Lightsource opportunities using coherent X-ray diffractive imaging to visualize dark matter and neutrino tracks in the rock record at scale

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SLAC NATIONAL ACCELERATOR LABORATORY

Stanford University | U.S. DEPARTMENT OF ENERGY

Visualizing damage tracks from Dark Matter and neutrinos in 2D and 3D

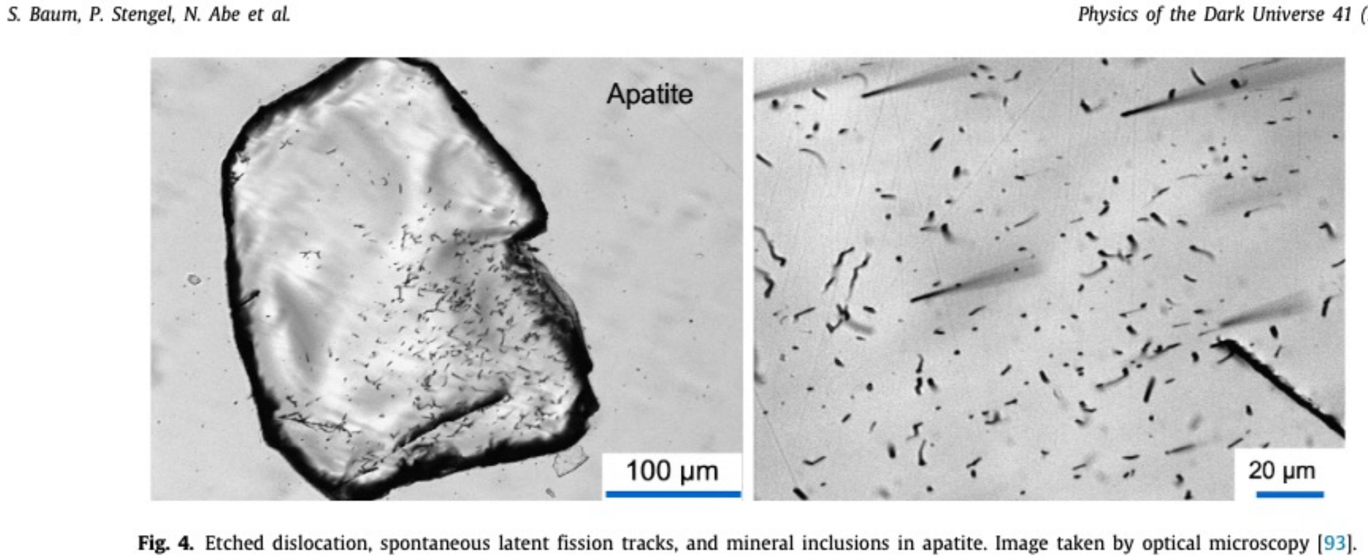

S. Baum, P. Stengel, N. Abe et al. Physics of the Dark Universe 41 (2023) 101245

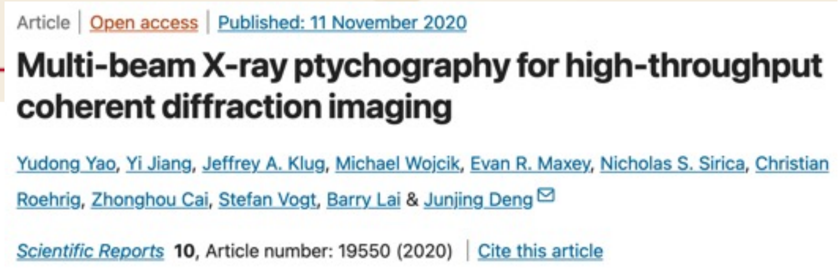
Fig. 4. Etched dislocation, spontaneous latent fission tracks, and mineral inclusions in apatite. Image taken by optical microscopy [93].

- Optical microscopy
- Electron microscopy: SEM/TEM/SFM
- Etching to enhance pits and tracks
- Soft X-ray microscopy
- Hard X-ray computed tomography
  - Lab-based sources
  - Lightsources

Large amounts of energy are deposited into minerals: characteristic damage (e.g., localized amorphization, phase change, grain morphology modification)

Using minerals as Dark Matter ‘paleo-detectors’ requires large volume imaging

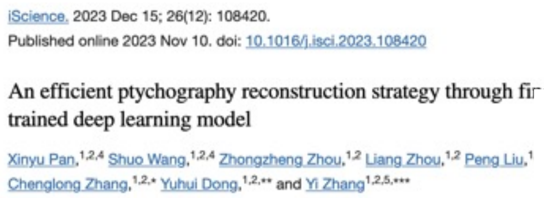
- Multiple samples of same material different locations?
- Multiple materials of similar ages
- Samples from different depths (background understanding)
- Samples of different age to provide stop-action video of Earth’s neutrino and DM environment over cosmic time
  → Need to scan 10 mg with 1nm resolution in 3D track length
  → Need to scan ~400 cm^2


Article | Open access | Published: 11 November 2020

Multi-beam X-ray ptychography for high-throughput coherent diffraction imaging

Yudong Yao, Yi Jiang, Jeffrey A. Klug, Michael Wojcik, Evan R. Maxey, Nicholas S. Sirica, Christian Roehrig, Zhonghou Cai, Stefan Vogt, Barry Lai & Junjing Deng

Scientific Reports **10**, Article number: 19550 (2020) | Cite this article


iScience. 2023 Dec 15; 26(12): 108420. PMCID: PMC10687283
Published online 2023 Nov 10. doi: 10.1016/j.isci.2023.108420 PMID: 38034346

An efficient ptychography reconstruction strategy through fi
trained deep learning model

Xinyu Pan,[1,2,4] Shuo Wang,[1,2,4] Zhongzheng Zhou,[1,2] Liang Zhou,[1,2] Peng Liu,[1]
Chenglong Zhang,[1,2,*] Yuhui Dong,[1,2,**] and Yi Zhang[1,2,5,***]


scientific reports

OPEN **Scalable and accurate multi-GPU-based image reconstruction of large-scale ptychography data**

Xiaodong Yu[2], Viktor Nikitin[2], Daniel J. Ching[2], Selin Aslan[2], Doğa Gürso
Tekin Biçer[1,2]


Research Article Vol. 30, No. 15 / 18 Jul 2022 / *Optics Express* 26027

Optics EXPRESS

High-resolution ptychographic imaging enabled by high-speed multi-pass scanning

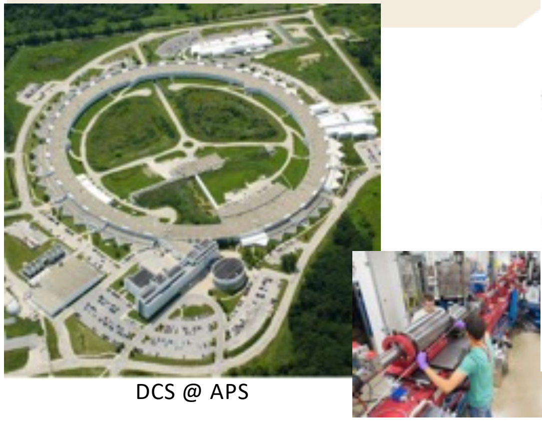
JUNJING DENG,* YUDONG YAO, YI JIANG, SI CHEN, TIM M. MOONEY, JEFFREY A. KLUG, FABRICIO S. MARIN, CHRISTIAN ROEHRIG, KE YUE, CURT PREISSNER, ZHONGHOU CAI, BARRY LAI, AND STEFAN VOGT

3rd & 4th generation lightsources

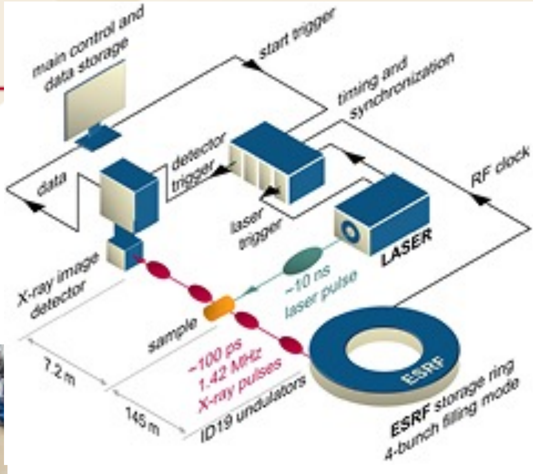
Synchrotron: Work horse of x-ray imaging
(MHz, ~10^3 coherent x-rays per pulse, 80-ps duration)

- -Multibend achromat (MBA) upgrades (APS-U)
- Increase coherent flux by 100 times, making DCS and other beamlines at APS more powerful
- -ESRF, microtomography BL ID19

