Frontier of Dynamic Materials Using Ultrafast X-ray Radiography

A. Gleason, SLAC/Stanford University

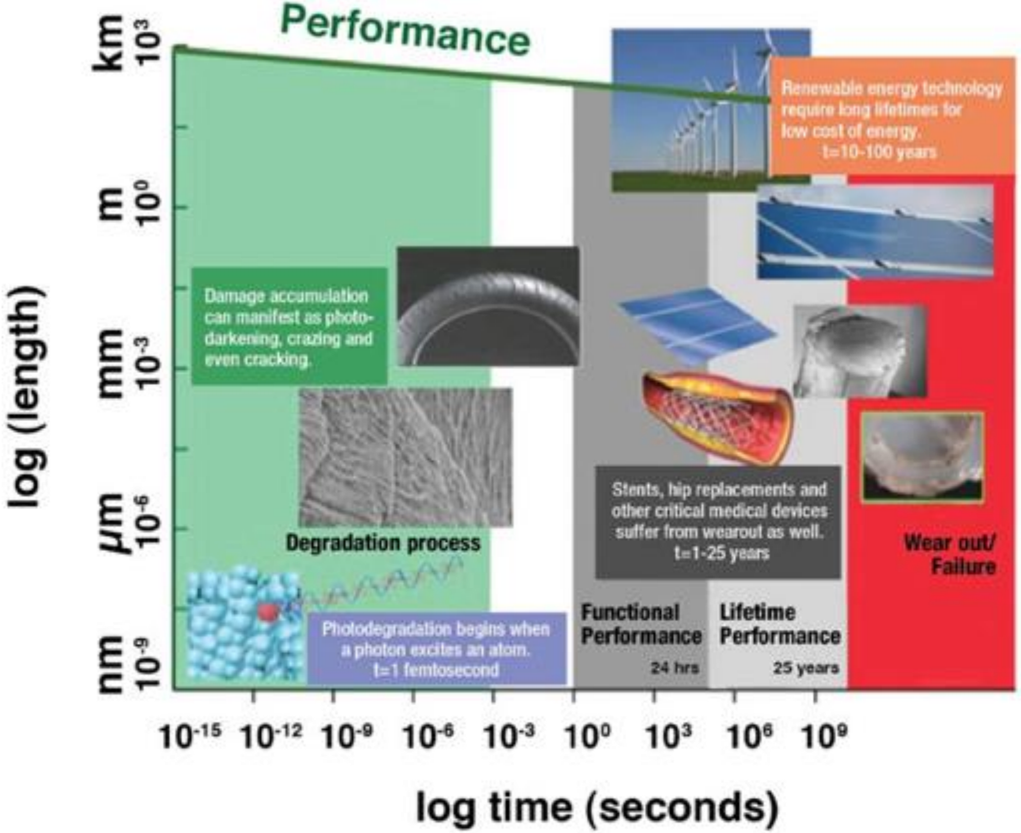
HEDS Seminar Series at LLNL

July 1, 2021

Outline

- Introduce X-ray imaging platforms for high-pressure science
- Case-studies
  - ICF ablator materials
  - Geomaterials & possibilities in astrobiology
- Outlook

Dynamic X-ray Imaging Is the Key to Solving Structure-Properties-Performance Challenges



Materials Genome

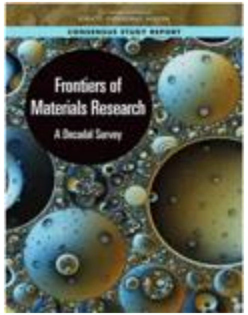
BESAC 2012

NAS 2015

BESAC 2015

NAS 2017

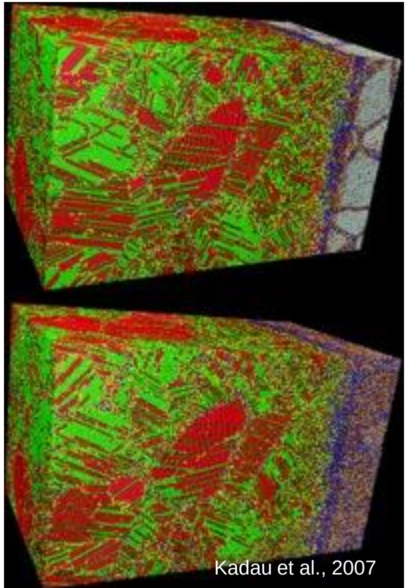
NAS 2019

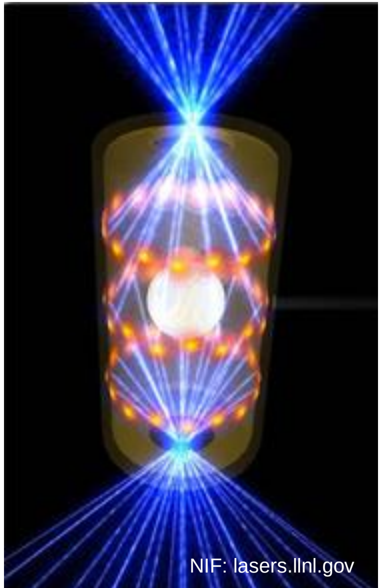


Frontier in Condensed Matter, Materials Science and Plasma Physics

To understand the fundamental physics that govern atomic interactions in High Energy Density (HED) materials, measurements are required at relevant temporal- and spatial-scales.

→ dynamic-loading + ultrafast X-ray techniques (XRD, imaging, spectroscopy)



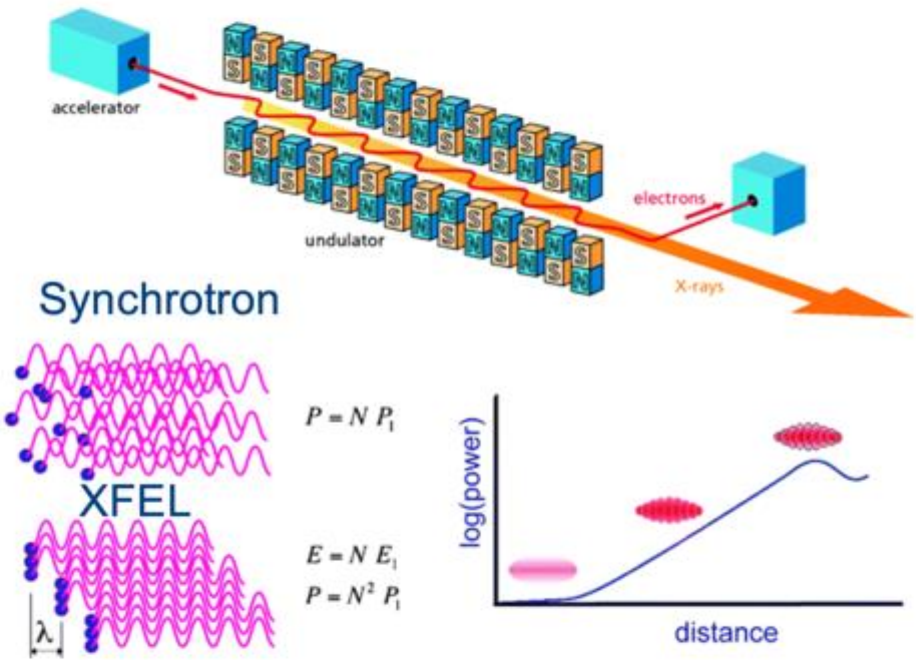


Good news: temporal- and spatial-fidelity of experiments now rival the best simulations

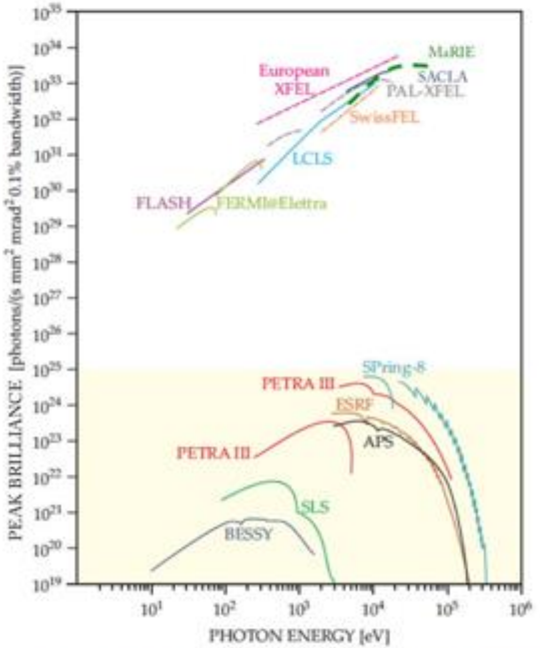
Bad news: cannot accurately model the behavior of materials at extreme conditions without including the microphysics

Why make a bright, coherent source?

Femtosecond, brilliant (10^{13}), coherent hard X-ray pulses



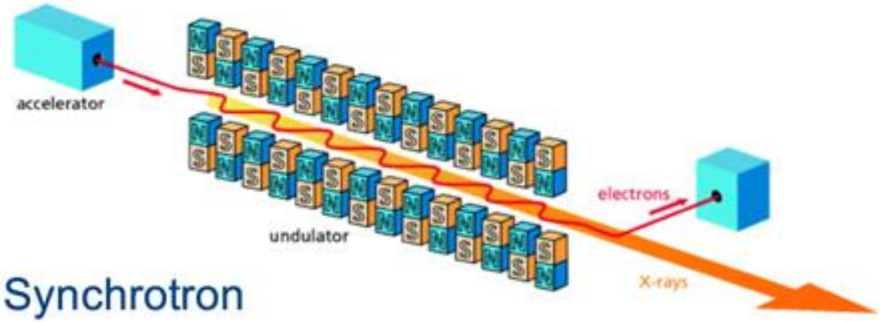
Patterson, B. D. & Abela, R. *Phys. Chem. Chem. Phys.* **12**, 5647–52 (2010).

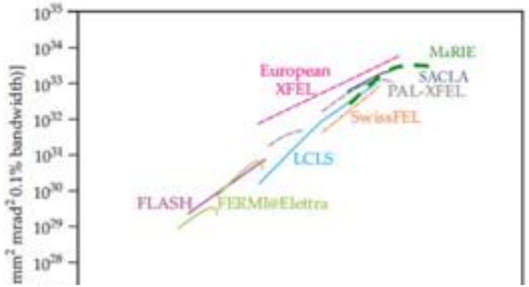


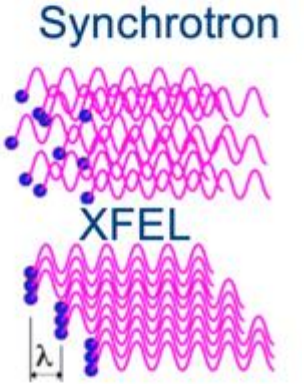
Modified from E. Weckert, *IUCrJ* 2, 230–245 (2015).

Why make a bright, coherent source?

