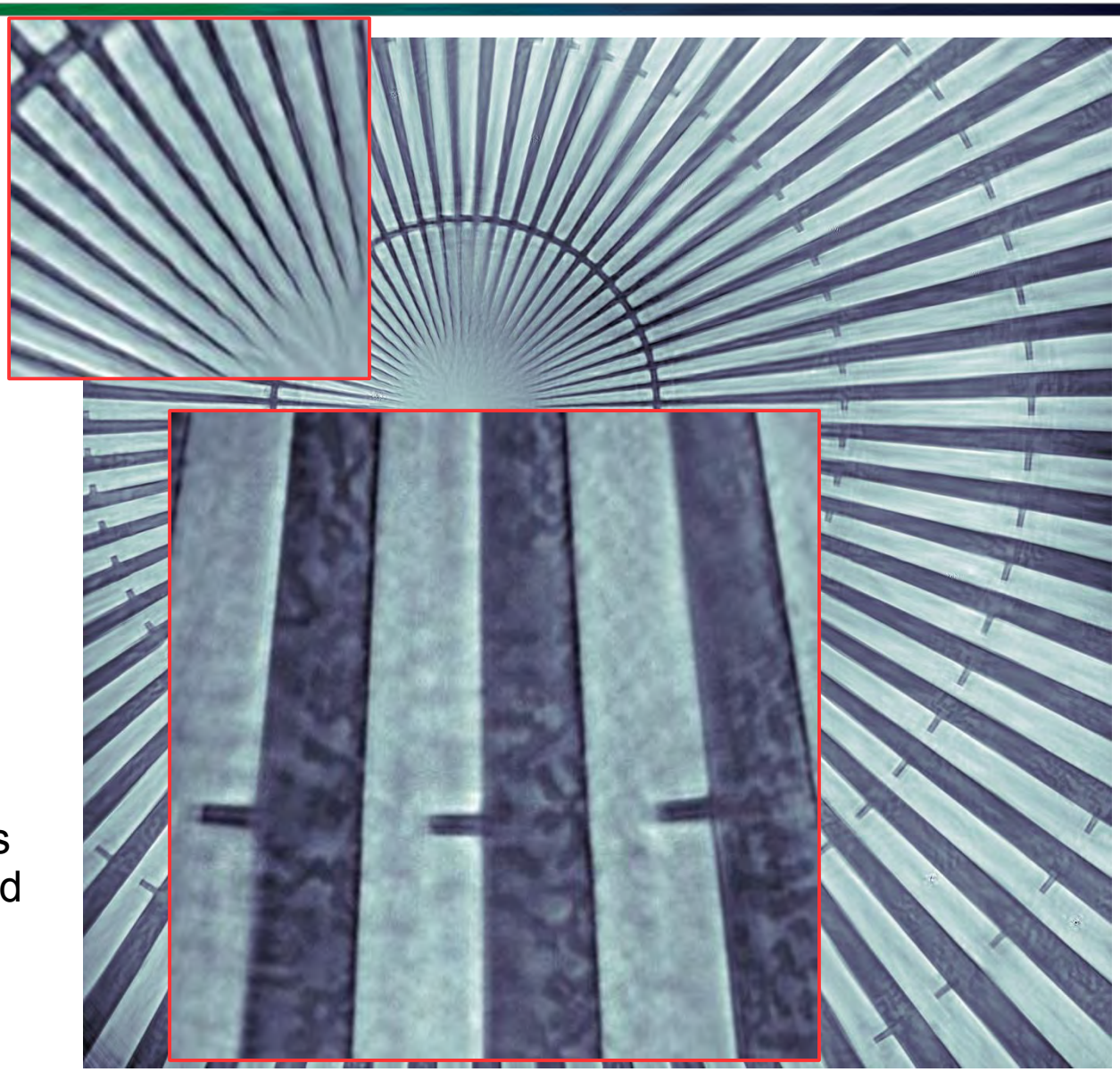
Data Acquisition Time 50 ms x-ray exposures 20 ms fCCD readout 10 ms motor move	10 s / um^2
Data Pre-Processing Time	1 s / um^2
GPU Reconstruction Time	1.6 s / um^2
CPU Reconstruction Time	7.5 s / um^2

“Nanosurveyor”: high performance computing

- Pre-processor: python + MPI
- Reconstruction: CUDA or python + MPI
- MPI4PY Reconstruction scales well, pre-processor and CUDA code do not
- Streaming pre-processor needed with pipe to cluster or NERSC
- Real time feedback critical for experiment control
- No job scheduler!



Nanosurveyor: High Throughput Ptychography



- 750 eV
- 250 nm zone plate
- 50 ms exposures
- 150 nm steps
- 8 nm pixels
- 20 nm resolution
- 1500 resolution elements (image pixels) per second

Nanosurveyor: Tomography of Cement

Calcium Silicate Hydrate
Paulo Monteiro
UCB

- 100 projections
- 9 nm voxel
- Acquisition: 30 minutes / um^3
- Reconstruction: 3 minutes / um^3
- Data Volume: 70 GB / um^3
- COSMIC will be 10X faster

Yttria Stabilized Zirconia

Klaus Van Benthem (UCD)
Hasti Majidi (UCD)
Maryam Farmand (ALS)

Nanosurveyor: Tomography of Porous Ceramics

Yttria Stabilized Zirconia
Klaus Van Benthem (UCD)
Hasti Majidi (UCD)
Maryam Farmand (ALS)