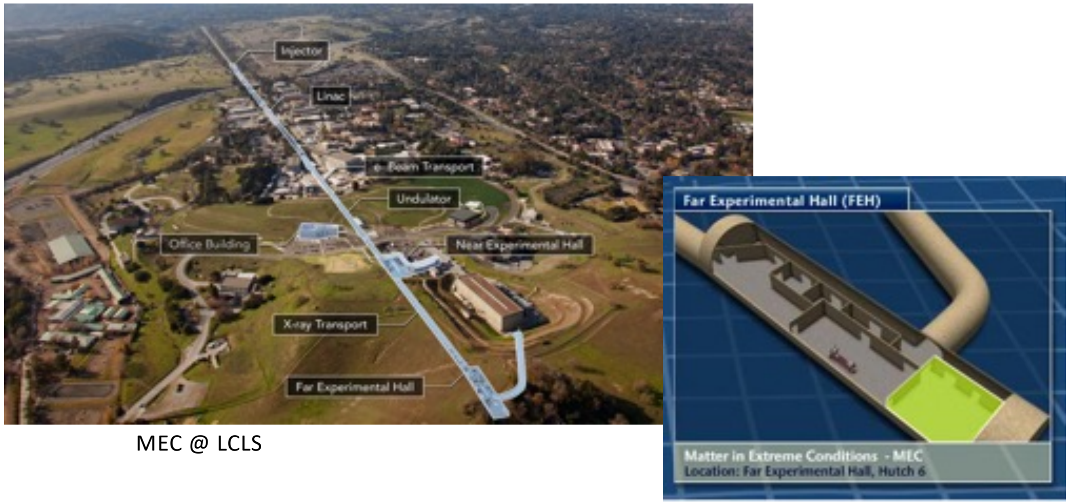
X-ray free electron lasers
(120 Hz - MHz, 10^{13} coherent photons per pulse, attosec-10s fs duration) Coherent buildup of photons, full spatial coherence



DCS @ APS



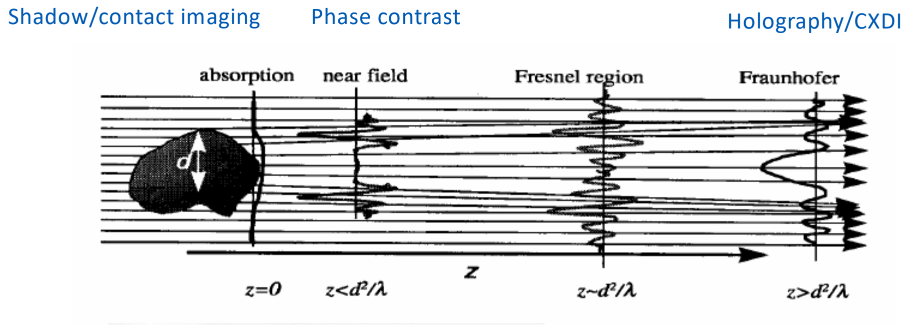
ID19 @ ESRF; Olbinado et al., 2018



MEC @ LCLS

X-ray imaging at 3rd & 4th generation lightsources will bring a revolution in nanoscale visualization

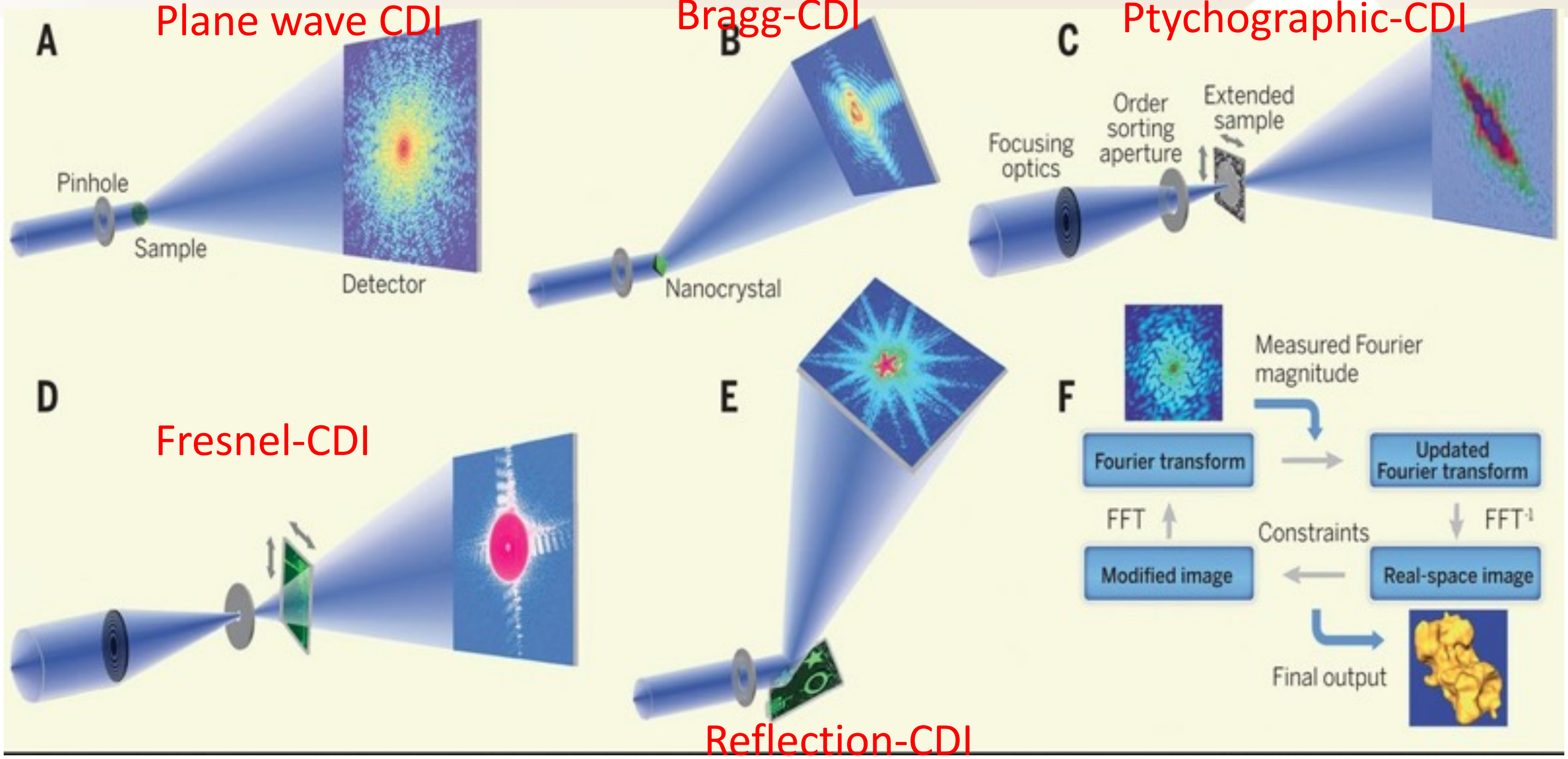
- **Traditional imaging (think lens)**
  - Fresnel, Kirz, Laue, Kinoform lenses for hard x-rays (up to 0.5 MeV)
  - Resolution: down to ~100s nms
- **Radiography approaches (line-projection, tomography, phase contrast imaging (PCI) and divergent beam PCI)**
  - Resolution typically scales with pixel size (max r ~ pixel/100 > 100 nm, typically 1 µm)
- **Coherent approaches (holography, PCI, coherent diffraction imaging (CDI))**
  - Resolution: Few nanometer resolution possible



CXDI can provide 3D information, but has only been demonstrated for softer x-rays (<1 keV) and small samples (few micron)

slide courtesy R. Sandberg

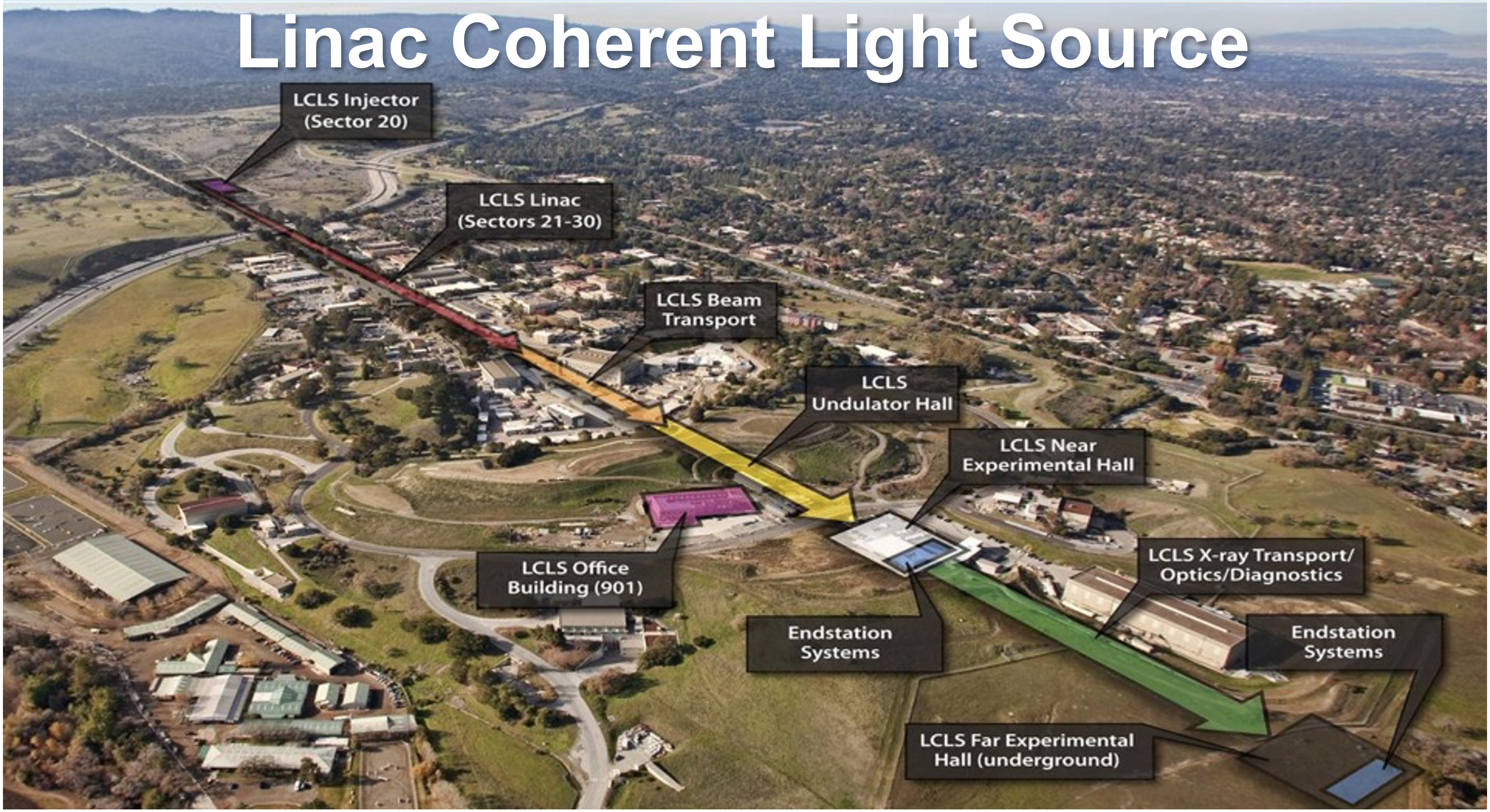
Coherent X-ray Diffractive Imaging (CXDI) can provide 3D information