Femtosecond, brilliant (10^{13}), coherent hard X-ray pulses

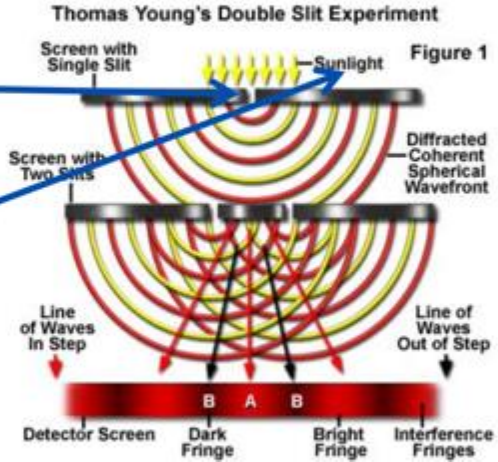






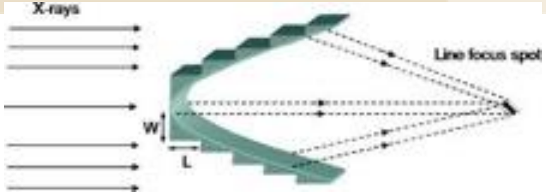
Patterson, B. D. & Abela,

- **Transverse (spatial) coherence related to the source size**
  - Defines a transverse coherence length ($\xi_t \sim 1/d$)
- **Longitudinal coherence (temporal) coherence is related to the bandwidth**
  - Defines a longitudinal coherence length ($\xi_l \sim \lambda/\Delta\lambda$)



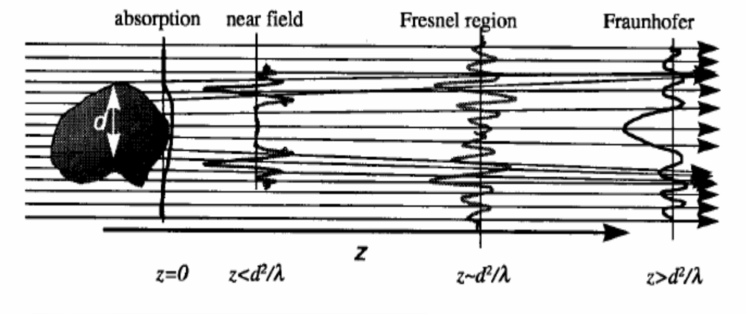
Moving toward the far-field in dynamic hard X-ray imaging: coherent X-ray diffractive imaging (CXDI)

- **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

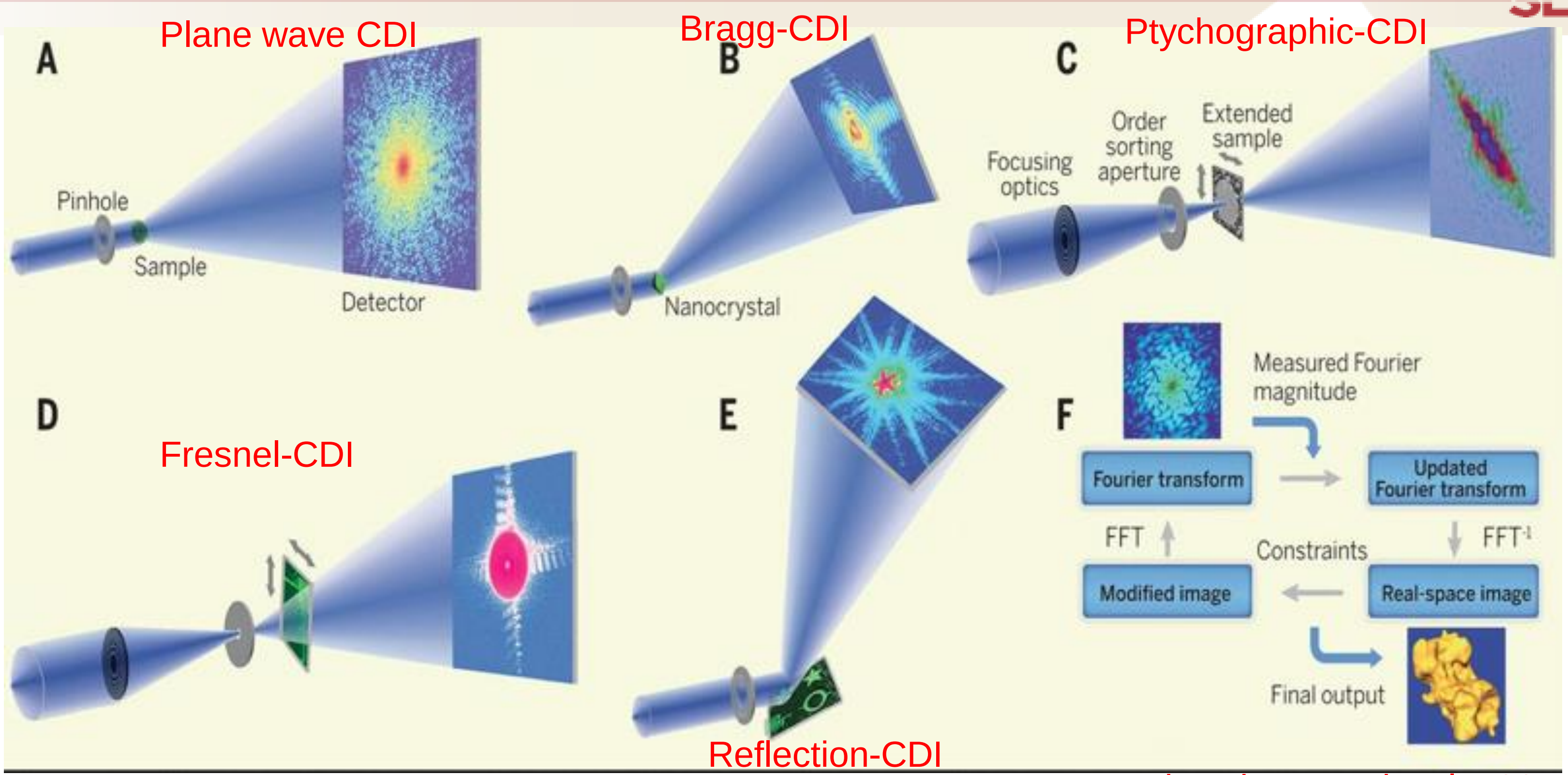
Shadow/contact imaging Phase contrast Holography/CXDI