Pore evolution during fast sintering

9 nm voxel, 120 degree rotation

70 nm average pore diameter

BL11.0.2: Highest Measured Resolution in 1D

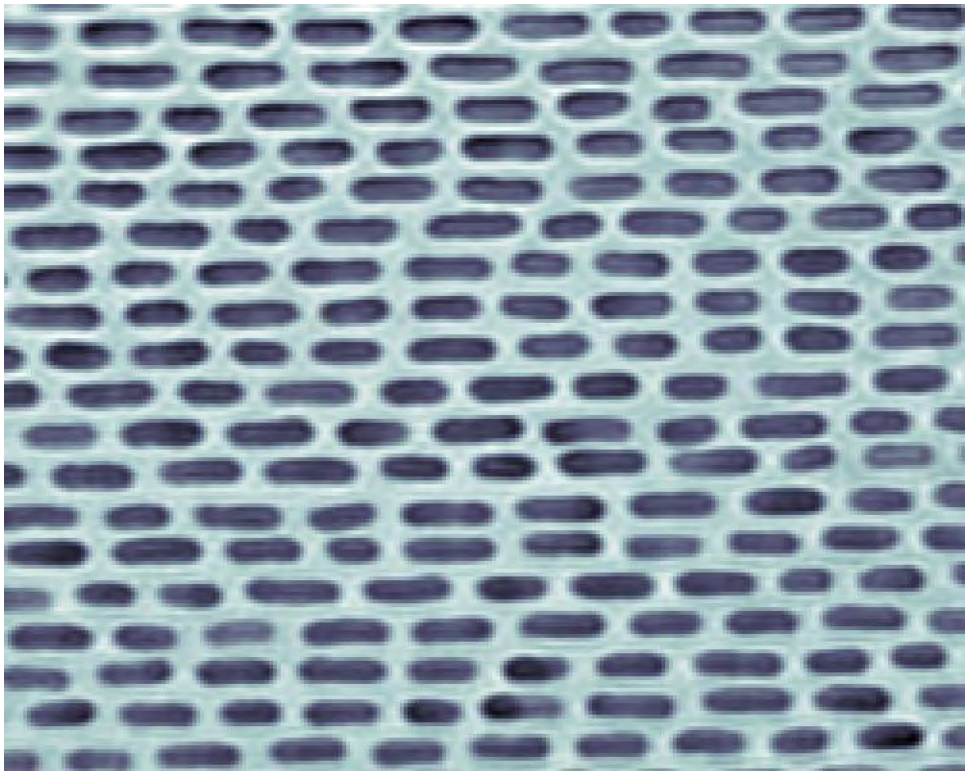
- SiMo multilayer, 100 nm thick
- 1500 eV
- 60 nm zone plate
- 150 ms exposures
- 40 nm steps
- 11% contrast at 3 nm
- 25% contrast at 5 nm
- 2 nm pixels

Manuscript submitted

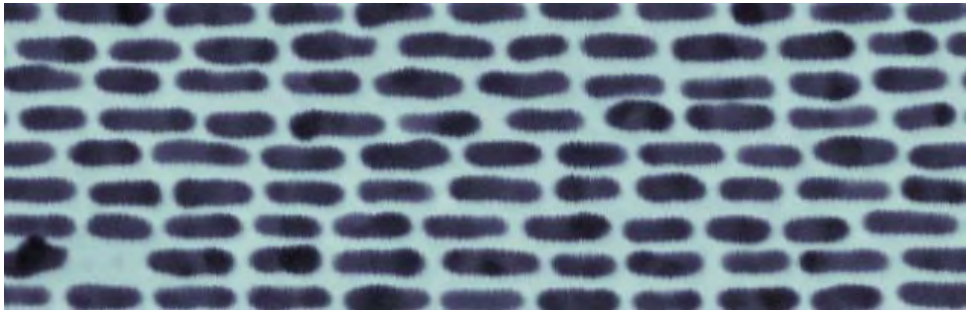
BL11.0.2: Highest Measured Resolution in 2D

10 x 6 nm
Resolution
Element

Ptychography
60 nm zp



SEM



STXM
25 nm zp

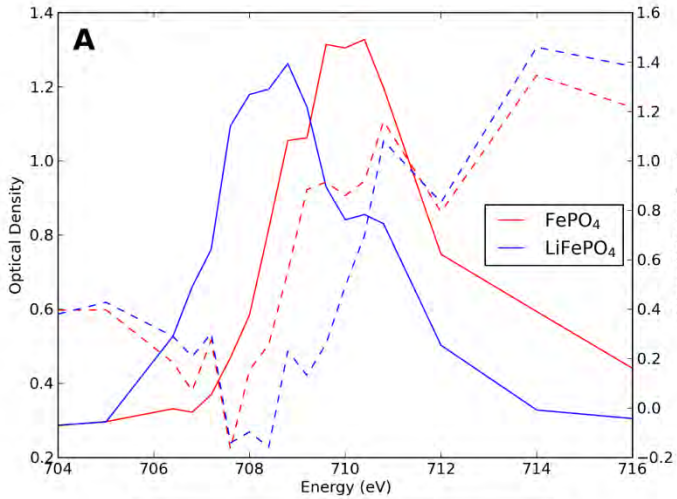
BL5.3.2.1: spectro-ptychography

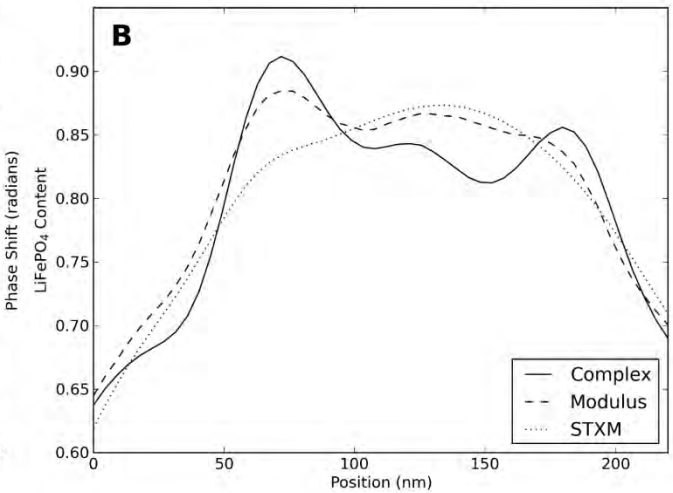
STXM – 25 nm zone plate Ptychography – 60 nm zone plate