Miao et al., 2015

Iterative phase retrieval; 100s-1000s iterations can find the correct phase

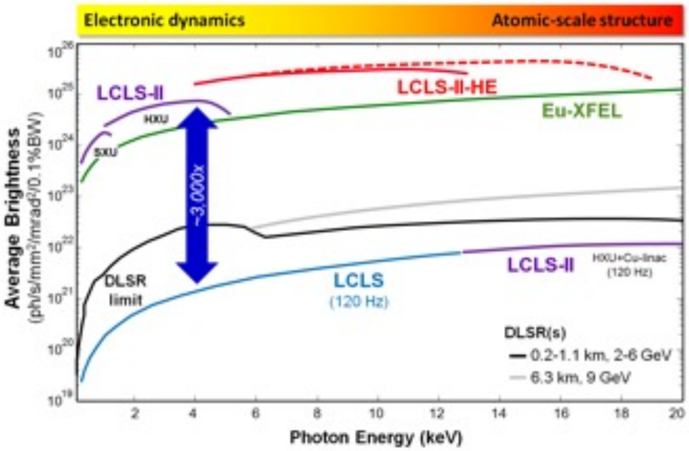
Linac Coherent Light Source

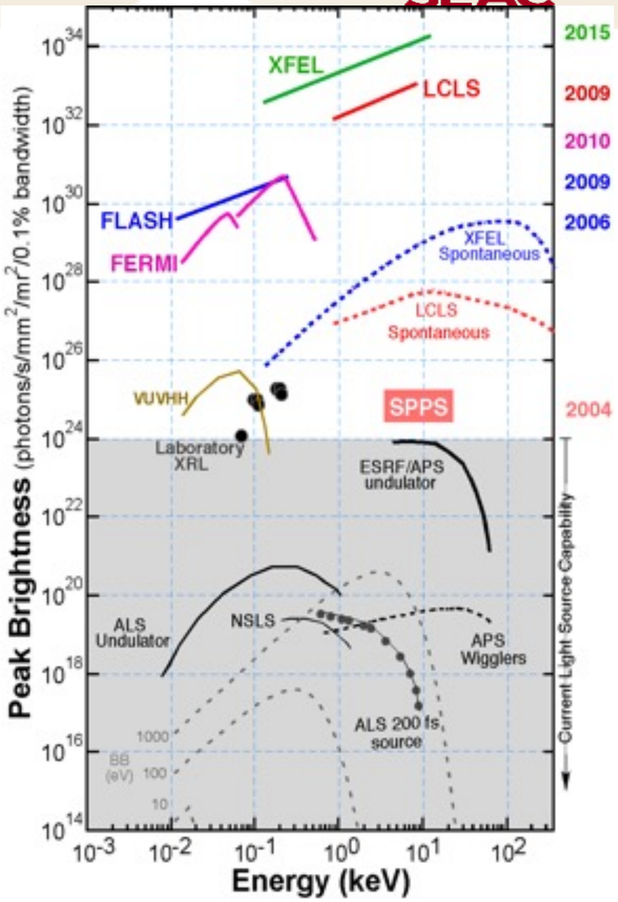


Revolution in X-ray sources is enabling a revolution in condensed matter physics & materials science

- bunch duration: 50 fs
- full transverse coherence
- high repetition rate: 120 Hz
- tunable from 600 to 12000 eV
- photons per bunch > 10^{12}
- 4 mJ/pulse

Doubles accelerator energy, extending X-Rays from 5 keV limit to 12 – 20 keV
(at high repetition rate)





https://portal.slac.stanford.edu/sites/lcls_public

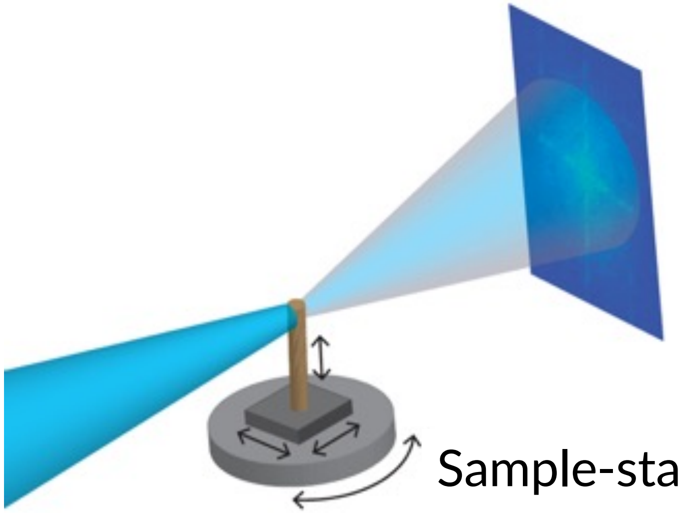
Example case study of nanofoam microstructure studies for fusion energy science

Foundational foam measurements:

Static

- Dry foam 3D characterizations to 10s nm (e.g., the pore-structure morphology, pore size distribution, pore wall density, spatial distribution of impurity/chemical concentration at pore intersection, and pore shape distribution)
- Characterizations as function of fabrication process / composition

Use XFEL-based ptycho-tomography to image nanofoams in 2D & 3D

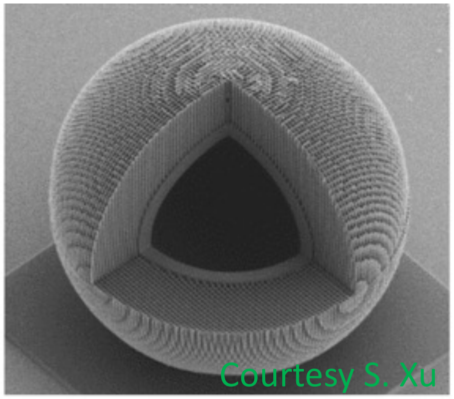


Sample-stage stack-up

Similar to Pound et al., 2020

Polymer nanofoam fabrication-dependent microstructure is not well mapped & cryo-D/T wetting process is unknown

There are many foam types: two-photon polymerization (TPP); chemical processes; molds



Courtesy S. Xu

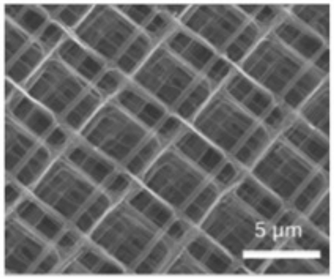
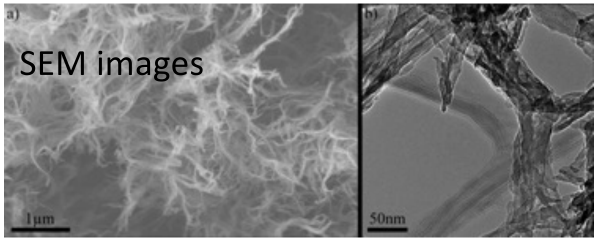
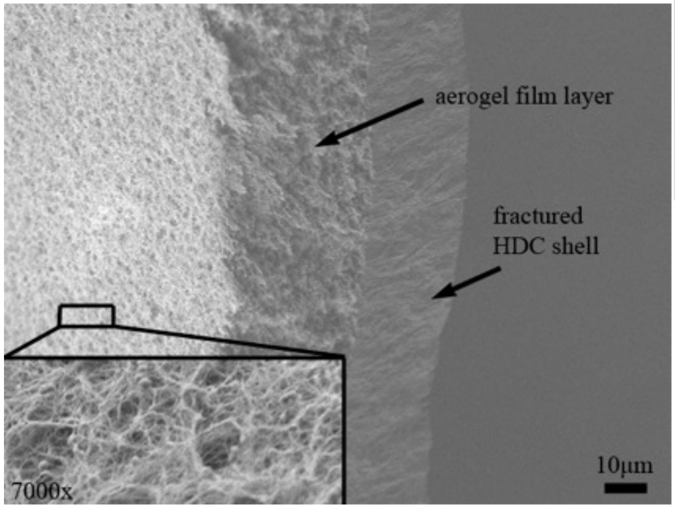
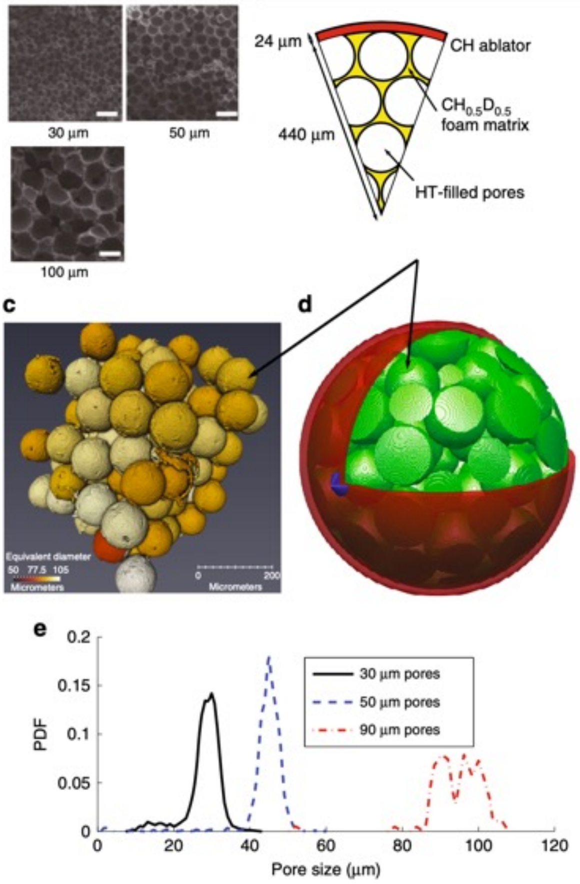


FIG. 3. 16 mg/cc log-pile carbon foam with hollow filaments separated by ~5 μm.