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

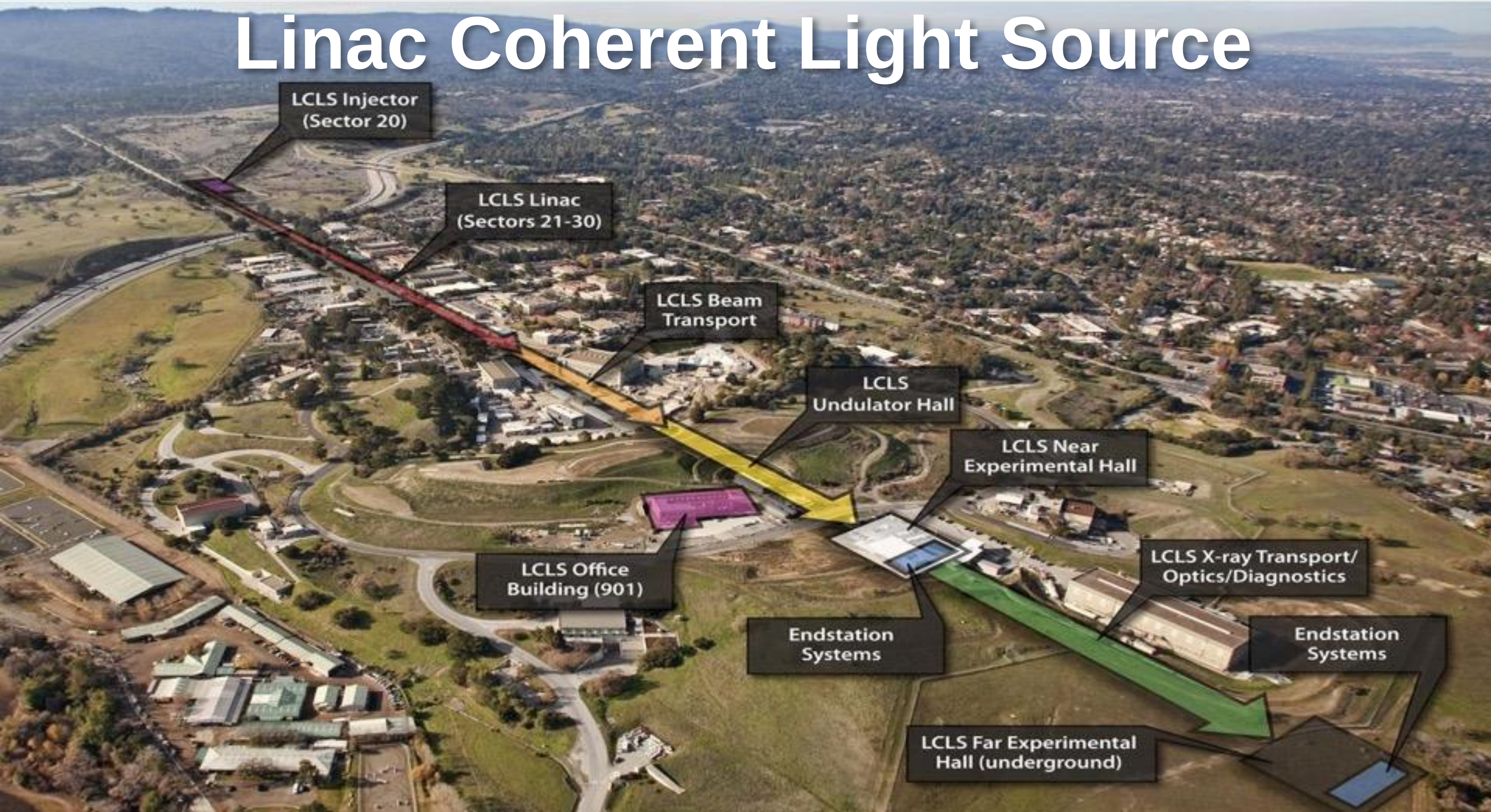
CXDI can provide 3D information



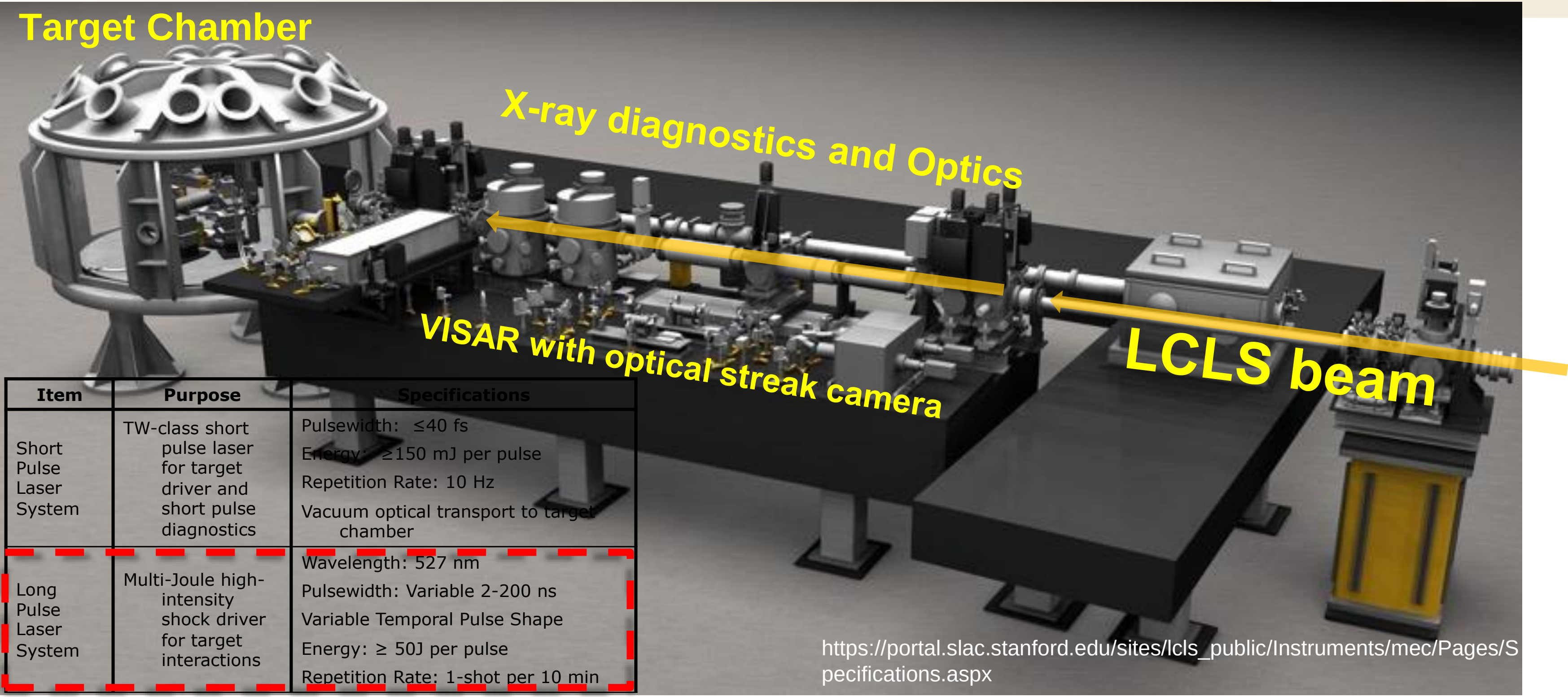
Miao et al., 2015

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

Linac Coherent Light Source



MEC instrument optics and diagnostics

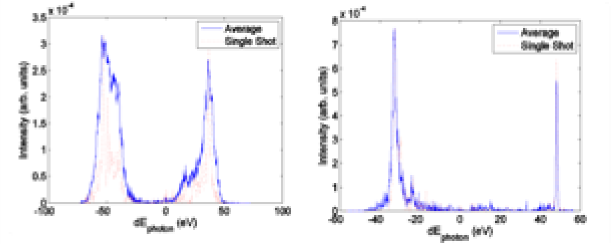


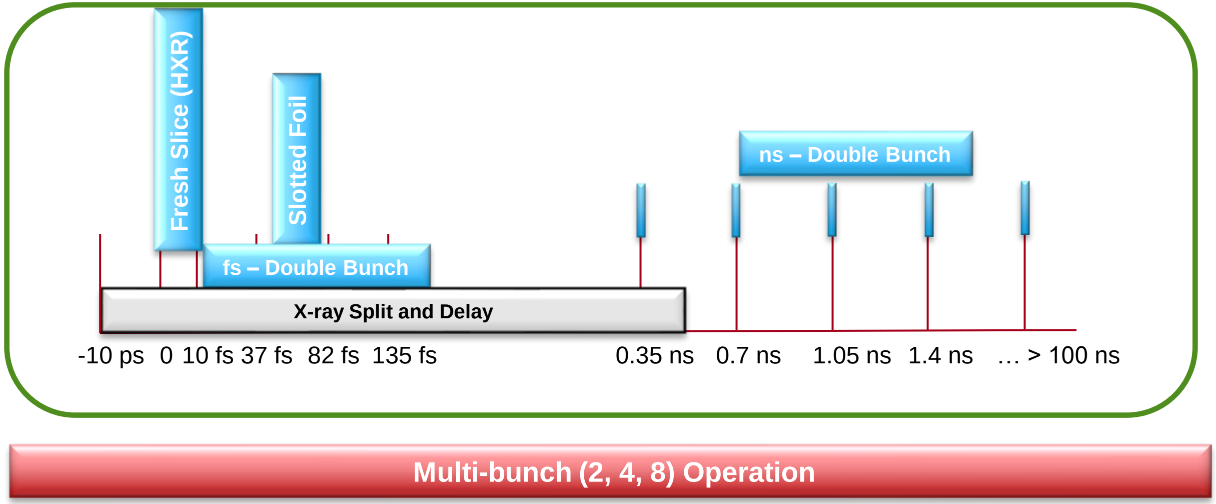
Item	Purpose	Specifications
Short Pulse Laser System	TW-class short pulse laser for target driver and short pulse diagnostics	Pulsewidth: ≤40 fs Energy: ≥150 mJ per pulse Repetition Rate: 10 Hz Vacuum optical transport to target chamber
Long Pulse Laser System	Multi-Joule high-intensity shock driver for target interactions	Wavelength: 527 nm Pulsewidth: Variable 2-200 ns Variable Temporal Pulse Shape Energy: ≥ 50J per pulse Repetition Rate: 1-shot per 10 min

The Matter in Extreme Conditions (MEC) instrument combines the unique LCLS beam with high power optical laser beams, and a suite of dedicated diagnostics tailored for the study of Warm Dense Matter, High Pressure Physics, Shock Physics, and High Energy Density Physics.

LCLS has a wide range of dual-pulse / dual-color modes available & ability to select Δt, ΔE, seeding, polarization

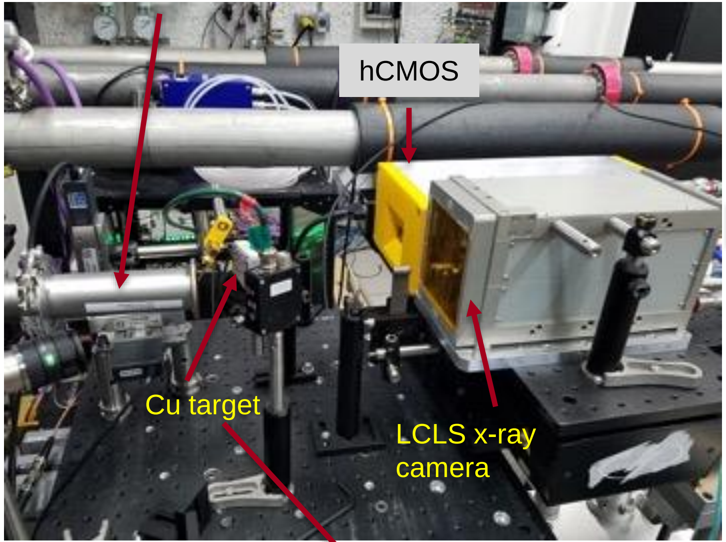
- Double Slotted Foil
- Split Undulator
- Injector laser pulse splitting
- Multiple laser pulses at cathode (dual lasers)
- Fresh Slice Technique

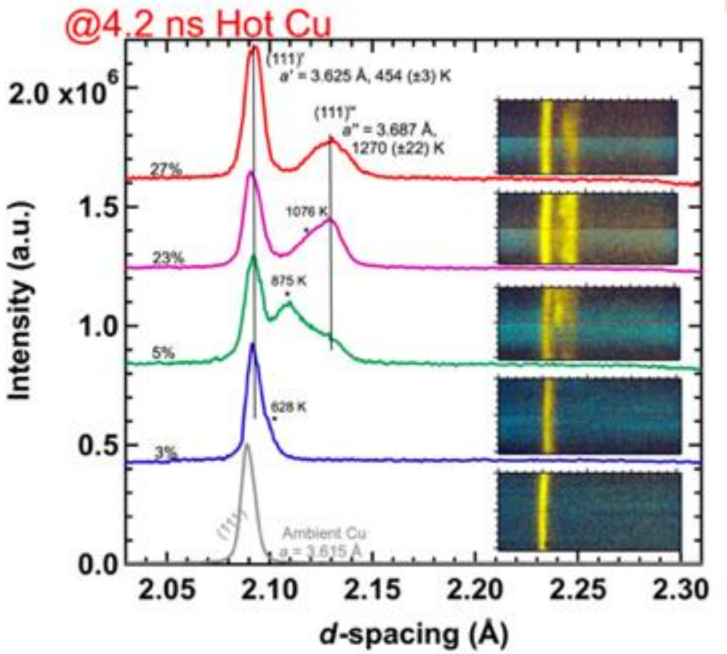


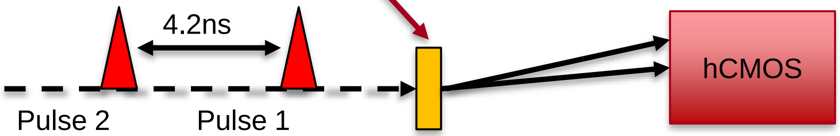


hCMOS camera developed by SNL/LLNL has been tested* using LCLS femtosecond x-ray pulses: linearity, gate profile, QE…

LCLS : Two x-ray pulses, 7.2keV, 4.2ns apart





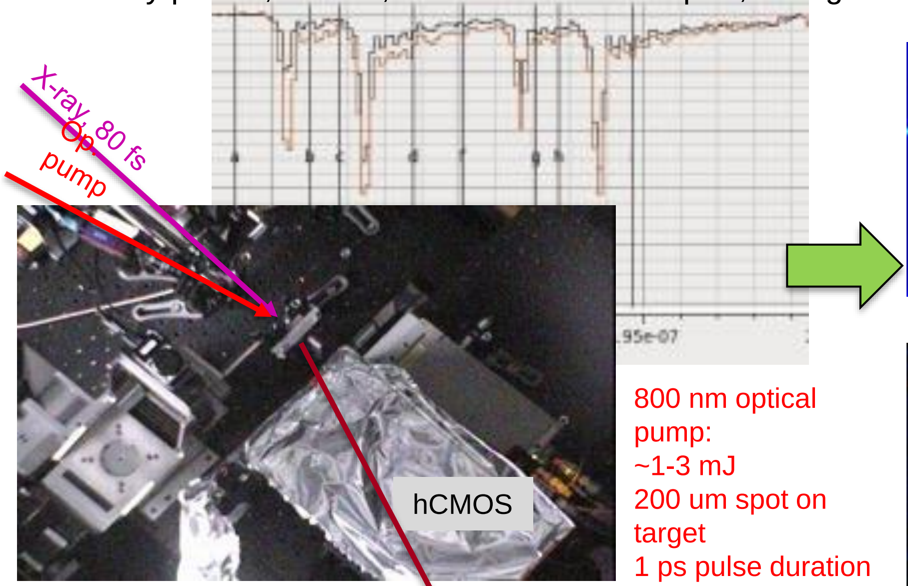


Hart et al., 2019

* Experiment led by P. Hart (SLAC)

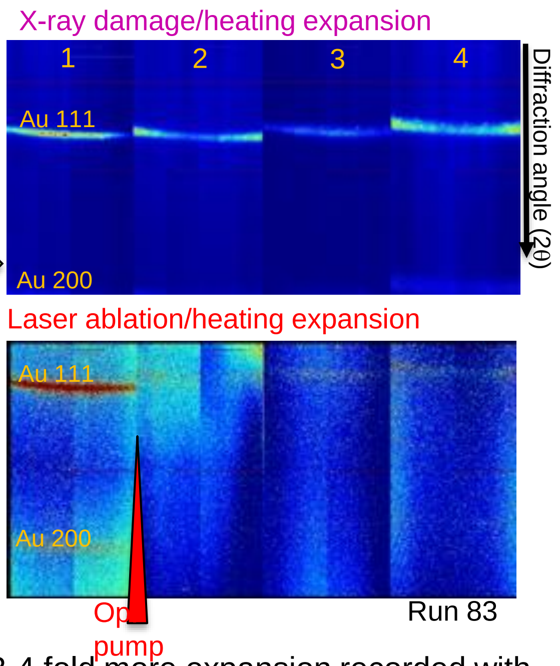
4-frame + 4 pulse test at XCS hutch, LCLS: camera characterization + optical laser pump experiment

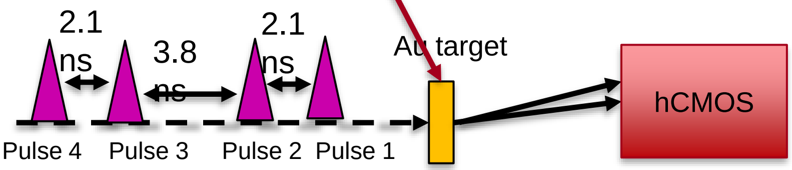
4 x-ray pulses, 7.2keV, 2.1 + 3.8 + 2.1 ns apart; 1 ns gate



800 nm optical pump:
~1-3 mJ
200 um spot on target
1 ps pulse duration

Icarus hCMOS Images

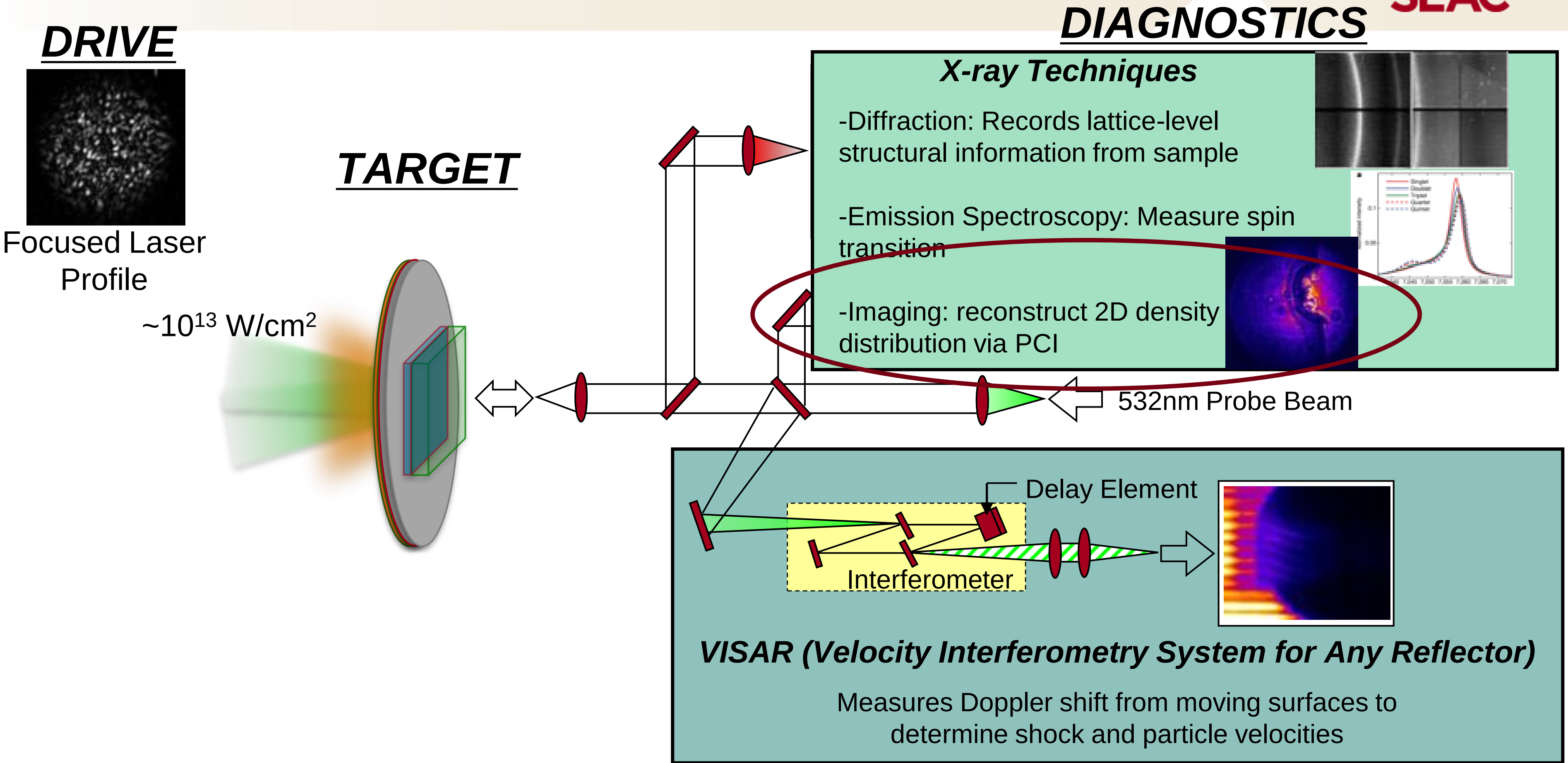




- 3-4 fold more expansion recorded with the optical pump
- Dynamic recrystallization