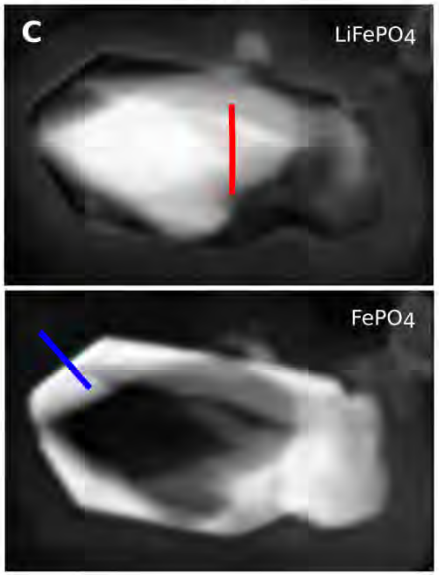
LiFePO4
Jordi Cabana (UIC)
Young-Sang Yu (EETD)
Shirley Meng (UCSD)

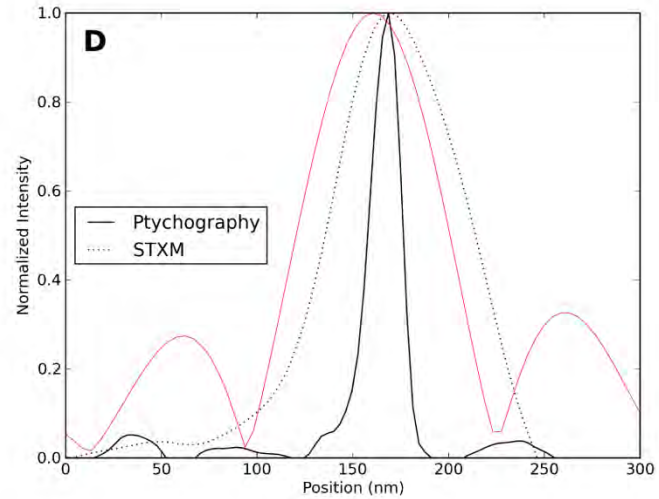
Manuscript submitted

The Complex Refractive Index Enhances Chemical Contrast





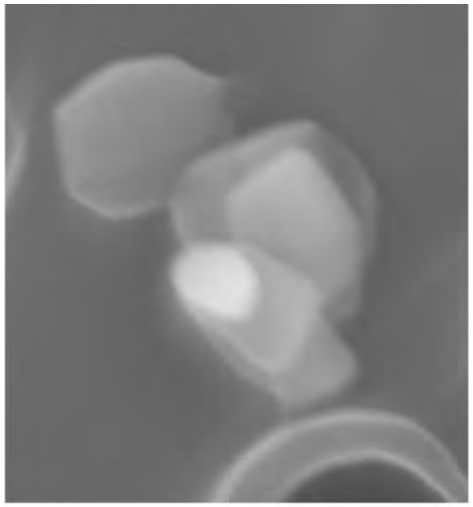


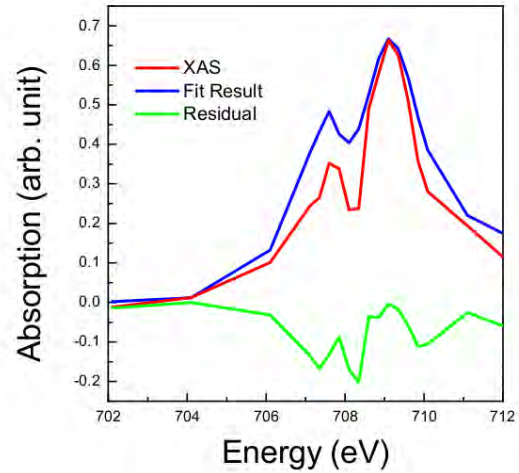


We measure the complex refractive index:
$n = 1 - \delta - i\beta$

PCA → k-means → SVD

Chemistry in Single Nano-Crystals



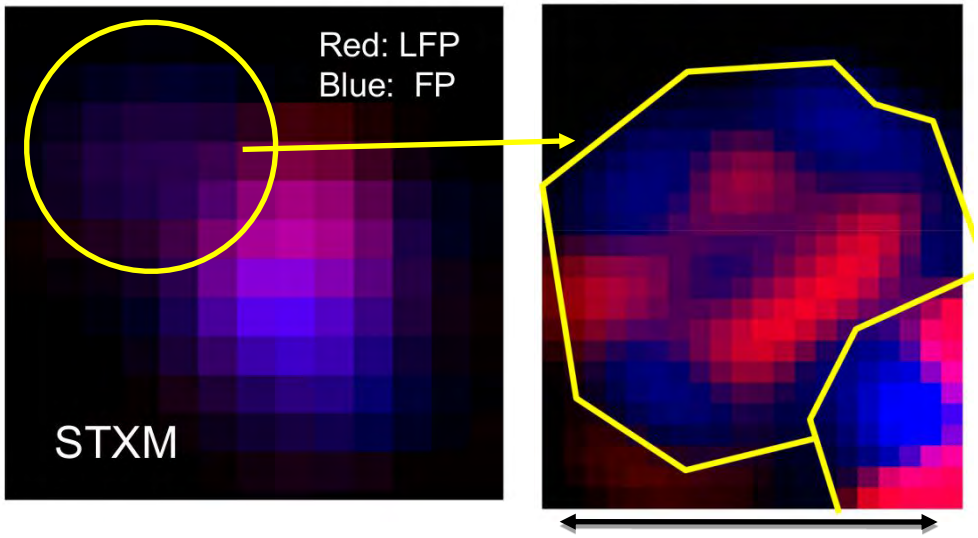


Young-Sang Yu
Maryam Farmand

LFP:FP = 2.5 : 97.5

STXM: Solid Solution

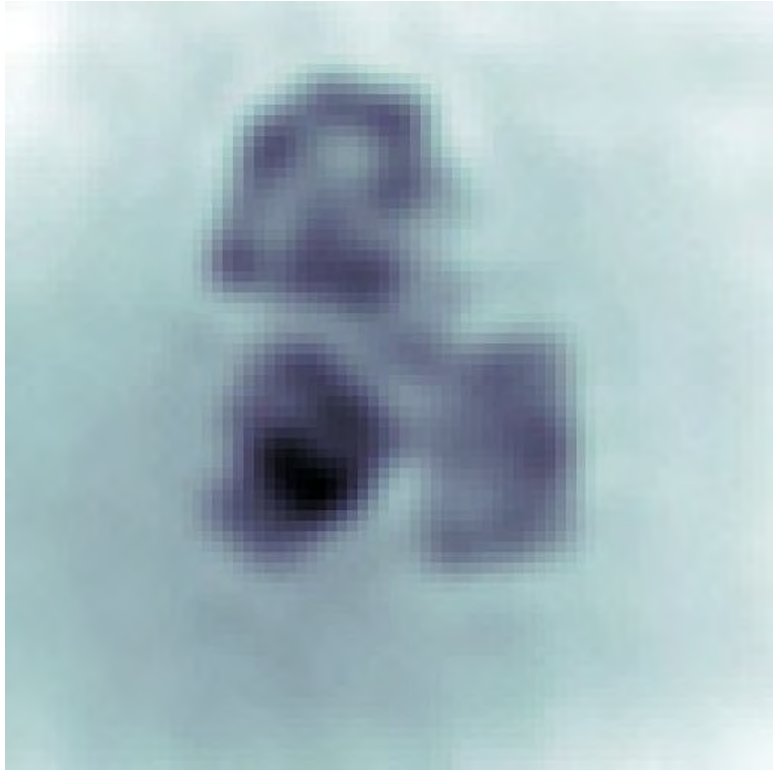
Ptychography: Two phase



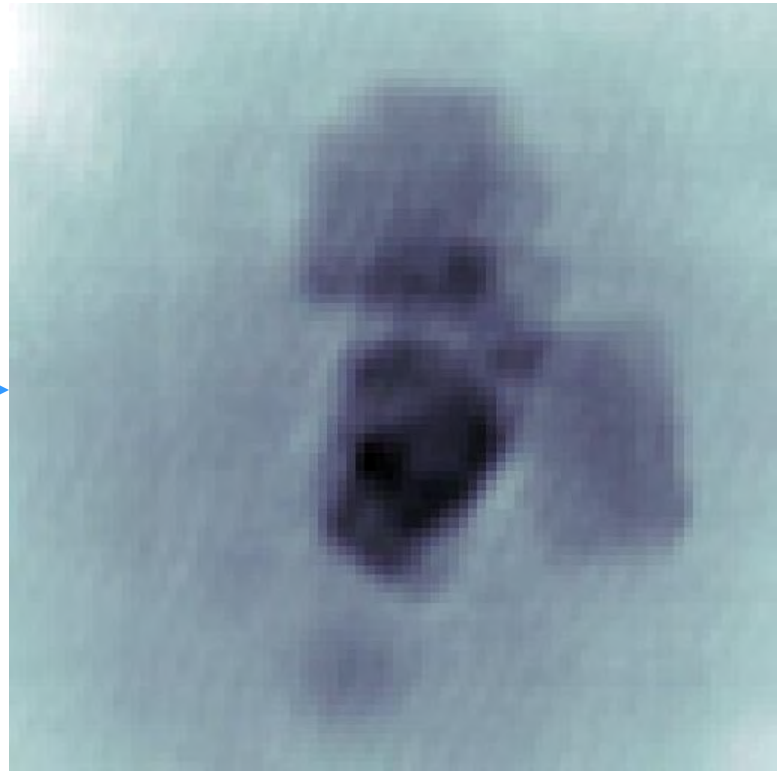
Manuscript in preparation