Figure 2. An example of a foam target with a solid shell inside. The external diameter is 860 μm, a shell thickness of 10 μm, and a foam density of 80 mg/cm^3.

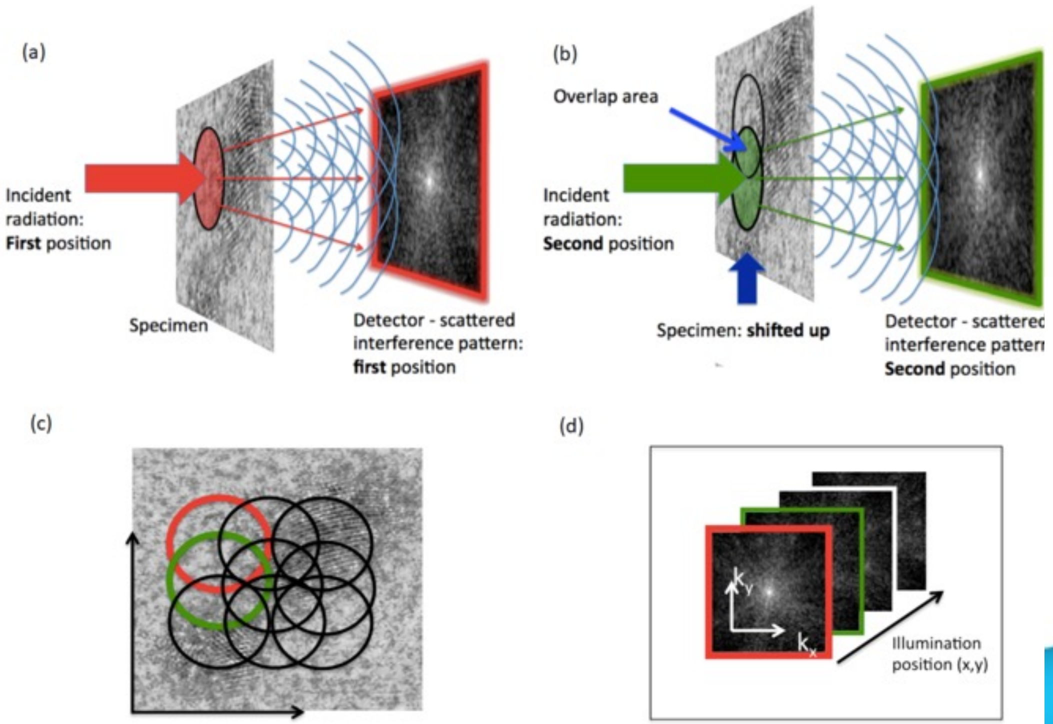




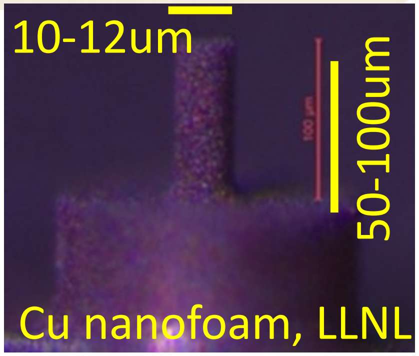


Haines et al., 2020

X-ray ptychography enables non-destructive, high-resolution imaging

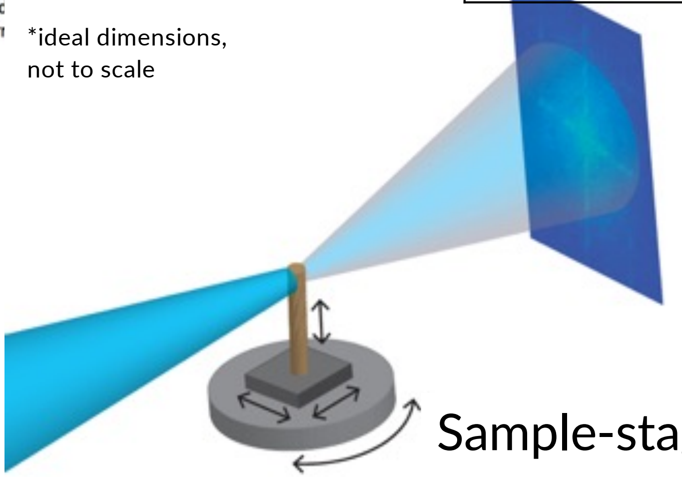


Wikipedia.org, 2018



*ideal dimensions, not to scale

Advantages
 - Image resolution only limited by detector - Can image large volumes - Quantitative phase information (absorption) of sample



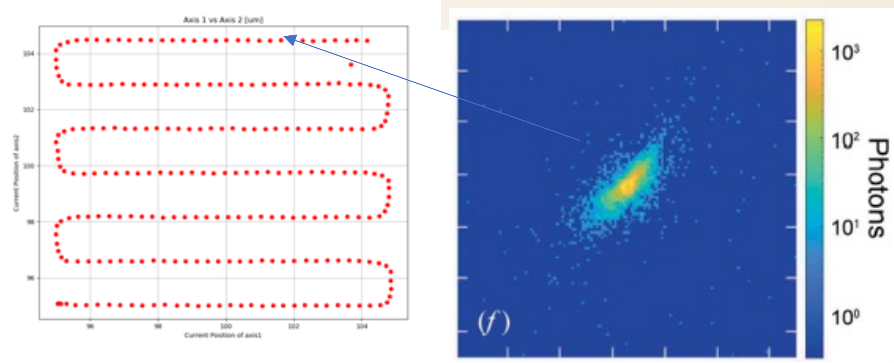
Sample-stage stack-up

Test Pattern

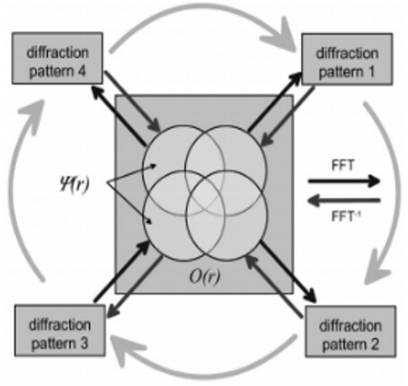
(1um W)

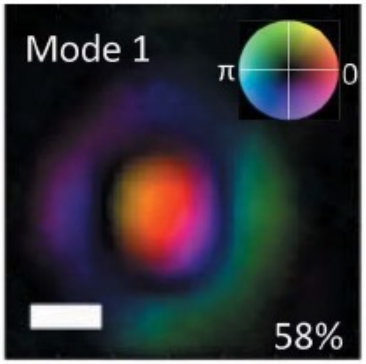
X-ray ptychography enables non-destructive, high-resolution imaging

- Oversampled diffraction patterns from an object
- Real-space structure determined by Fourier transformation
    - requires amplitude and phase of the diffracted X-rays
    - amplitude can be calculated directly from the measured intensity
    - phase is recovered separately by means of an iterative algorithm

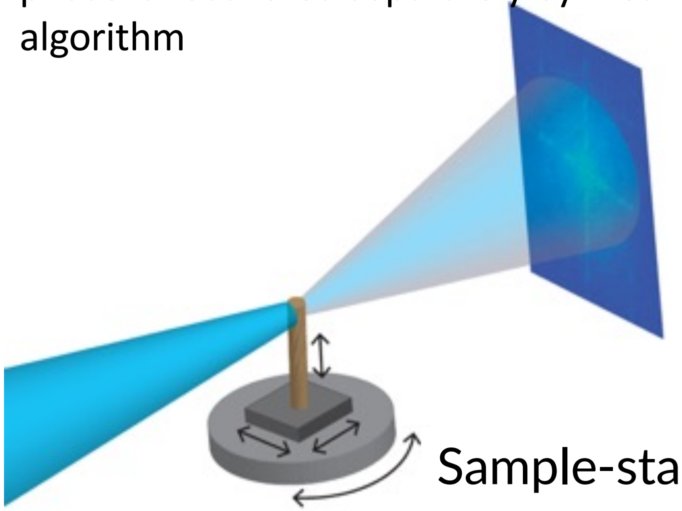


Iterative reconstruction algorithm (ptychography) for image and probe reconstruction