* Experiment led by **P. Hart (SLAC),** Dan Damiani, Arianna Gleason, Phil Heimann, Silke Nelson, Emma McBride, Sanghoon Song, Diling Zhu, Mike Glownia, XCS staff, ; LLNL: Arthur Carpenter, Matthew Dayton, Emily Hurd; SNL: Marcos Sanchez

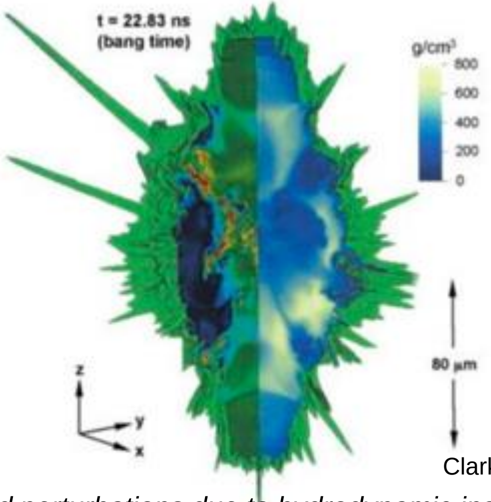
Laser driven shock compression + X-ray techniques



Void Collapse Physics: Mesoscale Materials Properties Control Functionality at Extreme Conditions

Fusion energy materials face harsh environments:
-structural materials in a reactor
-plasma facing materials / first walls of a tokamak
-ICF materials

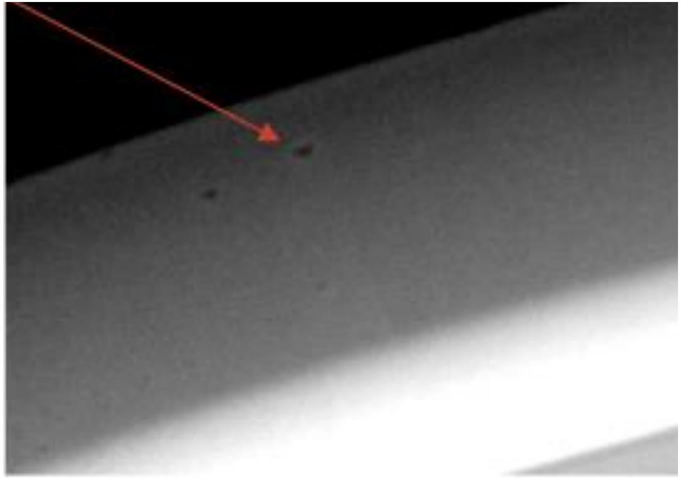
3D simulation of ICF implosion



Clark et al., 2015

Spiked perturbations due to hydrodynamic instability growth seeded by defects in the ablator.

X-ray radiograph of diamond-ablator showing voids



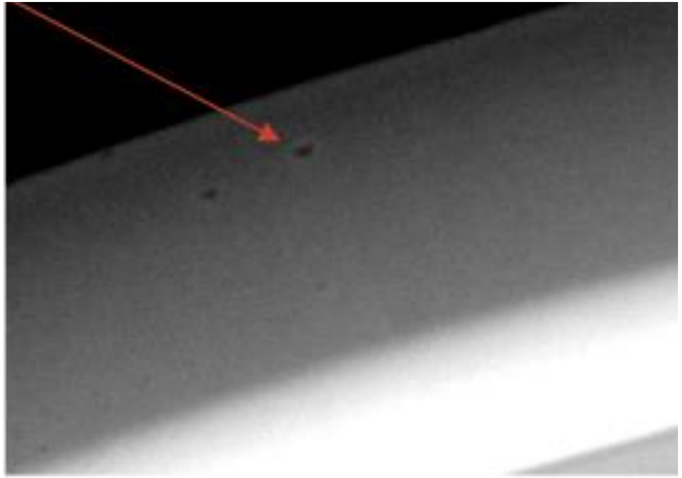
Courtesy T. Doeppner, 2019

Void Collapse Physics: Mesoscale Materials Properties Control Functionality at Extreme Conditions

Fusion energy materials face harsh environments:
-structural materials in a reactor
-plasma facing materials / first walls of a tokamak
-ICF materials

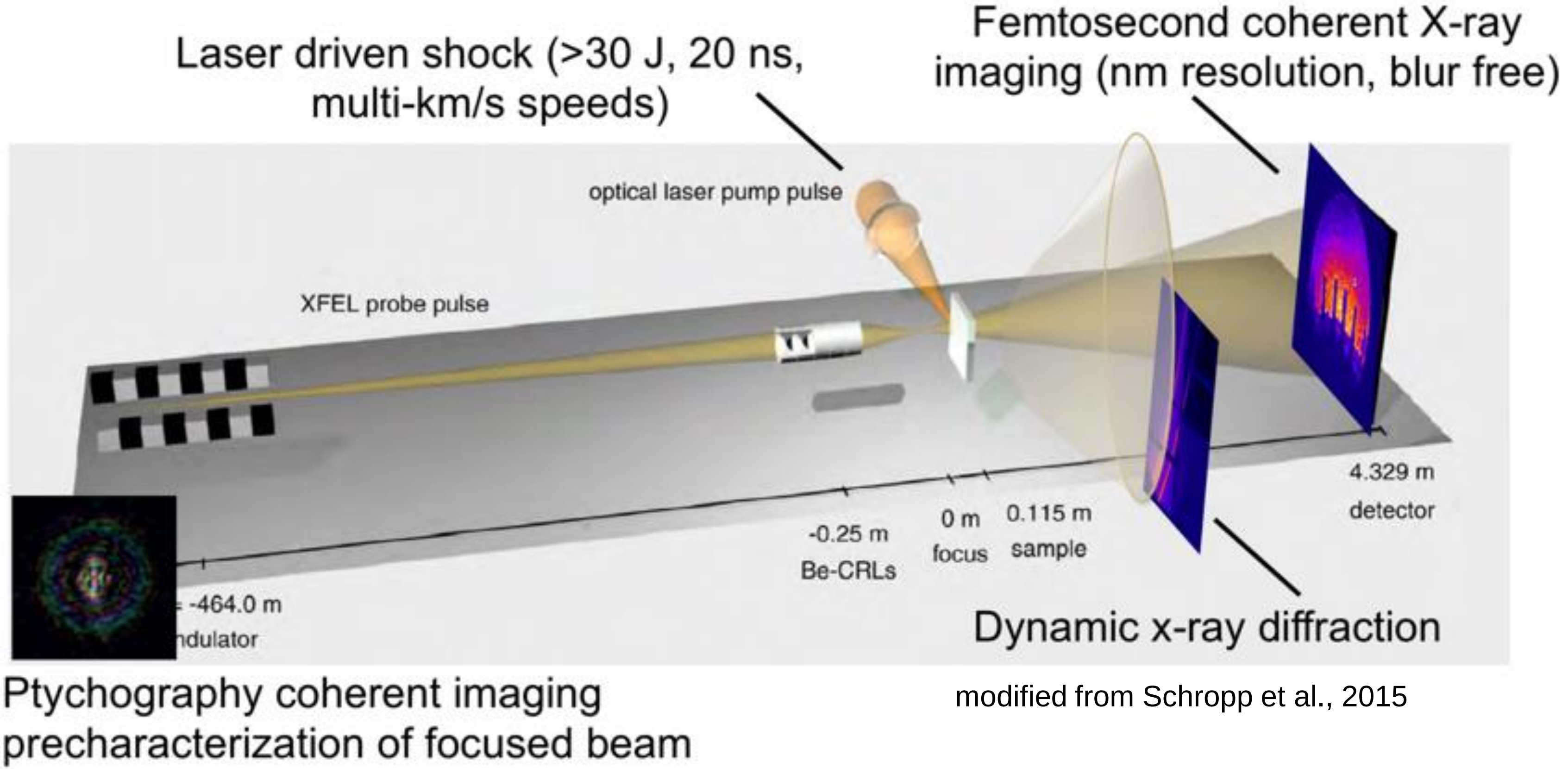
Key questions:
- How do we mitigate hydrodynamic instabilities plaguing ICF?
- What is the relationship between void size and collapse rate and interaction with the shock front?
- What are the plasma properties inside the void and what is the extent of jetting and how does that modify the surrounding material?

X-ray radiograph of diamond-ablator showing voids



Courtesy T. Doeppner, 2019

Revolution in X-ray sources is enabling a revolution in High Energy Density (HED) Science



modified from Schropp et al., 2015

Phase contrast imaging (PCI) for 2D density distribution @ MEC, LCLS

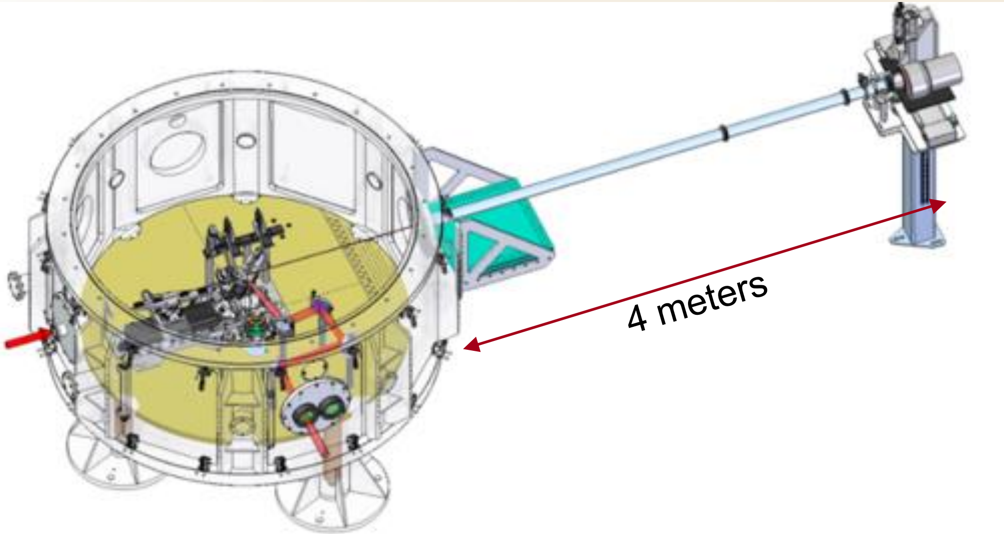


FIG. 1. 3D model of the PCI instrument in the MEC target chamber, and location of the x-ray cameras behind the MEC chamber. Different x-ray cameras can be translated into the beam on a motorized stage. Camera location can be varied between 1.2 m and 5 m from the target, by changing the length of the flight tube.