Ptychography Sees the Solid Solution

Chemically Delithiated
Two Phase



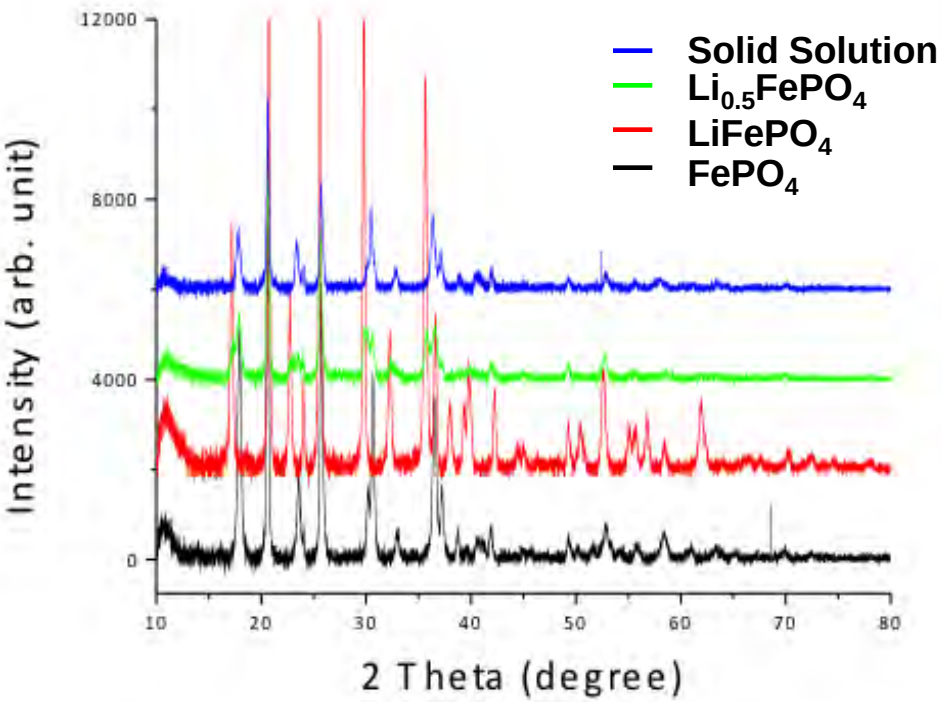
Annealed and Quenched
Solid Solution

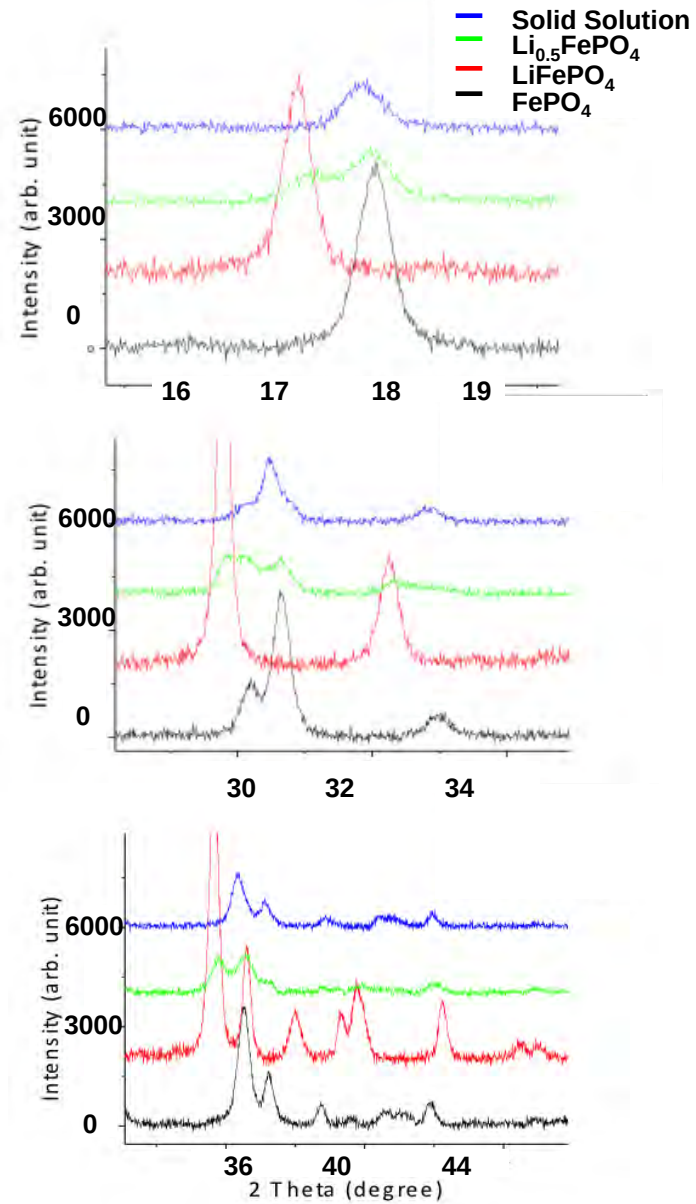


500 nm

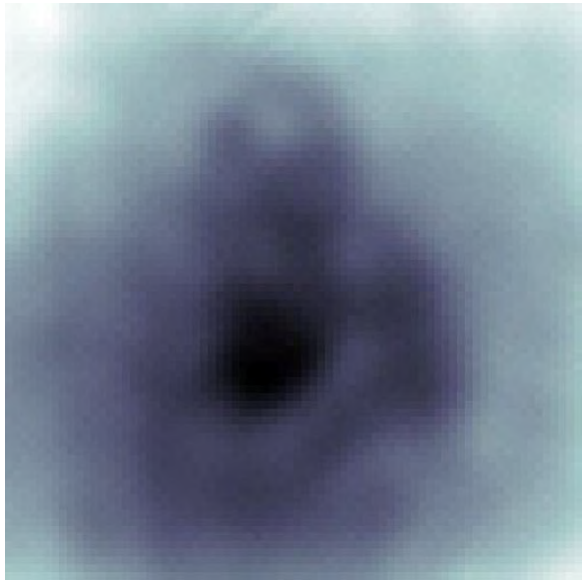
Jordi Cabana (UIC)
Robert Kostecki (EETD)
Young-Sang Yu (EETD)
Maryam Farmand (ALS)