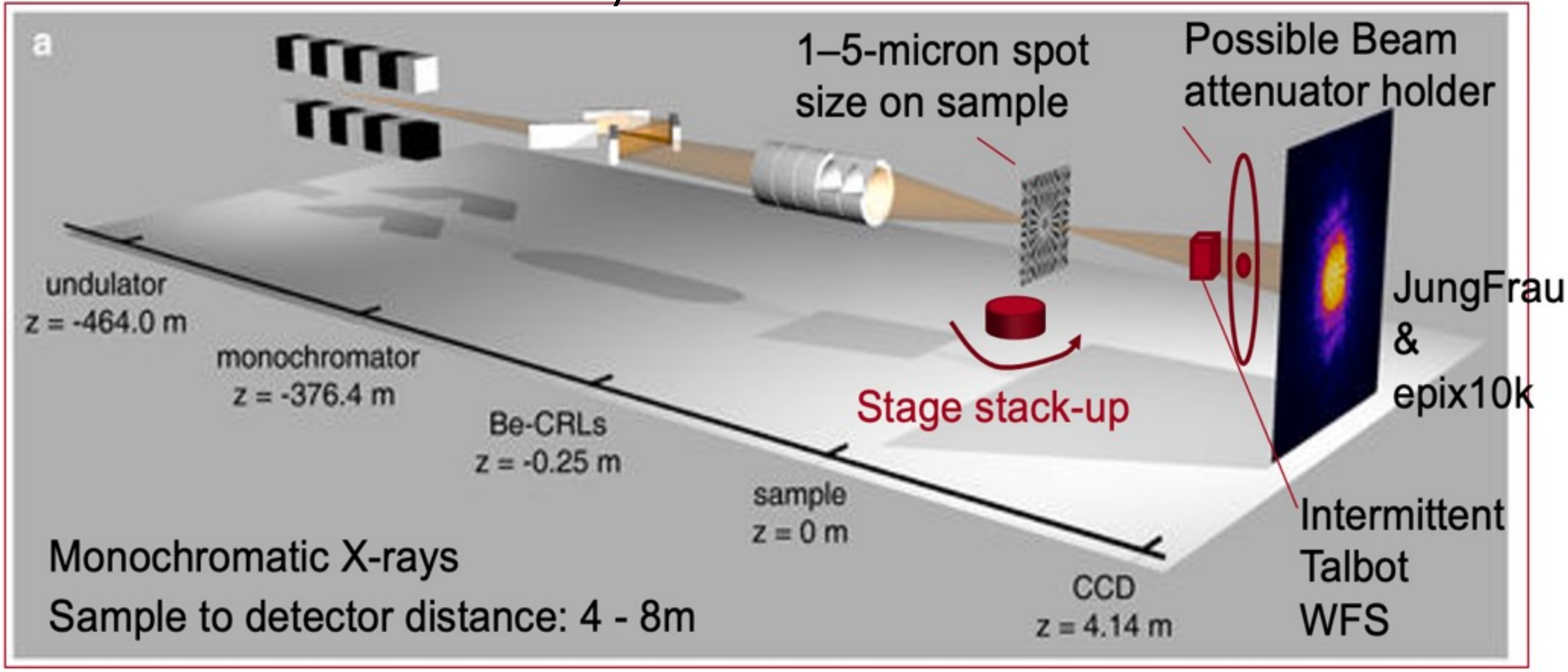
Ptychography algorithm diagram from Rodenburg and Faulkner, 2004



Sample-stage stack-up

X-ray Pump Probe (XPP) Instrument at LCLS demonstrates ~30 nm spatial resolution on Cu-nanofoam

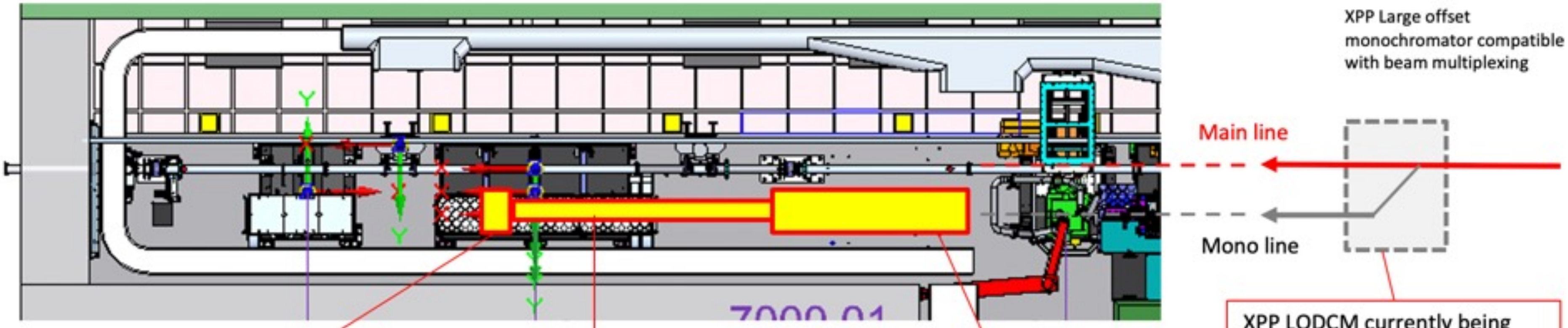
XPP Beamline schematic layout



- 8.8 keV
- diamond- and Si-mono design
- multiplexed-collection mode
- 2D X-ray ptychographic images collected at multiple angles

X-ray Pump Probe (XPP) End-station at LCLS: Setup

- **Goal: Demonstrate 3D ptycho-tomography in a multiplexed mode at XPP**
- Key steps
  - Set up automatic ptychographic reconstructions
  - Verify beam stability



Large area detector at ~ 3 meter from imaging endstation

Vacuum beam pipe for clean propagation of the scattering

Semi-permanent endstation with focusing optics and sample manipulation

XPP LODCM currently being modified to improve the angular stability of the diamond crystal optics.

Prior Work: Coherent X-ray Imaging and X-ray Pump Probe End-stations

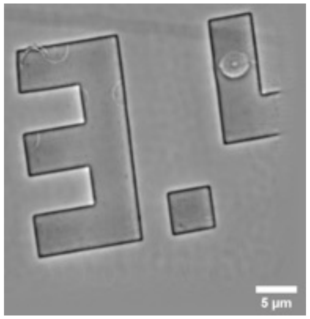
Parasitic mode at CXI: To our knowledge, 1st ptychography reconstructions at CXI (*Pound, B.A., Mertes, K.M., Carr, A.V., Seaberg, M.H., Hunter, M.S., Ward, W.C., Hunter, J.F., Sweeney, C.M., Sewell, C.M., Weisse-Bernstein, N.R. et al. (2020). J. Appl. Cryst. 53, https://doi.org/10.1107/S1600576720010778*).

Multiplexed mode at XPP

Evaluated reconstruction quality using ePix10k and JungFrau detectors

Test Pattern

(200nm Au)

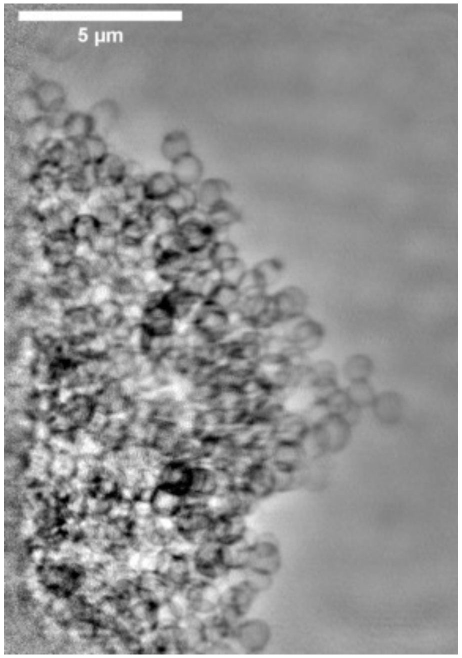


Test Pattern

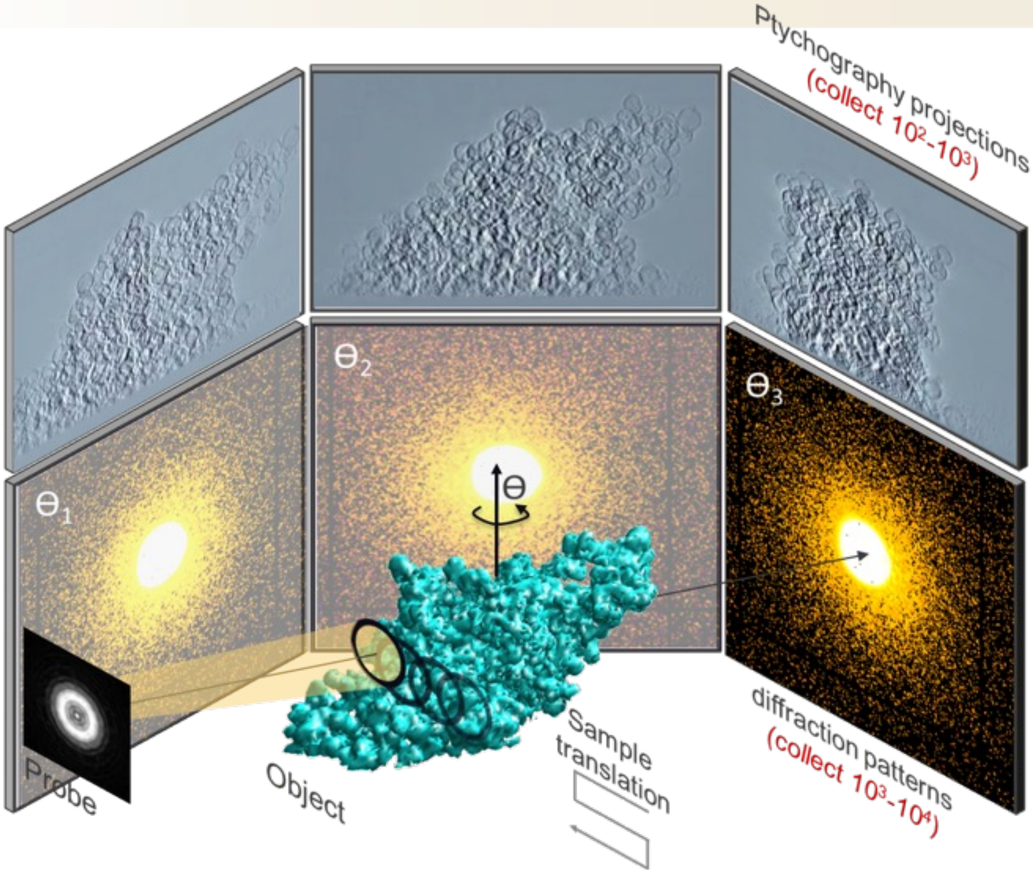
(1um W)