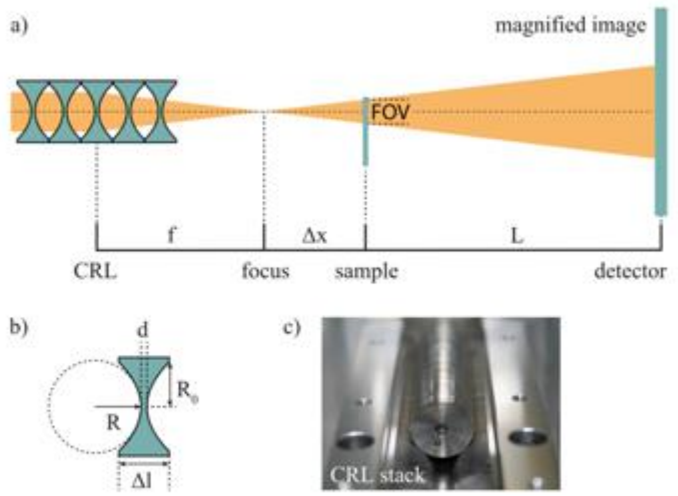
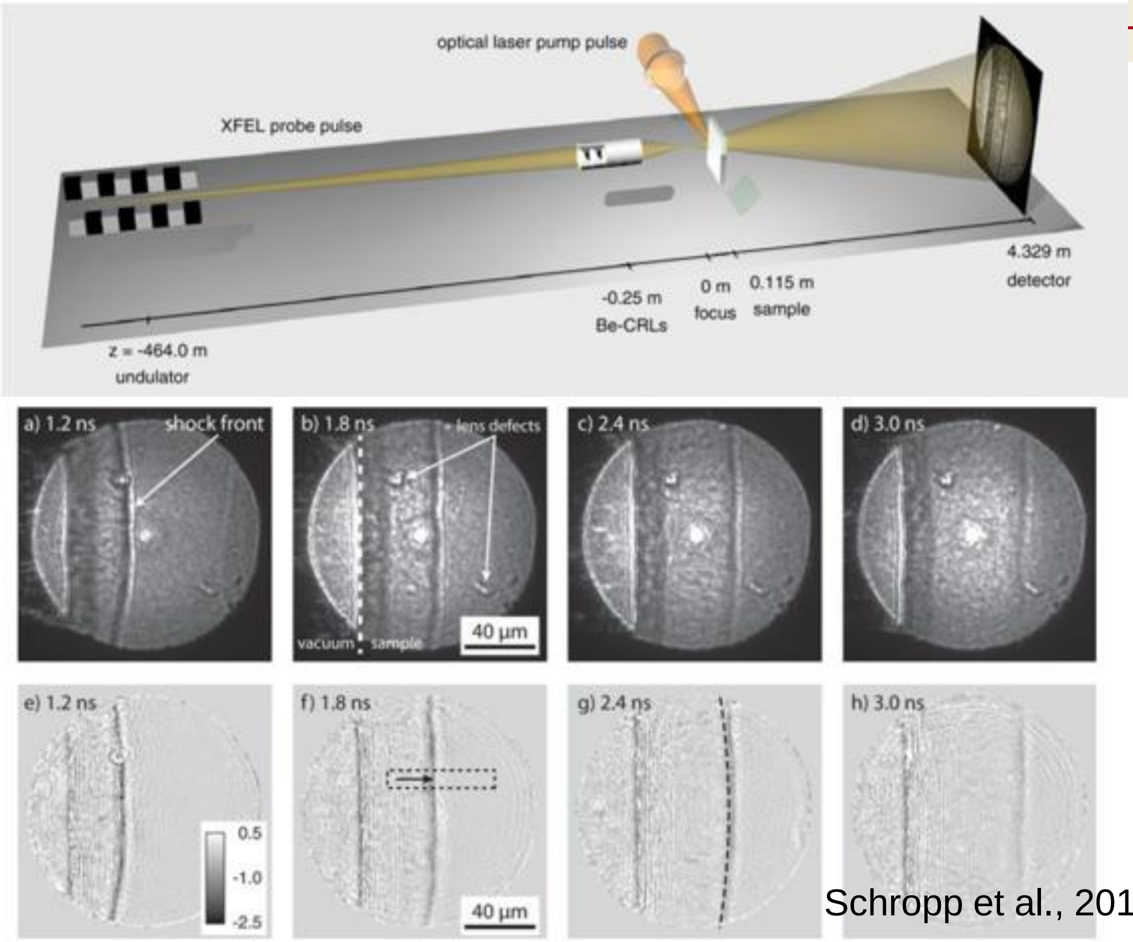


FIG. 3. (a) Schematic of the Be CRL setup in PCI geometry. The lens stack has a focal length f. The focus is placed at a distance Δx in front of the sample. A detector is then positioned at a distance L after the sample, leading to a magnification $M = (L + \Delta x)/\Delta x$. (b) Sketch of a single parabolic Be CRL indicating relevant geometric parameters. (c) Image of a stack of Be CRLs aligned in a lens holder.

Nagler et al., 2016

PCI + shock compression @ MEC in diamond

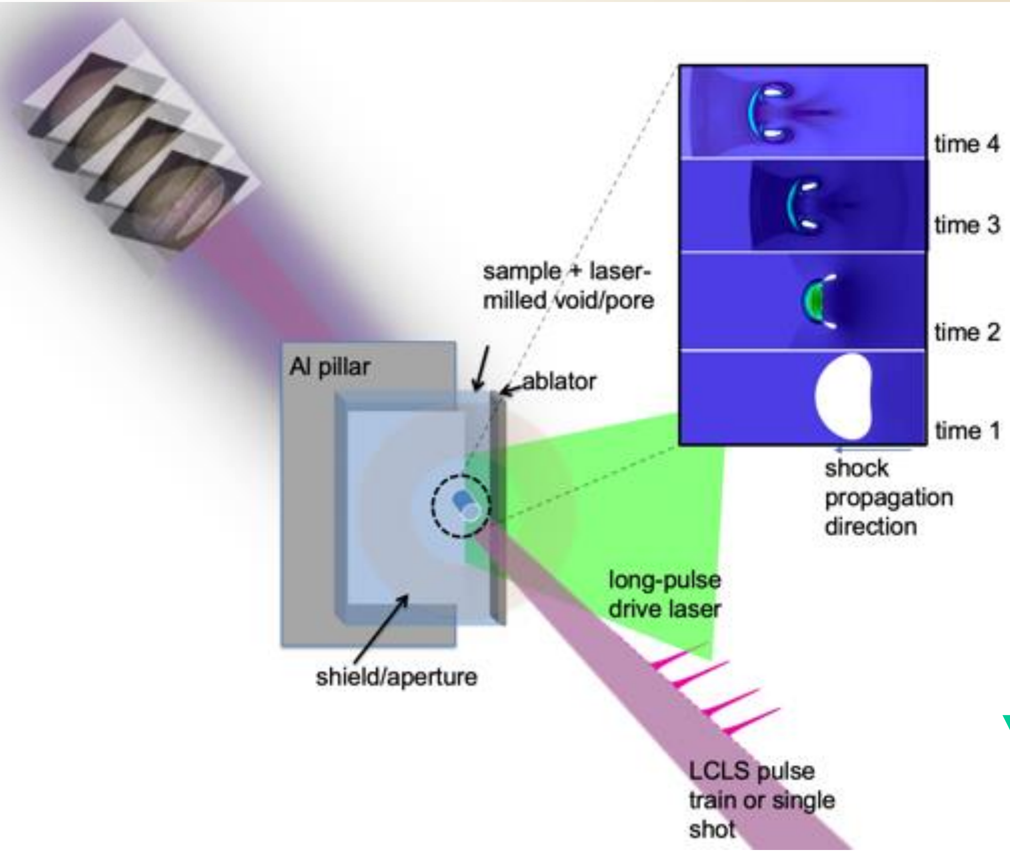


Schropp et al., 2015

Caveats/Notes:

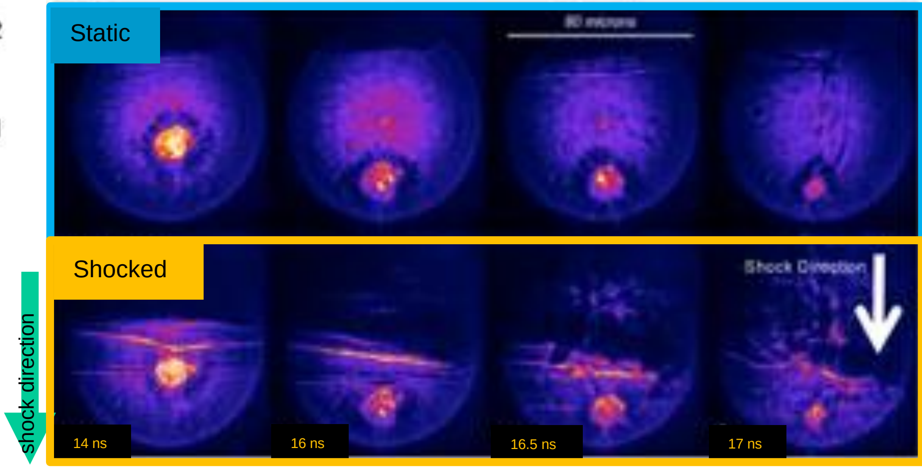
- → phase-contrast images measured at different time delays on different samples
- → recording the intensity only in the detector plane, so the phases of the x-ray wave field are lost.
- → do ptychography of incident beam enables calculation of transmission function via iterative phase-retrieval techniques
- → compression of the material by the shock wave introduces an additional phase shift in the x-ray wave field behind the sample
- → reconstructed phase change corresponds to an integrated value accumulated along the path of the x rays through the sample
- → assume spherical symmetry use tomography to reconstruct local phase change per voxel

Dynamic process timeseries in a single sample



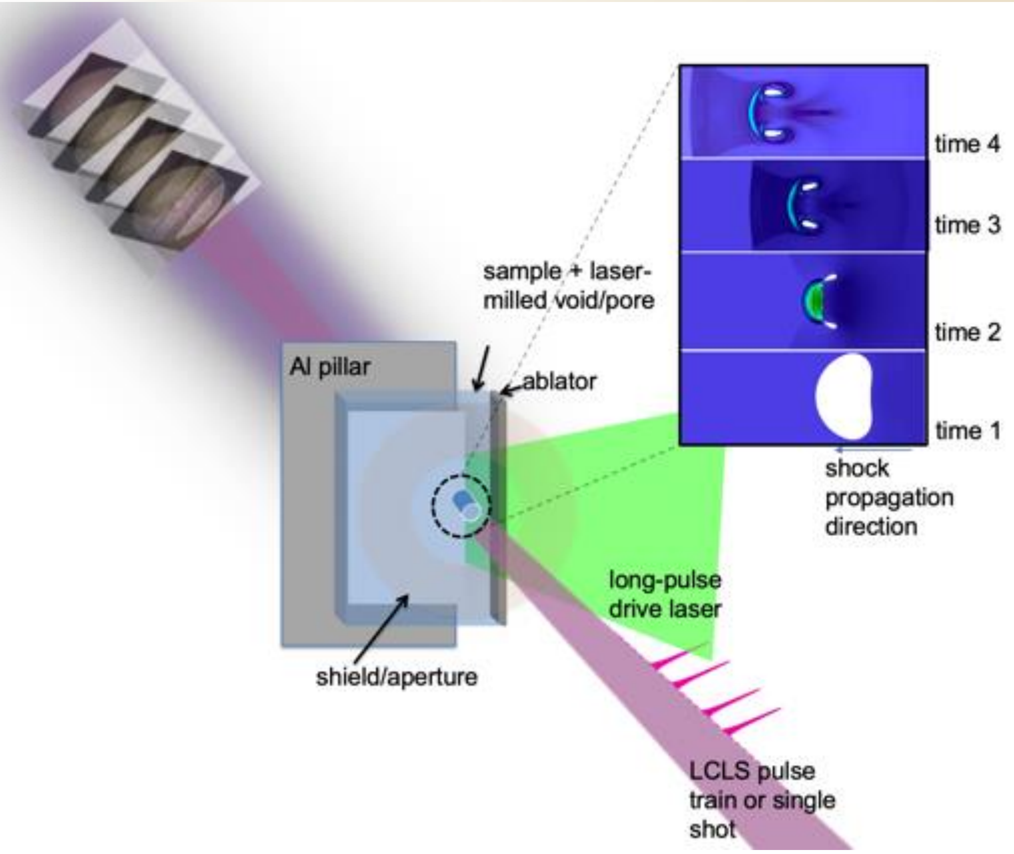
Ultrafast movie of a shock front traversing a void

Void collapse during a shock at MEC



Sandberg et al.