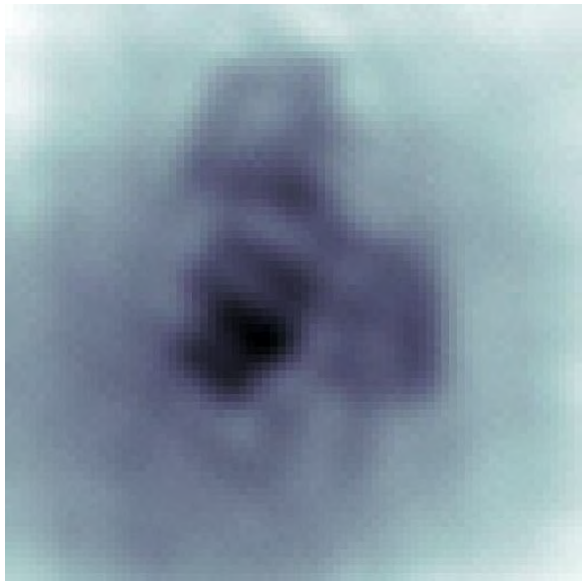
Solid Solution Confirmed by XRD

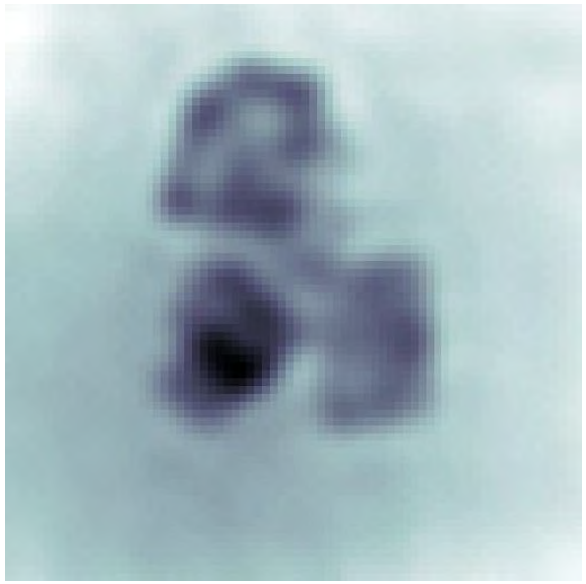


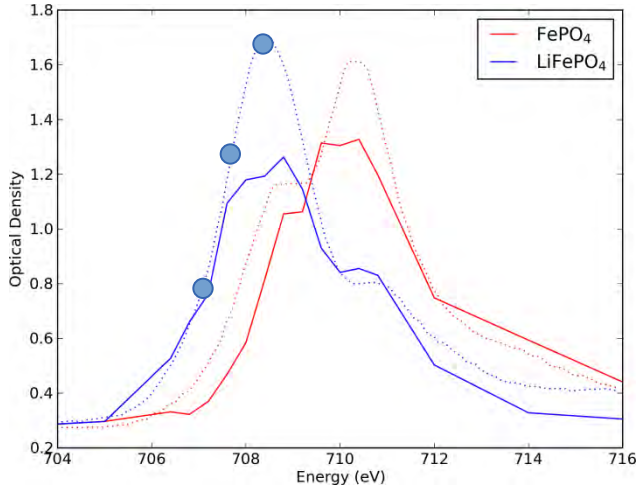


Resolution (Contrast) is Sample (Energy) Dependent







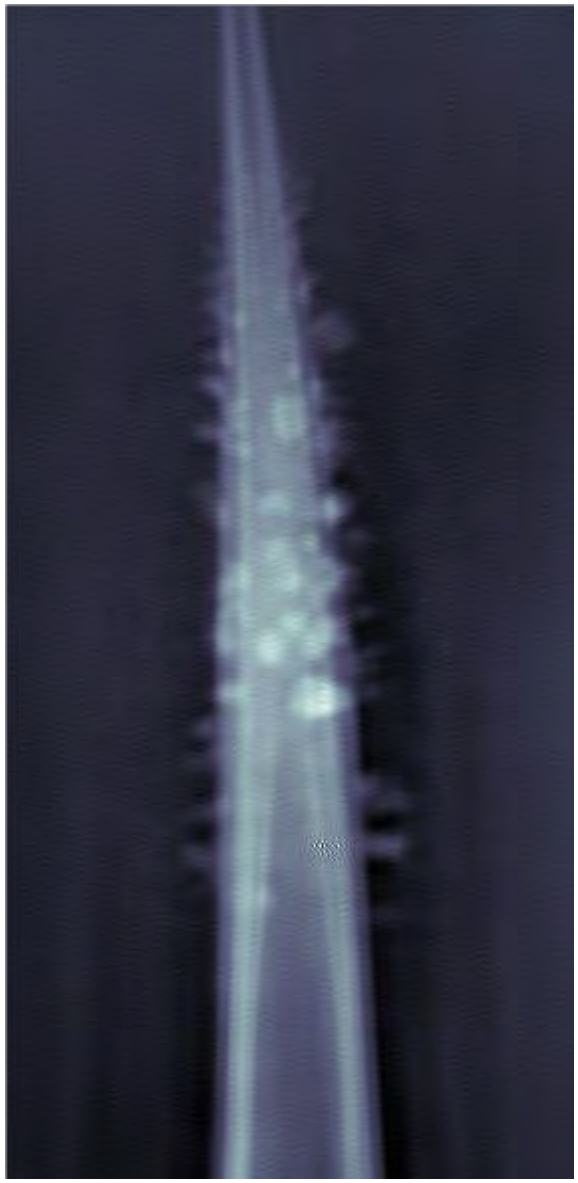


Is increased exposure needed off resonance?

How does the chemical resolution compare?