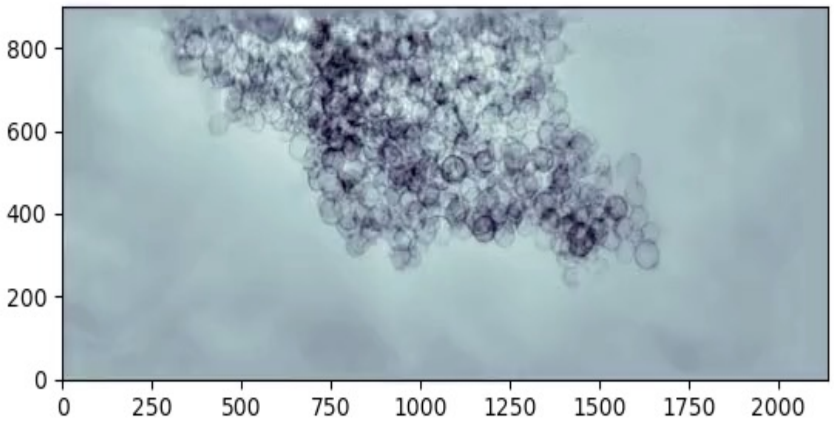
Nanofoam (XPP)

(Cu 100nm-300um void features)



X-ray Pump Probe (XPP) Instrument at LCLS demonstrates ~30 nm spatial resolution on Cu-nanofoam





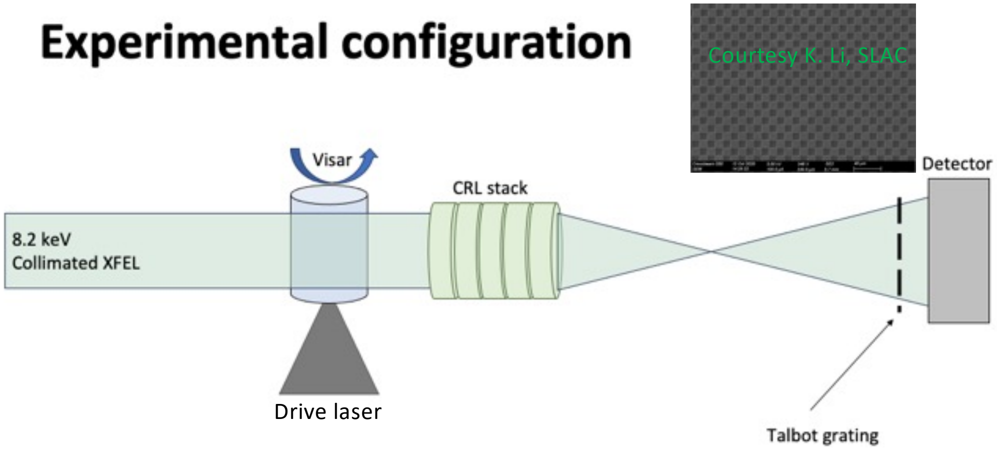
**More detail in paper: A. Carr et al., 3D Ptycho-tomography of nanofoams for radiation hydrodynamics and fusion applications, to be submitted 2024

Investigation of shock dynamics in laser-driven foams using Talbot X-ray Imaging

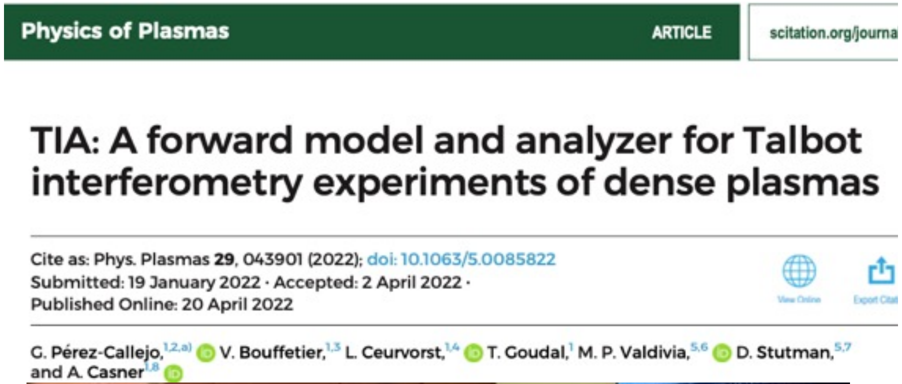
L-1011021 -- PI: M.P. Valdivia (UCSD), V. Bouffetier (ExFEL) , P. Kozlowski (LANL)

Goal: Collect high-resolution Talbot phase-contrast images of laser-driven foams at the Matter in Extreme Conditions (MEC) end-station, Linac Coherent Source (LCLS), SLAC

Experimental configuration



- Talbot imaging accentuates the visibility of highly dense structures and density gradients
- Talbot effect: a Fresnel phenomenon in which self-images of a periodical structure are reproduced at specific planes under coherent illumination
- A phase grating placed at a Talbot distance from a detector enabling phase-contrast imaging → simultaneous retrieval of refraction and absorption



Physics of Plasmas ARTICLE scitation.org/journa

TIA: A forward model and analyzer for Talbot interferometry experiments of dense plasmas

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G. Pérez-Callejo,[1,2,a)] V. Bouffetier,[1,3] L. Ceurvorst,[1,4] T. Goudal,[1] M. P. Valdivia,[5,6] D. Stutman,[5,7] and A. Casner[1,8]

Investigation of shock dynamics in laser-driven foams using Talbot X-ray Imaging: preliminary results

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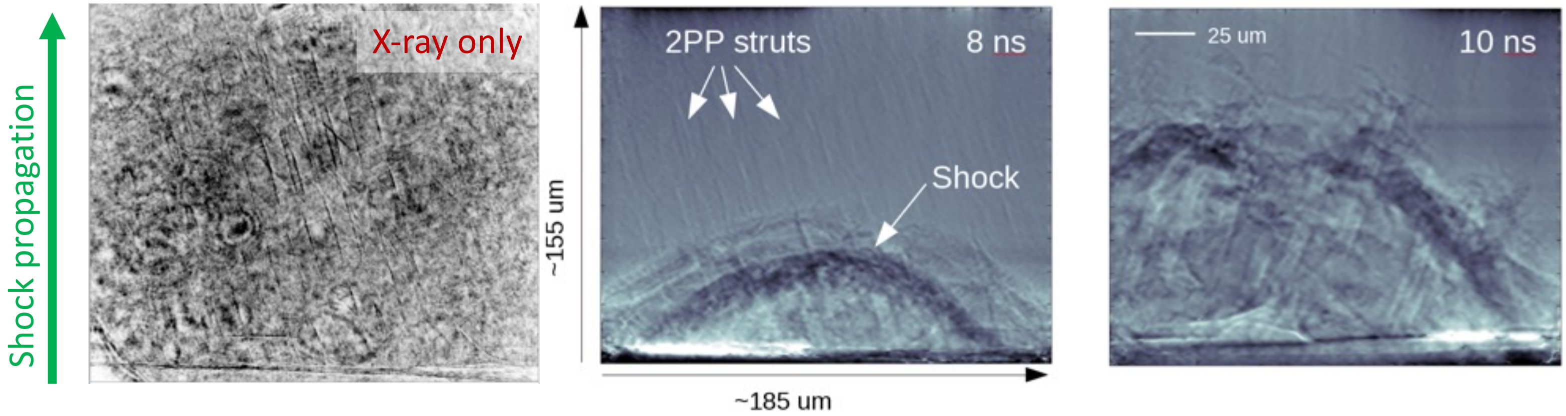
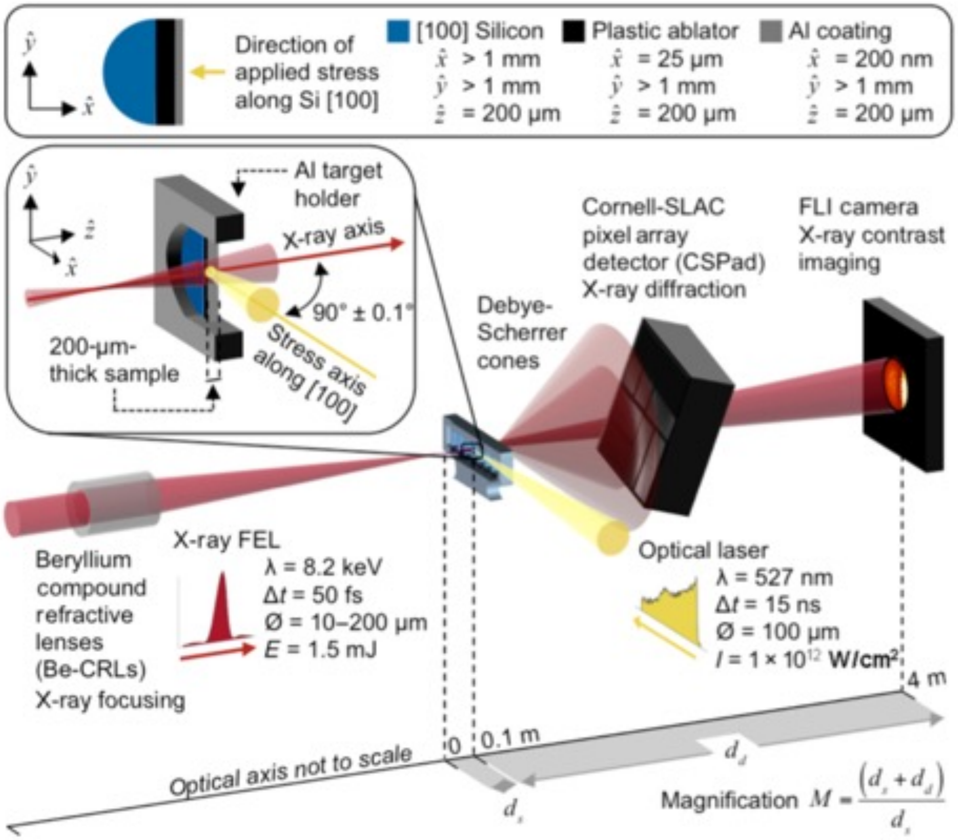
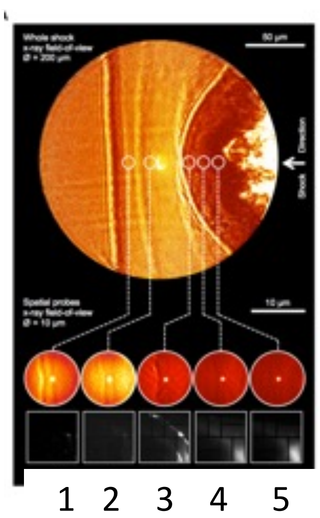