Dynamic process timeseries in a single sample



Ultrafast movie of a shock front traversing a void for *2-D & 3-D image reconstruction*

- ICF ablator materials with natural or synthetic voids:
  -Be & diamond (with LLNL)
  -polystyrene (with LLE)

- Robust image algorithm deployment/development

- X-ray optics design/testing for multi-zone plate or design + split and delay

Fabricating synthetic voids

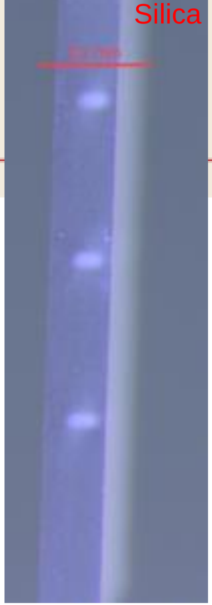
Laser Milled:

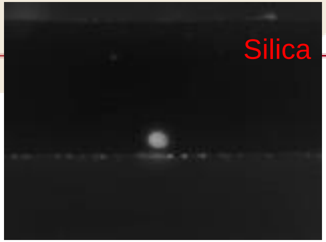
Femtosecond laser milled voids:

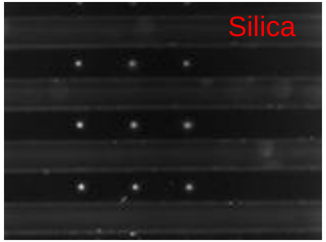
- in polystyrene (10-20 um diameter)
- in silica glass (20 um diameter)

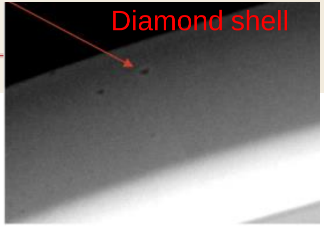
Photoresist spin + hollow shell :

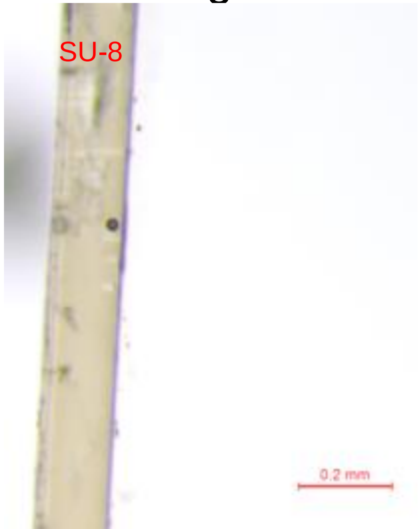
- in SU-8 + hollow glass shell (40 um diameter)

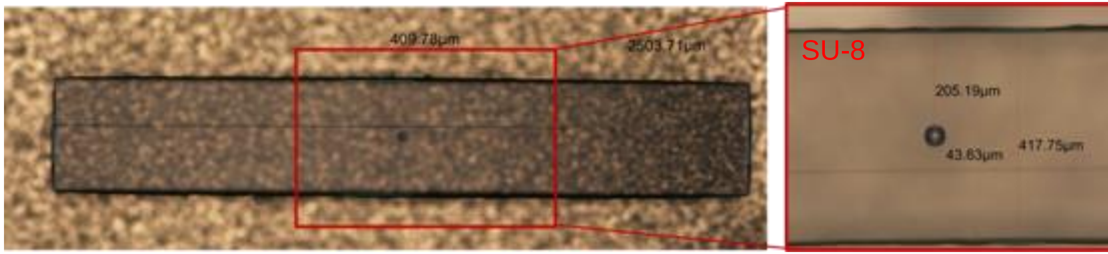


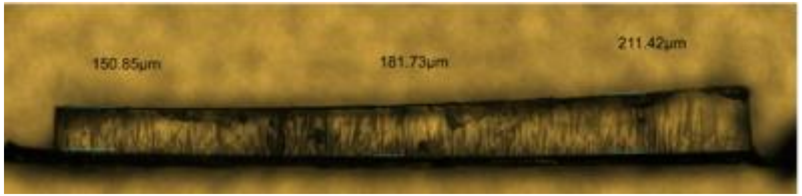












Void collapse in energetic materials at HP-CAT & DCS, APS

Time-resolved x-ray imaging of void collapse at 10 micron length scales

Michael R. Armstrong[1, a)], Ryan Austin[1], Eric Bukovsky[1], Paul Chow[2], Yuming Xiao[2], Paulius Grivickas[1], Joshua Hammons[1], Batikan Koroglu[1], Andrew Robinson[1], William Shaw[1], and Trevor Willey[1]

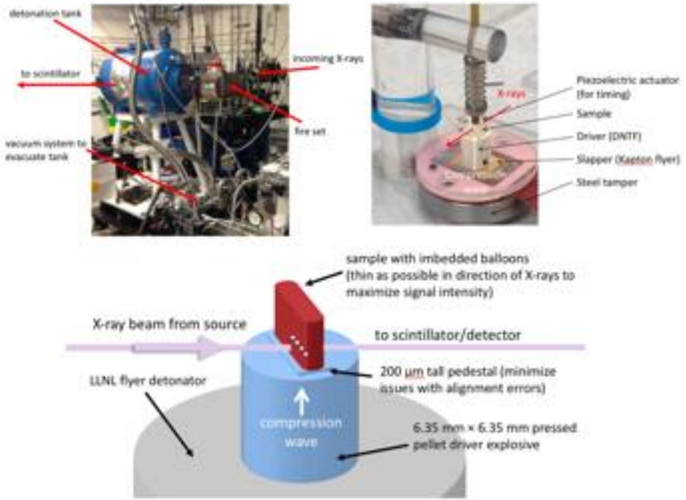


FIGURE 3. (top left) The containment chamber, associated equipment, and orientation with respect to the x-ray beam. (top right) A close-up picture of the sample configuration outside the chamber. (bottom) A schematic of the experiment.

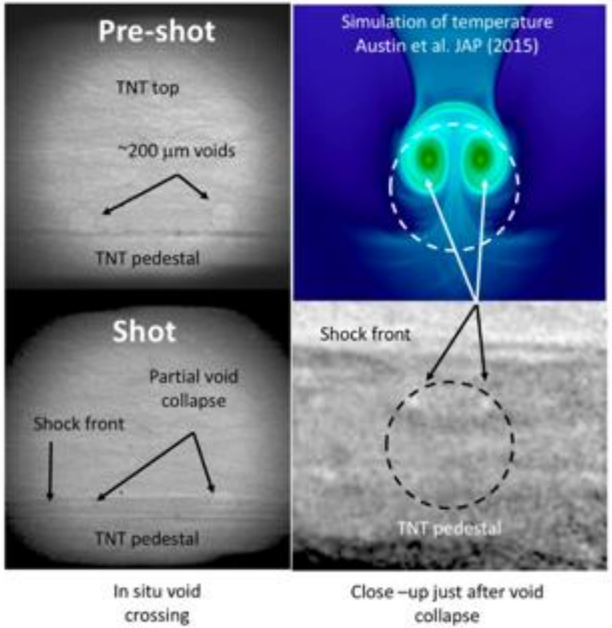
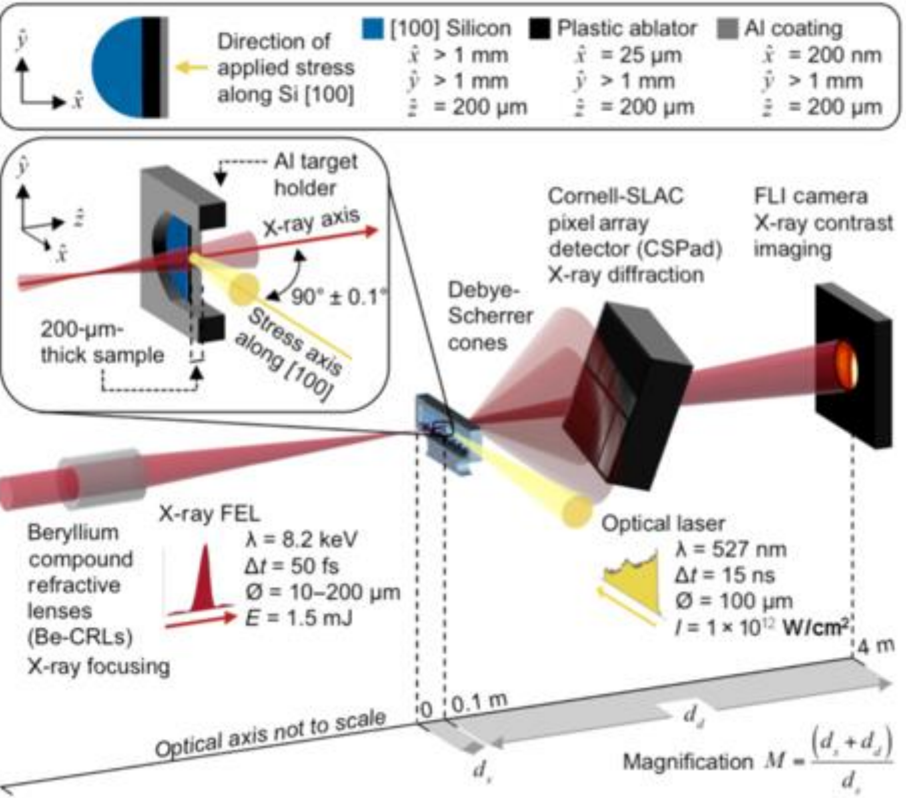


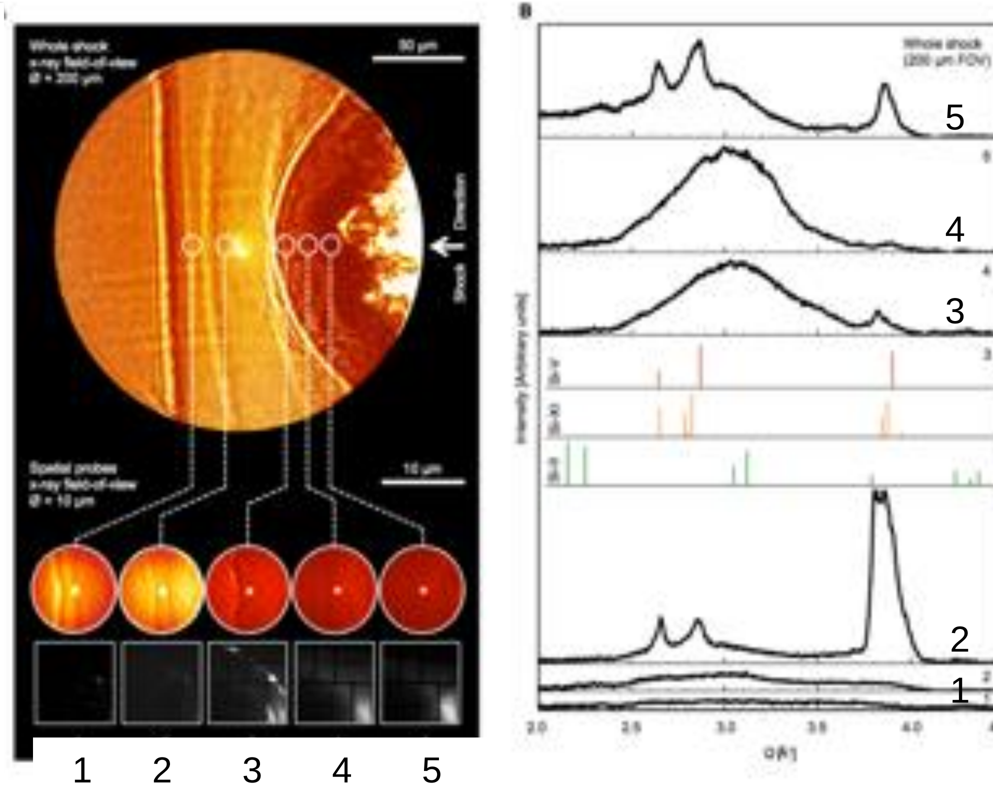
FIGURE 7. Images from shock compressed TNT samples, and a simulation (upper right) for qualitative comparison.