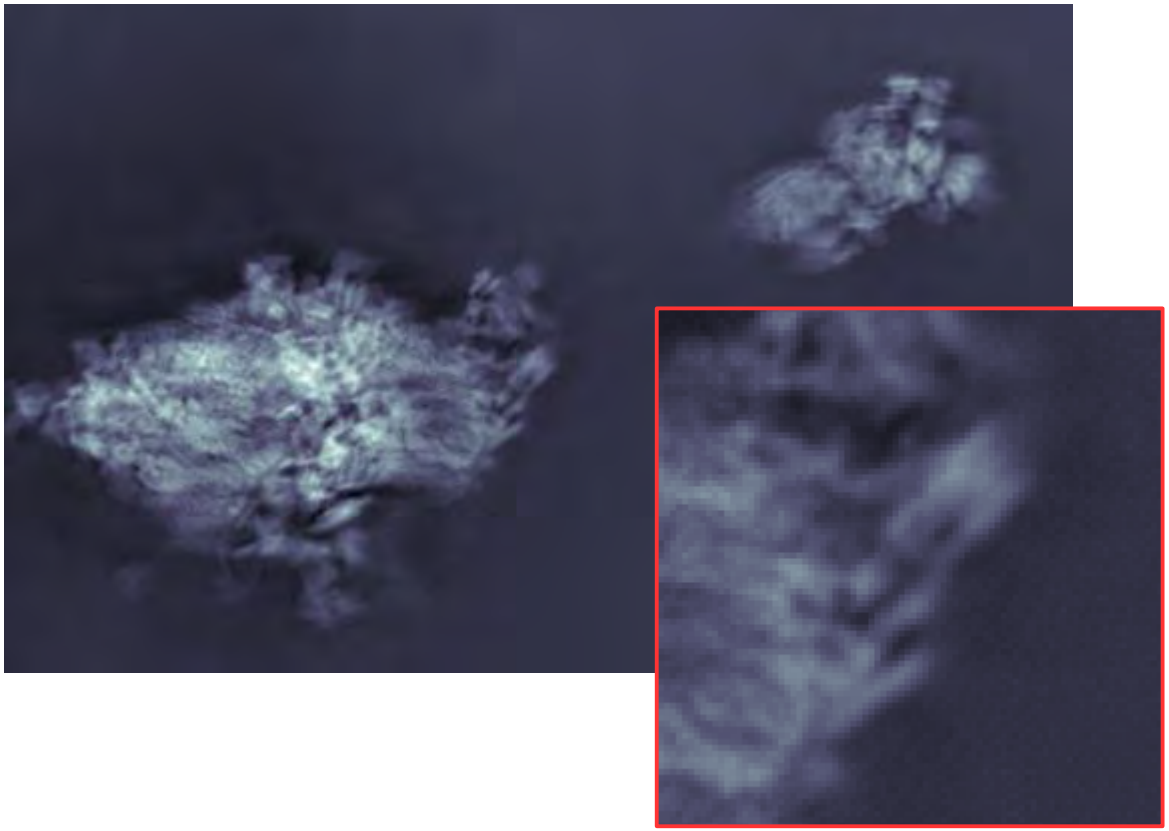
We can't increase contrast, only the SNR...

Towards Chemistry in 3D



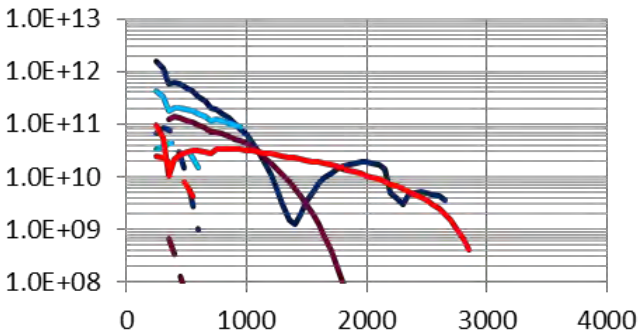
Spectro-tomography is needed to visualize chemistry in secondary particles