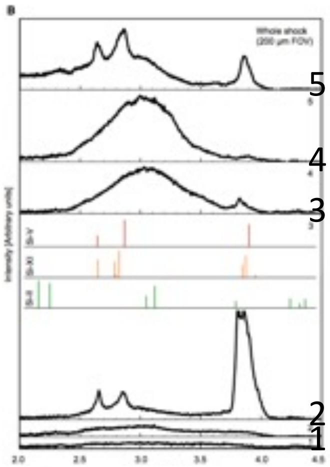
Talbot x-ray deflectometry (TXD) images printed foams shot at LCLS MEC reveal detailed shock front structures. International team of colleagues led by UCSD, have successfully fielded 3D printed lattices at MEC, and obtained phase contrast images using the TXD diagnostic capable of resolving features down to ~100 nm. Phase unwraps were generated using the Talbot Interferometry Analyzer (TIA) code.

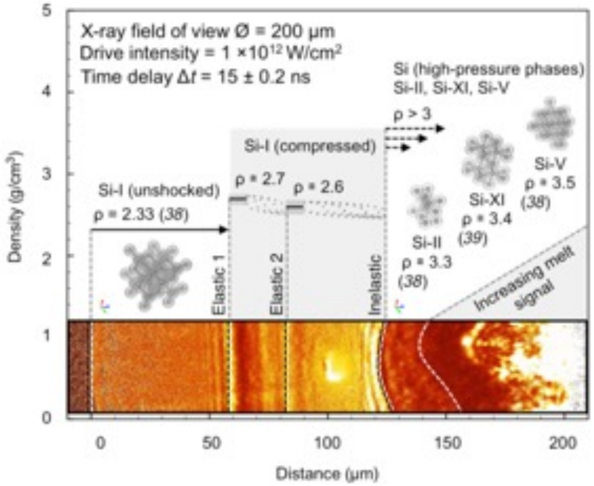
[LANL *P-4, MST-7, XCP-2*; UCSD, SLAC, Stanford University, Universidad de Valladolid, Eu-XFEL, HZDR, CEA, CELLS, Pontifica Universidad Catolica de Chile, Hellenic Mediterranean University]

Phase Contrast Imaging + X-ray diffraction capabilities, case study in Silicon



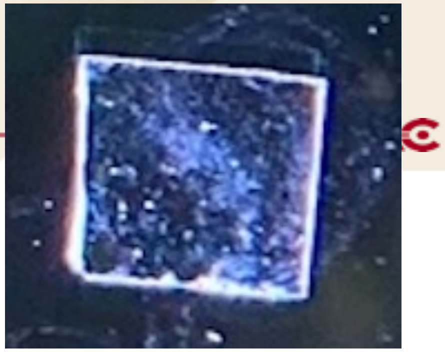






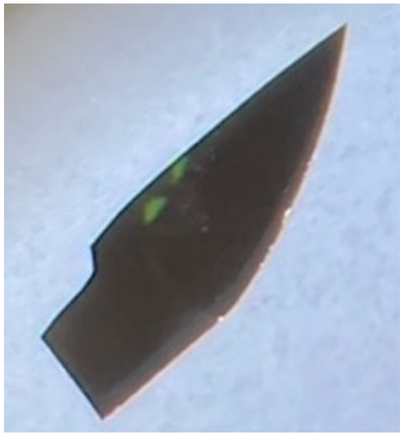
Brown et al.. 2019

Control Samples for Ptychography



Mica sample. 12 microns thick

- Want to mimic low-mass Dark Matter tracks
- Implant pristine silicon and mica sheets
- Four parameter sets:
    1. As ions, 30 keV, 15 um tracks, 6 degrees to normal
    2. As ions, 200 keV, 120 um tracks, 6 degrees to normal
    3. **As ions, 200 keV, 120 um tracks, 30 degrees to normal**
    4. As ions, 1 MeV, 500 um tracks, 6 degrees to normal
- Used parameter set #3 for first LCLS ptychography beam time
- Very rushed sample preparation ~ 1 hour to make beam time
- Significant detritus from cutting small samples