Armstrong et al., 2019

PCI + shock compression @ MEC in Si

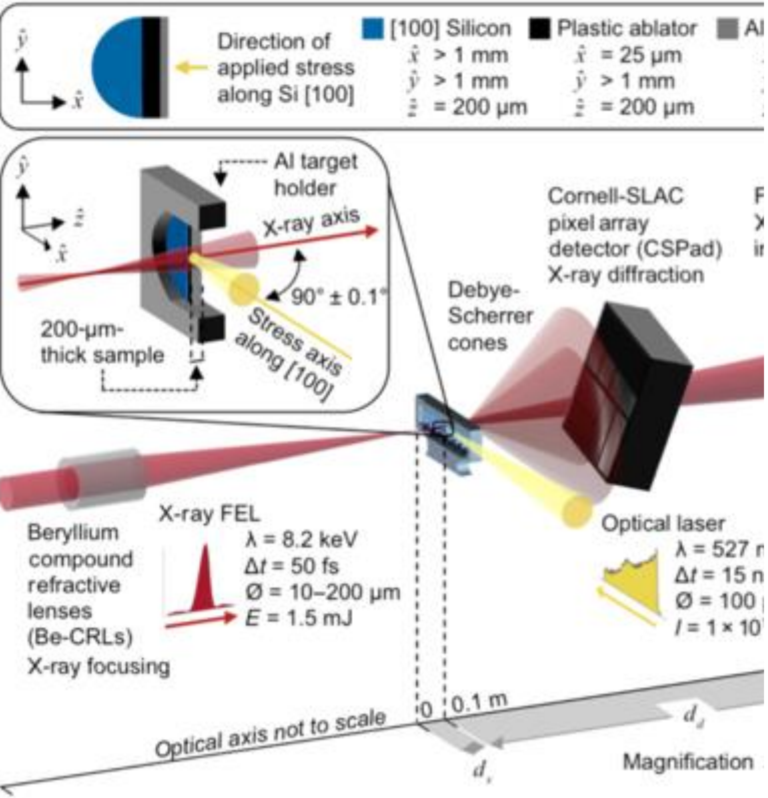


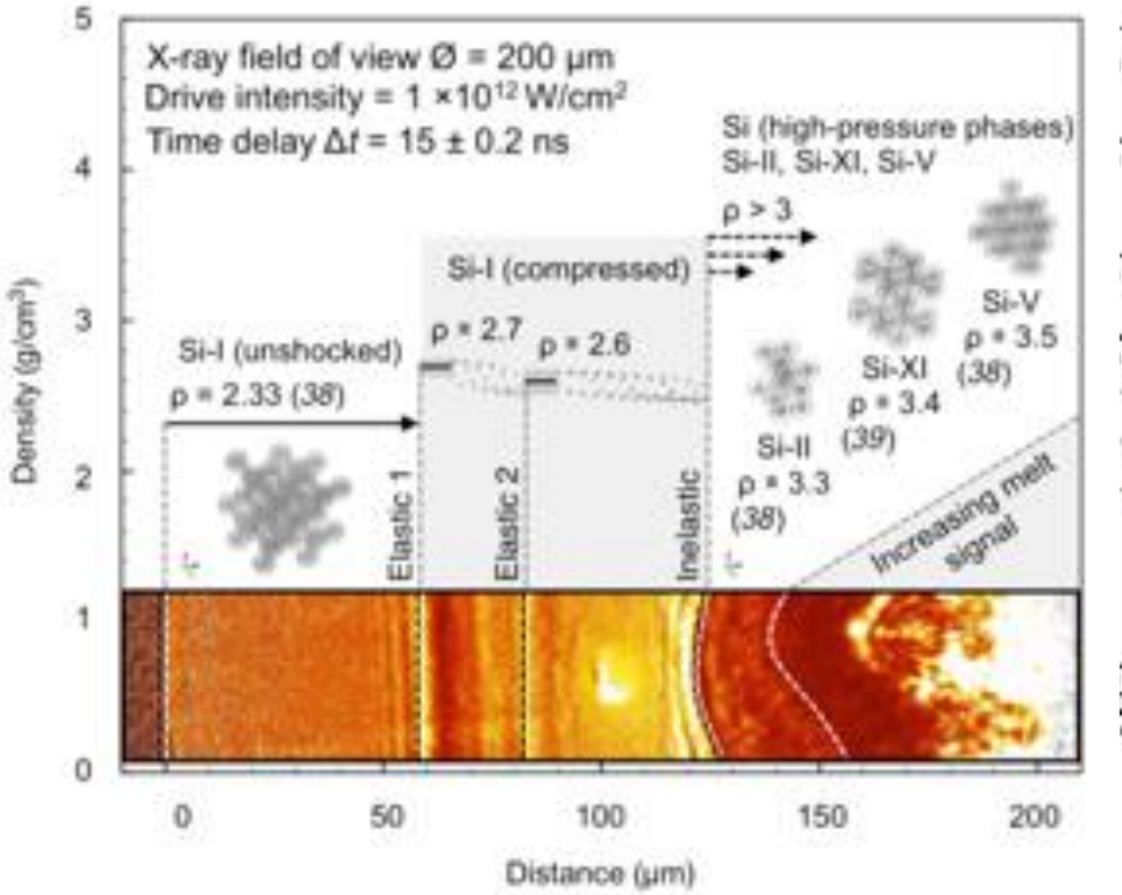
Brown et al., 2019



Pinpoint phase, density and microstructure in a single-shot down to sub um resolution

PCI + shock compression @ MEC in Si



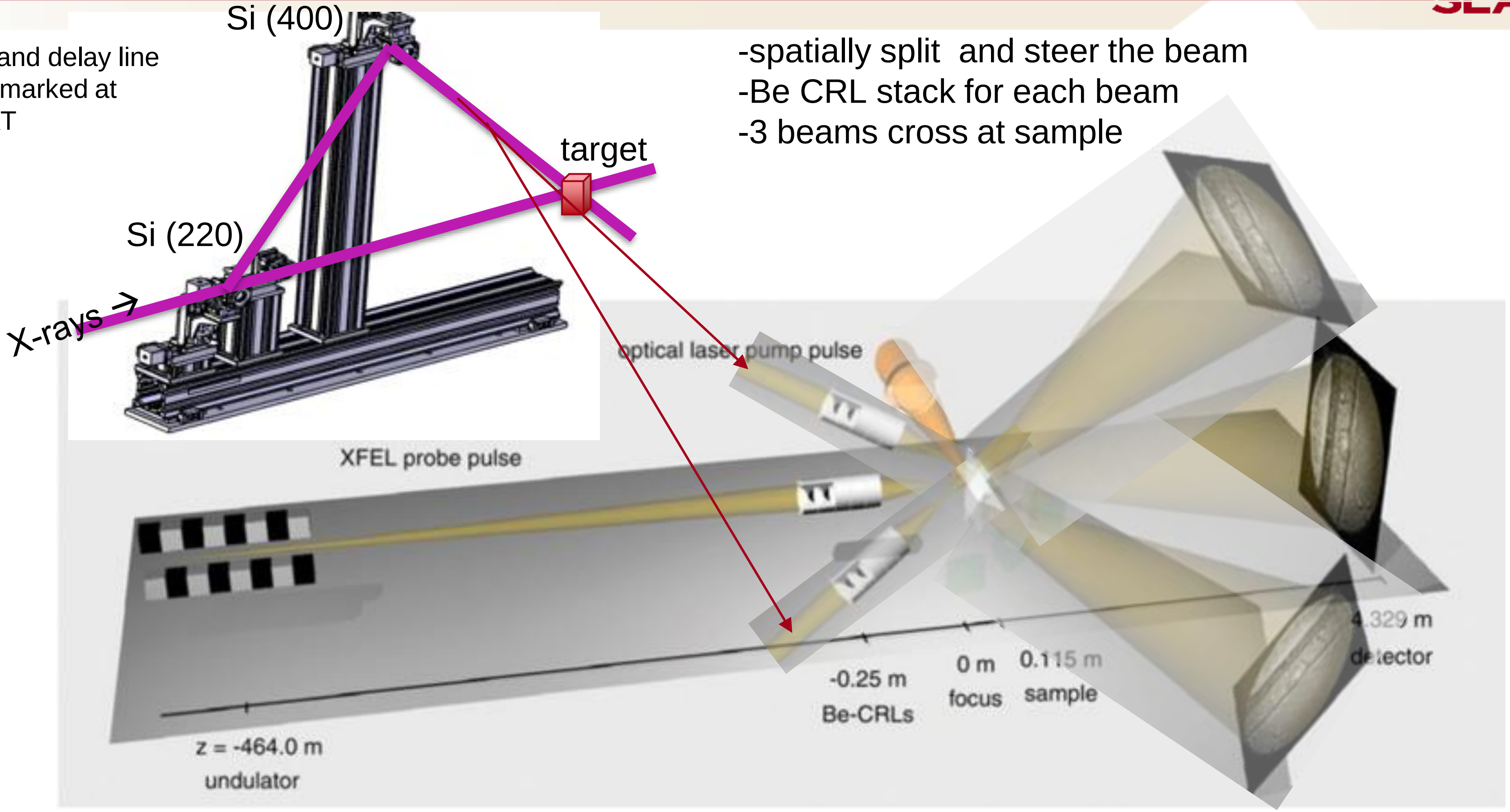


Brown et al., 2019

Stereo PCI + shock compression @ MEC via multi-angle imaging

*Split and delay line benchmarked at HPCAT

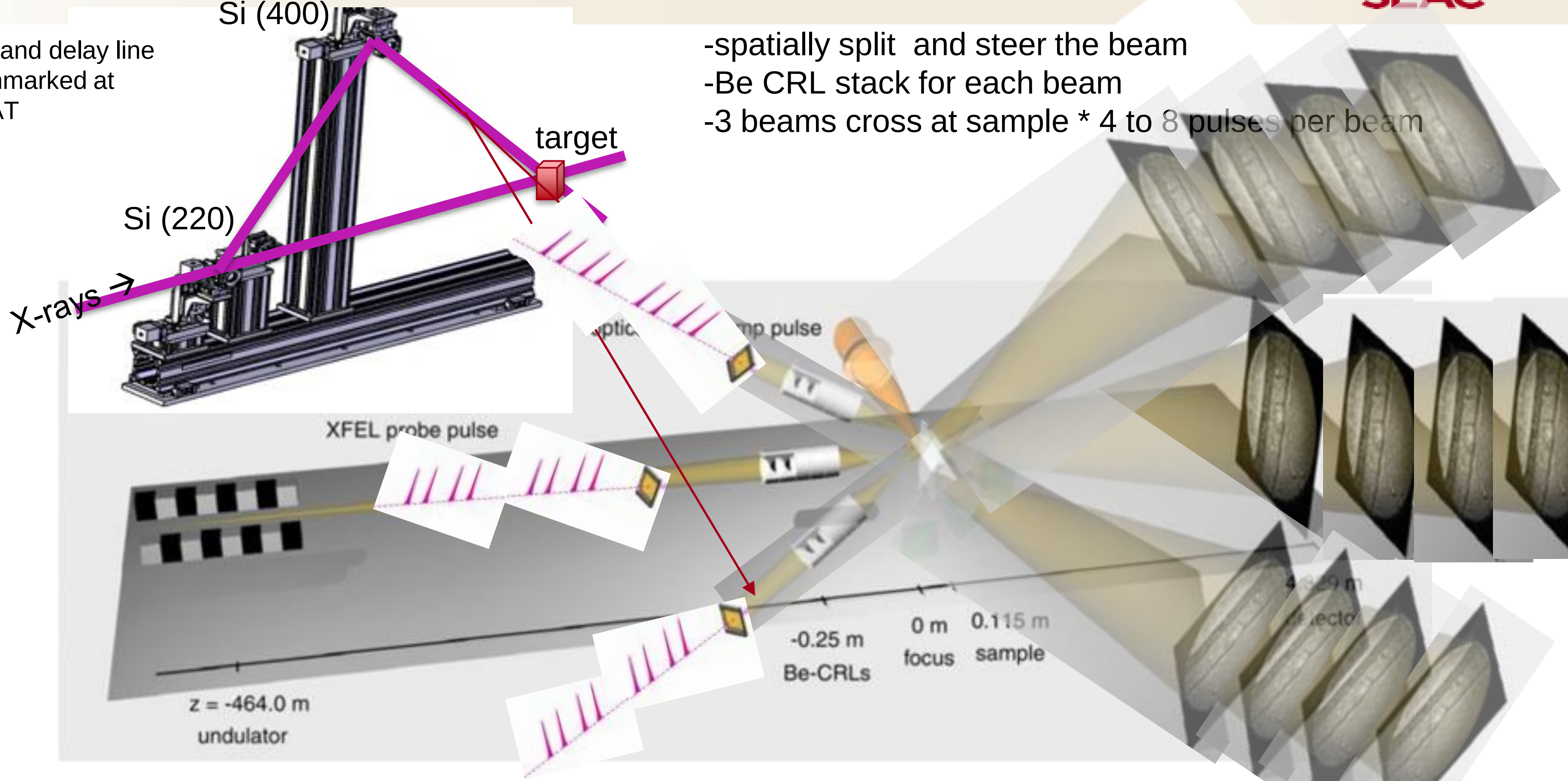
- -spatially split and steer the beam
- -Be CRL stack for each beam
- -3 beams cross at sample