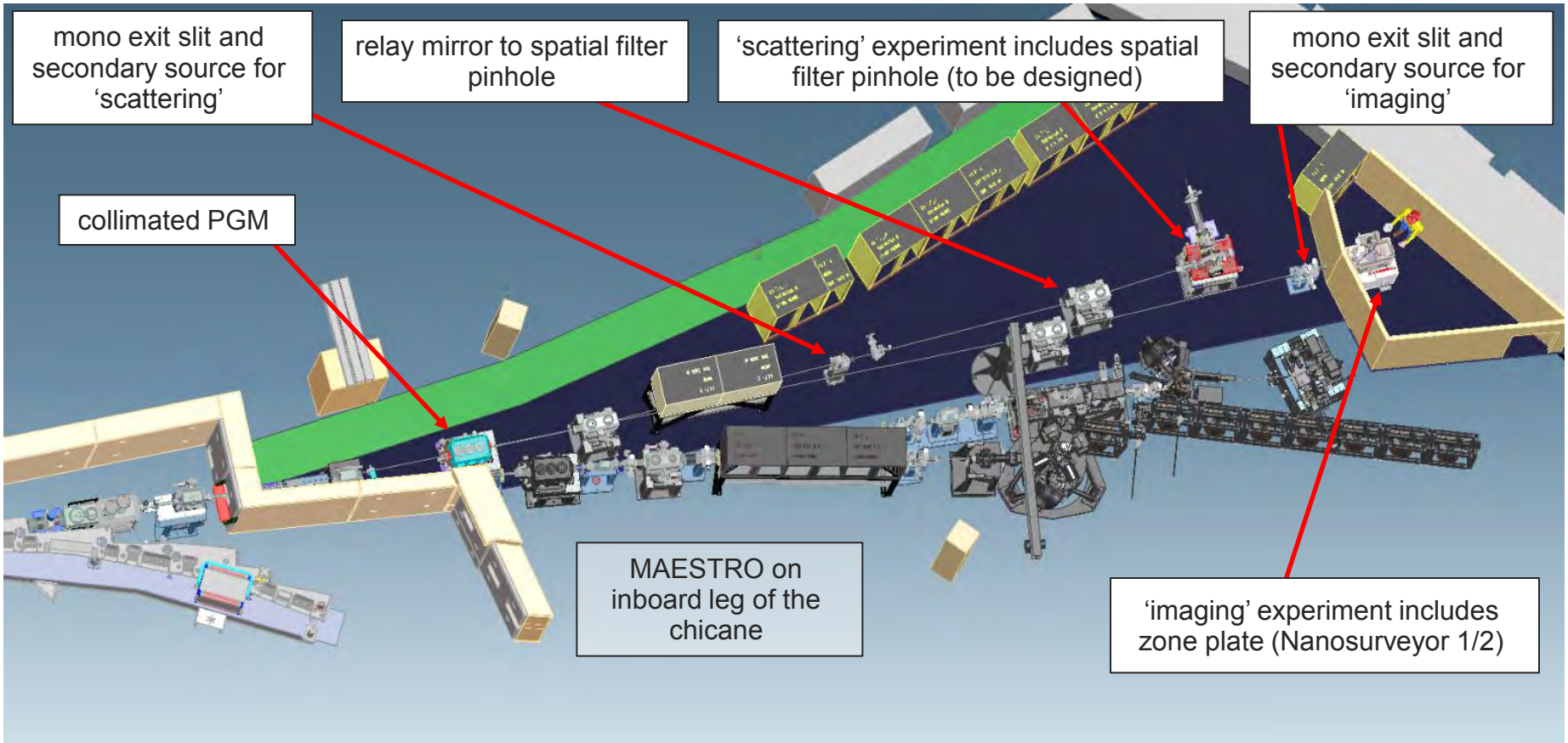
Nanosurveyor → BL5.3.2.1



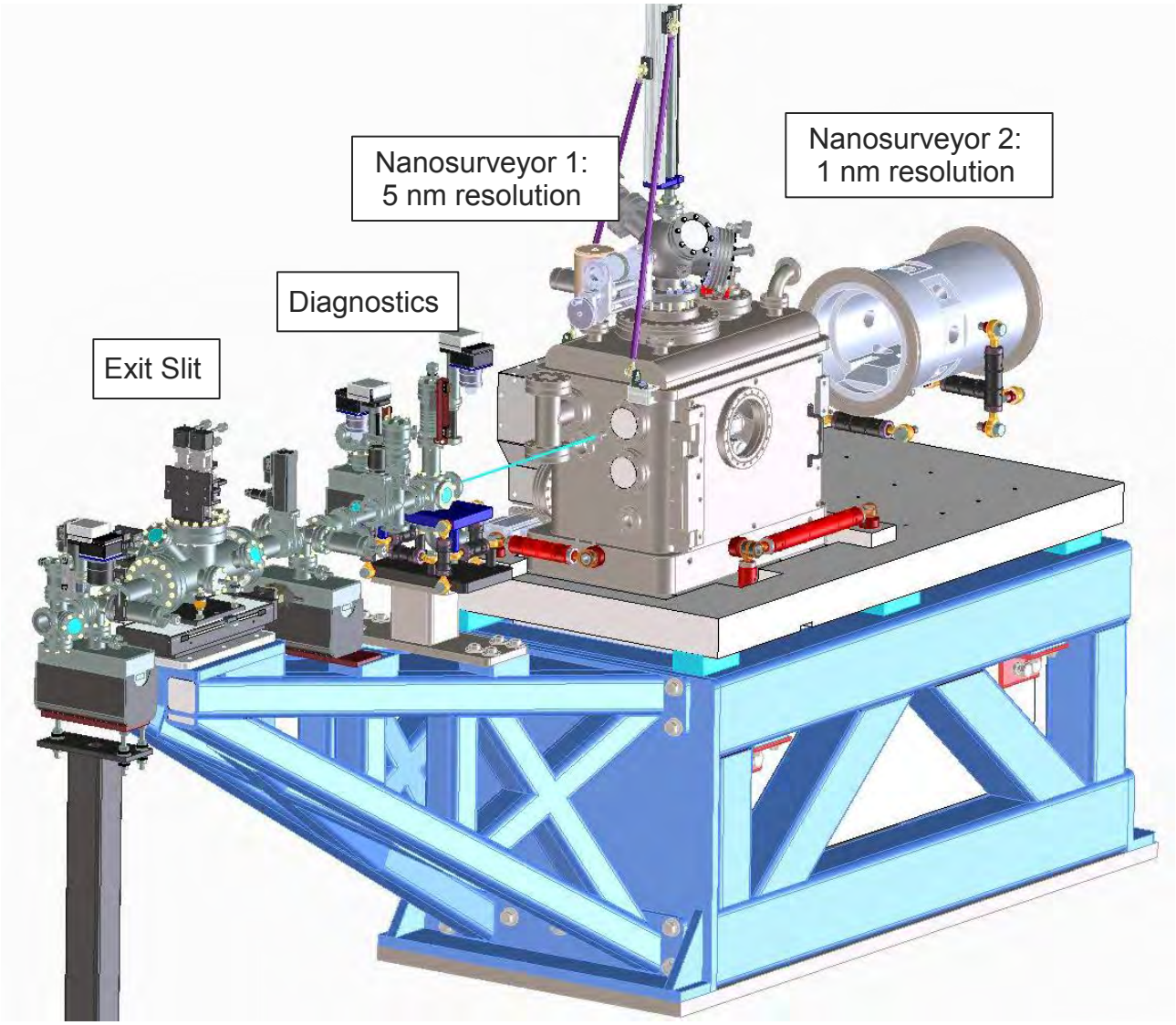
COSMIC: COherent Scattering and MICroscopy

- Optimized for high coherent flux
- Carbon to Sulphur
- 2 microscopes
- Environmental control





COSMIC Imaging Endstations



Nanosurveyor 2: based on TEAM-1(NCEM) Technologies

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National Energy Research Scientific Computing Center

COMPUTATIONAL RESEARCH
LAWRENCE BERKELEY NATIONAL LABORATORY

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LBNL LDRD

James Sethian
Hari Krishnan

UC DAVIS
UNIVERSITY OF CALIFORNIA

Klaus Van Benthem
Hasti Majidi

University of California San Diego

Shirley Meng

UIC
UNIVERSITY OF ILLINOIS AT CHICAGO

Jordi Cabana

UPPSALA UNIVERSITET

Filipe Maia

Cal

Paulo Monteiro

Coming in
2015...

Thank You!