Silicon sample. 10 microns thick

SLAC Collaboration: S. Baum, C. Kenney, P.A. Breur, A. Gleason, J. Segal

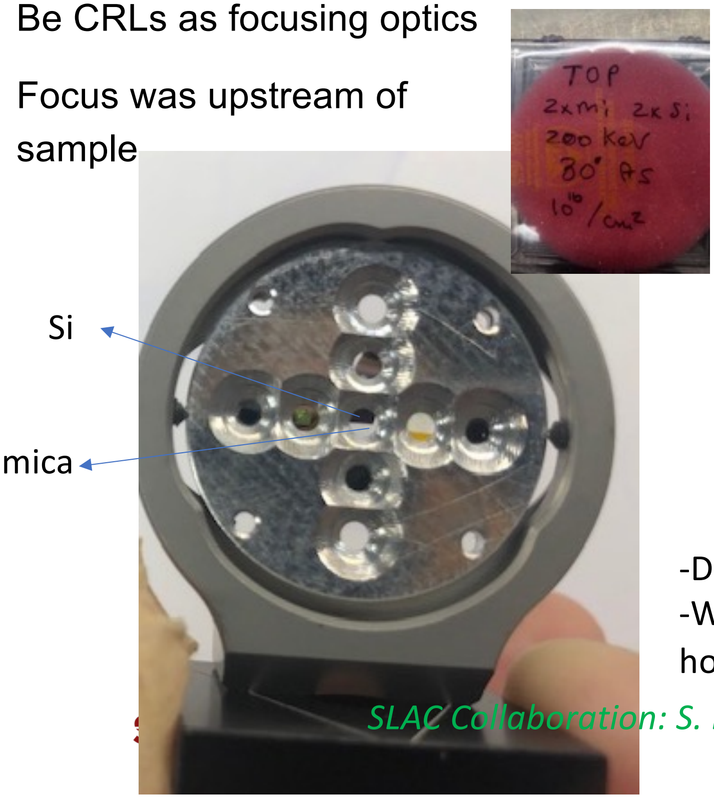
XPP Dark Matter test samples

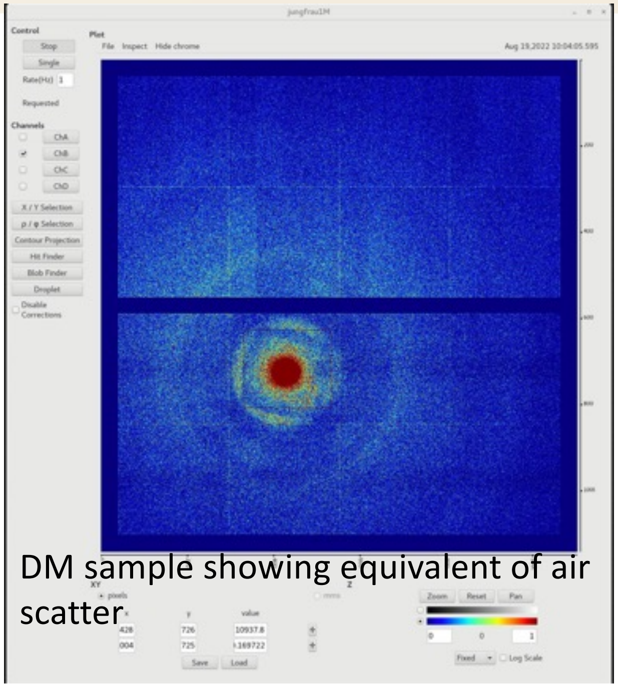
8.9 keV, 1.4 mJ, Si mono

4 um spot size on target

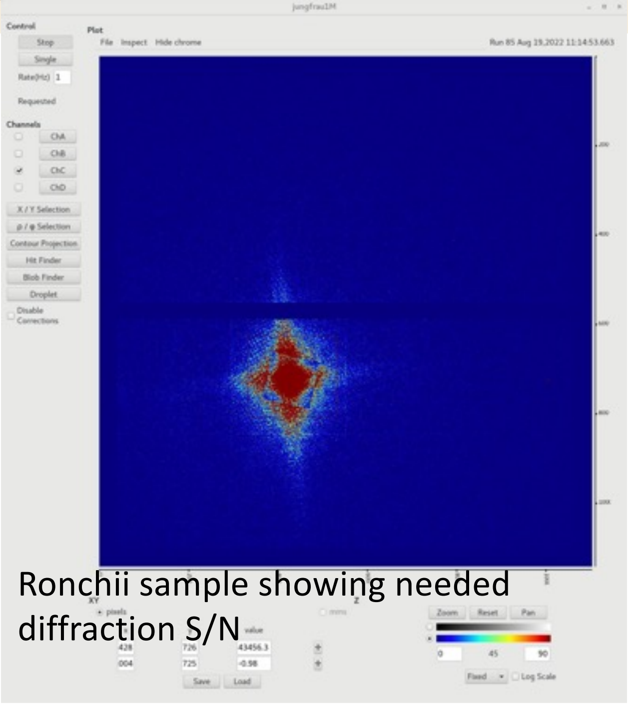
Be CRLs as focusing optics

Focus was upstream of sample





DM sample showing equivalent of air scatter



Ronchii sample showing needed diffraction S/N

-Did not see significant/any scatter from the either DM sample, unfortunately.

-We translated in steps of 5-20 um, laterally in each direction (vertically & horizontally)

SLAC Collaboration: S. Baum, C. Kenney, P.A. Breur, A. Gleason, J. Segal

Run 22 beamtime is possible (April 2024)

3D is possible if FIBed to ~10 um diameter

2D attempt again, maybe increase thickness to 40 um for Si or mica (~70% transmission at 8.9 keV, and etching for max density contrast)

Use known angle of control tracks to search for signal

Use known track geometry to enhance

Longer term exploit the full power of the 4 orders of magnitude increase in power of LCLS II

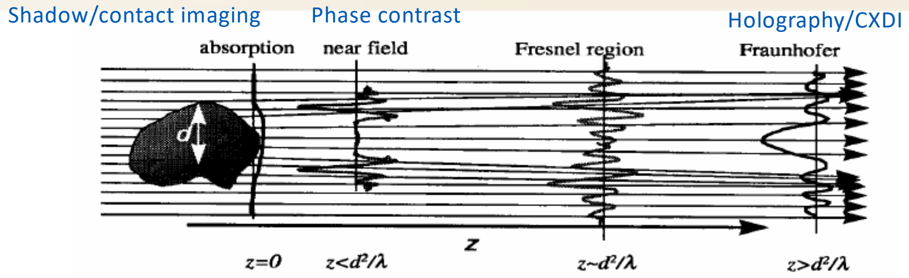
Developing ptychography is a major focus of facility

Ideally x-rays can provide complete track length spectrum

Enabling if can flag areas of possible tracks to decrease AFM workload

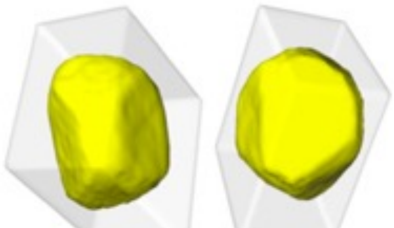
SLAC Collaboration: S. Baum, C. Kenney, P.A. Breur, A. Gleason, J. Segal

Single shot CXDI

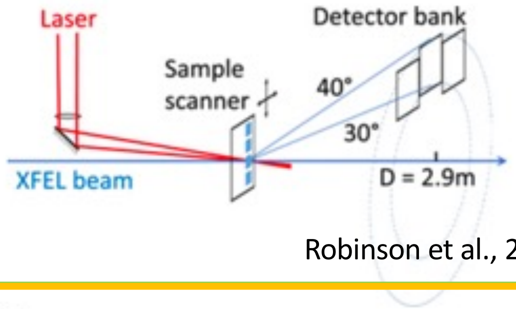


CXDI can provide 3D information, but has only been demonstrated for softer x-rays (<1 keV) and small samples (few micron)

Bragg-CDI



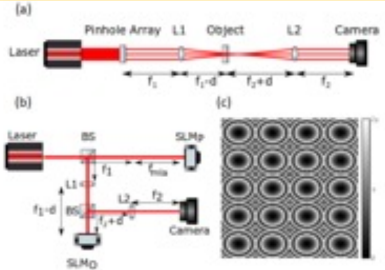
Au nano particle, 200 nm



Robinson et al., 2016

- 9keV
- crystalline sample
- bath the sample in X-rays

Multi-beam ptychography



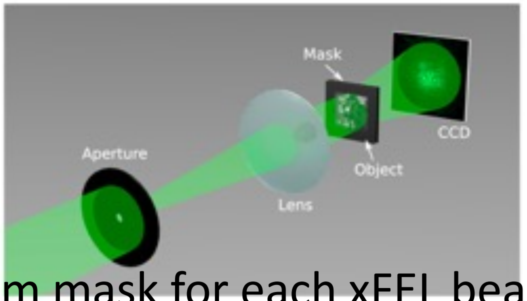
Sidorenko and Cohen, 2015
Wengrowicz et al, 2019

pinhole array for each xFEL beam

- maybe diffraction overlap on detector
- limited fov
- 70% overlap between spots

Single shot CXDI

time resolved ptychography

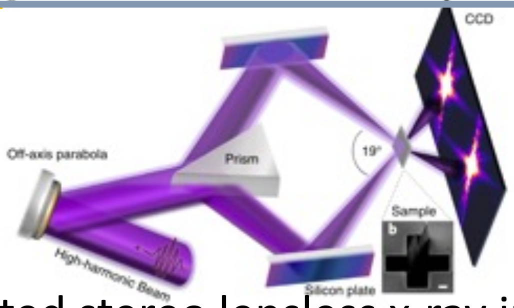


random mask for each xFEL beam

Seaberg et al, 2015

- so far only test with optical light & soft X-rays

ptychotomography

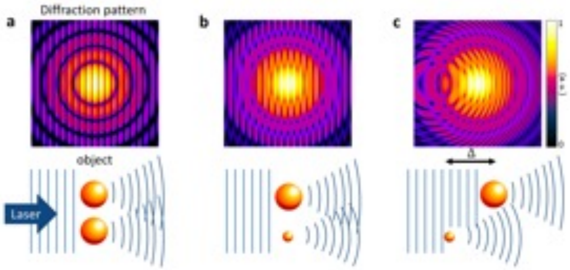


computed stereo lensless x-ray imaging

Duarte et al, 2019

- so far only soft X-rays

in-flight holography



Gorkhover et al, 2018

- so far only soft X-rays
- maintain know (unchanging or predictable) reference which must scatter more or equivalent to the sample

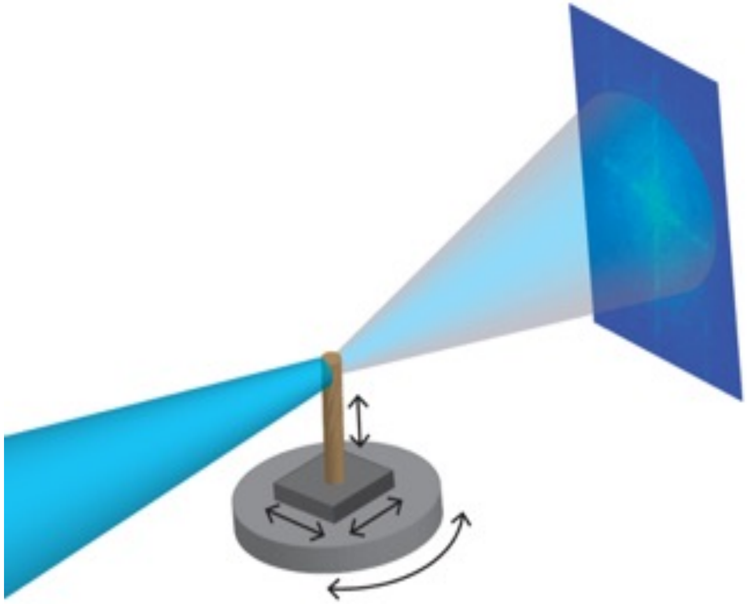
Using minerals as Dark Matter 'paleo-detectors' requires large volume imaging → Novel CXDI Techniques

- Multiple samples of same material different locations?
- Multiple materials of similar ages
- Samples from different depths (background understanding)
- Samples of different age to provide stop-action video of Earth's neutrino and DM environment over cosmic time
  - → Need to scan 10 mg with 1nm resolution in 3D track length
  - → Need to scan ~400 cm^2

Capabilities to date: 20µm x 50µm, 30 seconds

10 μm^3, 360 deg, 6-8 hours

Tiling, stitching & high-throughput compute strategies to improve speed and increase volumes



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