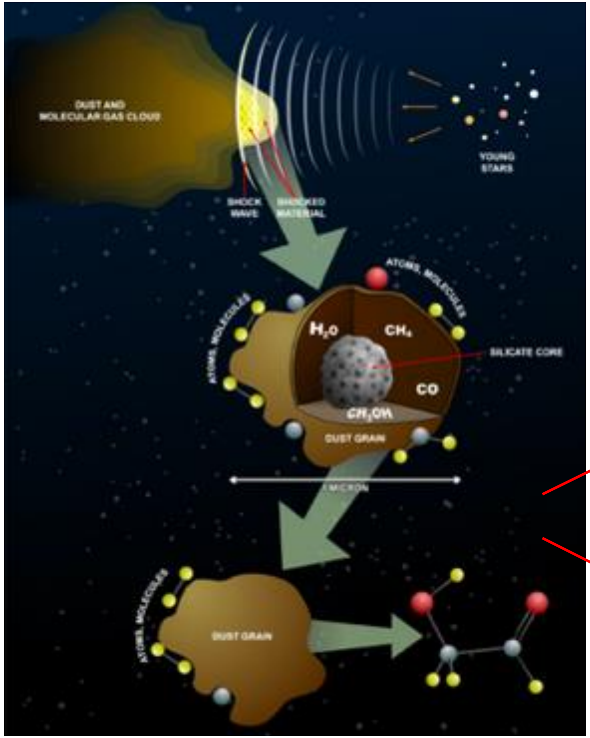
Stereo PCI + shock compression @ MEC via multi-angle imaging

*Split and delay line benchmarked at HPCAT

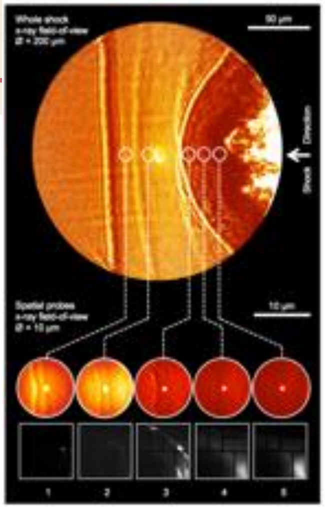
-spatially split and steer the beam
-Be CRL stack for each beam
-3 beams cross at sample * 4 to 8 pulses per beam



Evolution of prebiotic to biotic materials via shock wave interaction



https://www.nasa.gov/images/content/107500main_panel1_m.jpg



X-ray imaging
-visualize phase transformations in presence of trapped volatiles

X-ray absorption spectroscopy
-visualize chemical dynamics

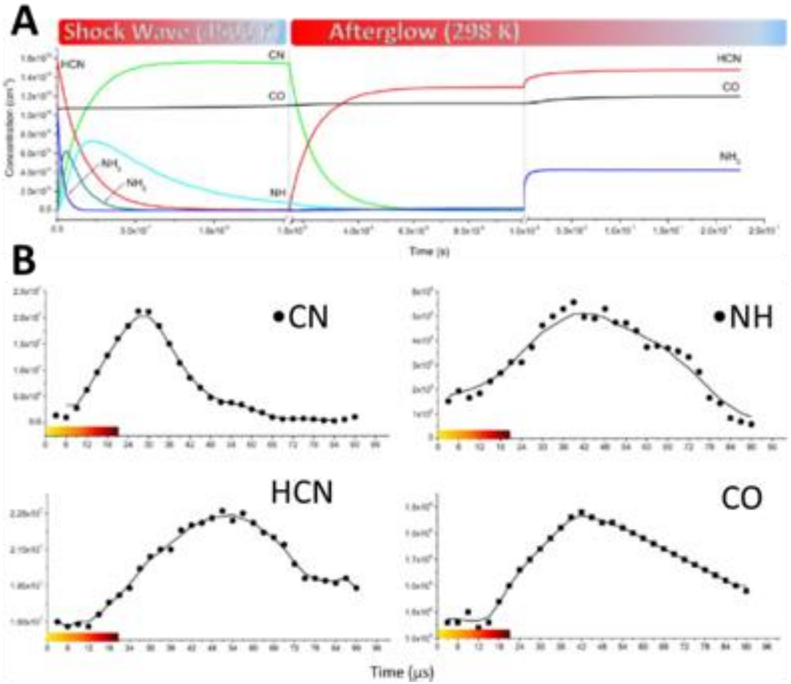
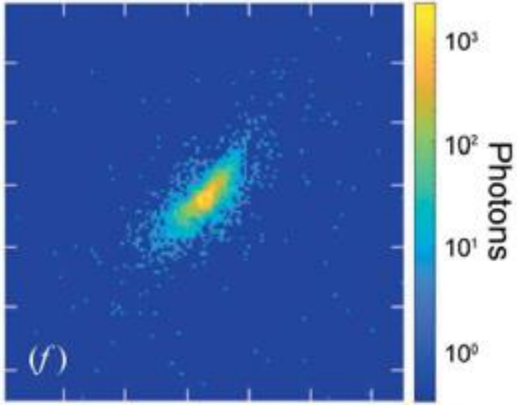


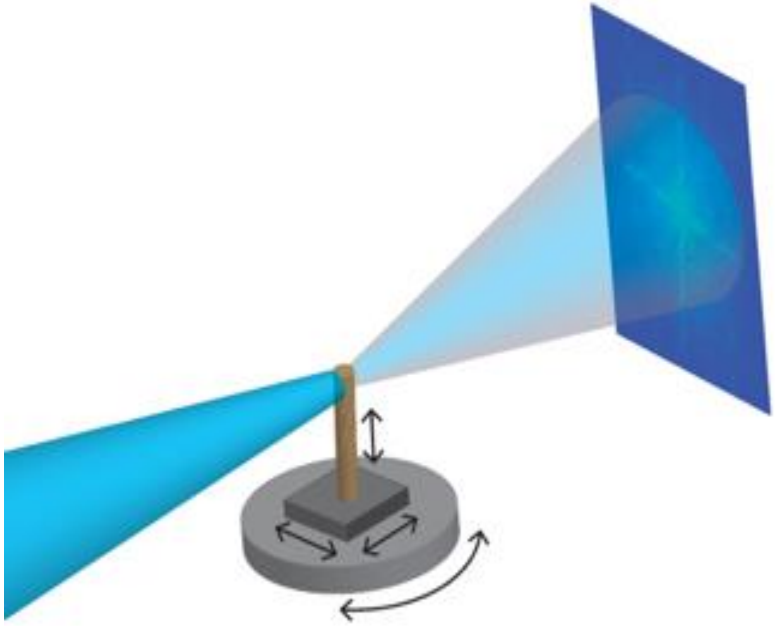
Figure 5. Previously reported kinetics data for simulated impacts with formamide showing the growth and decay of various intermediates, both from theoretical (a) and experimental (b) data. Adapted from Ferus *et al.* 2014.

Characterization of Materials with xFEL Ptychography

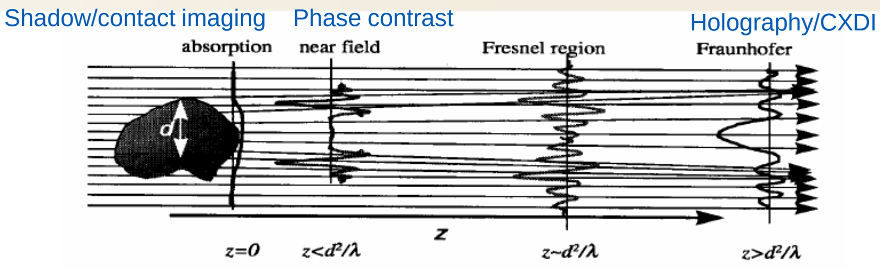
Demonstration of 2D & 3D ptycho-tomography with fly scanning at an XFEL

-high resolution (20-50 nm)
-operated in fly scan mode
-evaluated reconstruction quality using ePix10k and JungFrau detectors



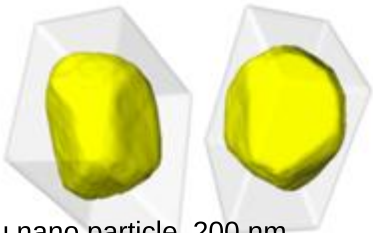


Single shot CXDI

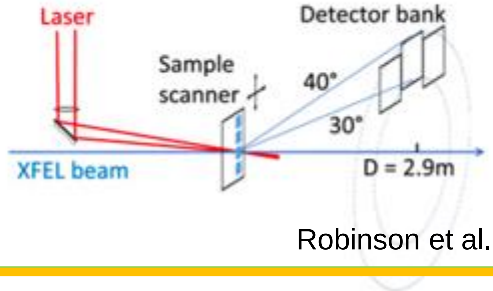


CXDI can provide 3D information, but has only been demonstrated for softer x-rays (<1 keV) and small samples (few micron)

time resolved Bragg-CDI



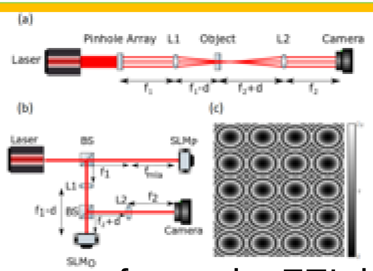
Au nano particle, 200 nm



Robinson et al., 2016

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

time resolved ptychography



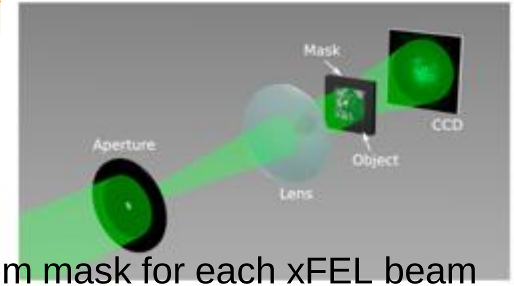
Sidorenko and Cohen, 2015
Wengrowicz et al, 2019

pinhole array for each xFEL beam

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

Single shot CXDI

time resolved ptychography

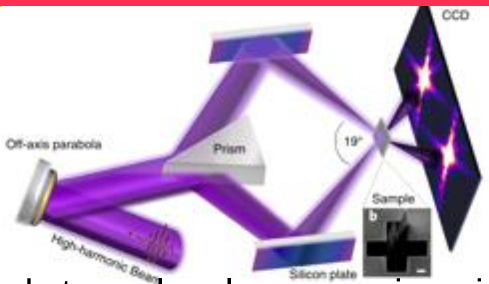


random mask for each xFEL beam

Seaberg et al, 2015

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

time resolved ptychotomography

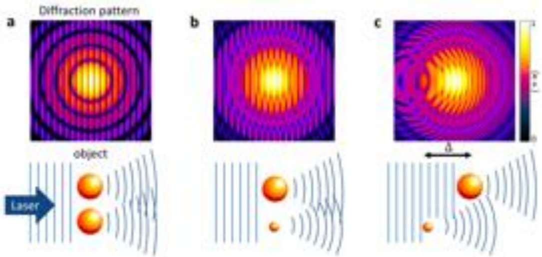


computed stereo lensless x-ray imaging

Duarte et al, 2019

- so far only soft X-rays

time resolved 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

Exp. techniques and sample environments for single pulse dynamic imaging

1. ***Biggest, current challenges***: (technical) Detectors, X-ray beam conditioning, experimental platform synergy; (logistical) beamtime and workforce
2. ***Current state-of-the-art methods & limitations***: single-shot coherent X-ray diffractive imaging (CXDI) methods with hard (>25 keV) X-rays for 2-D reconstructions are maturing; 3-D is more nascent; streamlining concurrent data collection – analysis/algorithms – reconstruction is paramount
3. ***Most promising current/new methods***: single-shot CXDI, e.g. phase contrast imaging (PCI), ptychography + multi-dimensional X-ray pulse train and gated detectors
4. ***Beneficial methods not yet under development***: hard X-ray single-shot holography; grating interferometry + dynamic compression

→ All of the above can be achieved in the next 5 years. This is not a one size fits all – different science scopes, with different spatial resolution requirements, will dictate which X-ray imaging methodology to adopt.

Thank you for your attention!!

Collaborators:

LANL: Cindy Bolme, Richard Sandberg* now at BYU, Don Brown, Pawel Kozlowski, Kyle Ramos, Michael Powell, David Montgomery
Stanford University: Wendy Mao, Silvia Pandolfi
SLAC: Hae Ja Lee, Bob Nagler, Eric Galtier, Eric Cunningham, Yanwei Liu, Kenan Li, Anne Sakdinawat, Philip Hart, Roberto Colina, Richard Walroth, Chandra Curry
DESY: Andreas Schropp, Frank Seiboth, Christian Schroer
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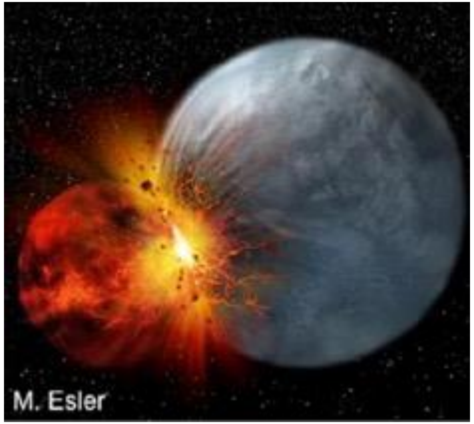
Geophysical Lab: Andrew Steele



- many more!!

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