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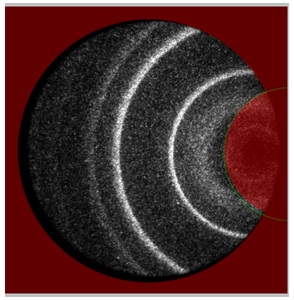
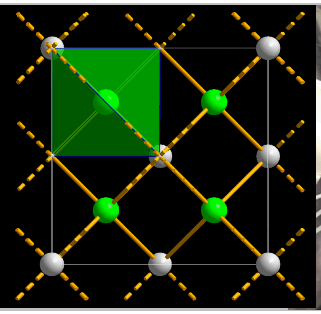
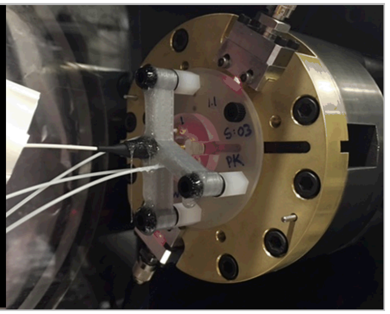

Real-Time Monitoring of Shock-Driven Phase Transitions with Synchrotron X-ray Diffraction

Patricia Kalita, Seth Root, Paul Specht, and Justin Brown

Sandia National Laboratories

Invited presentation at the American Crystallographic Association 68th Annual Meeting, July 20-24, 2018, Toronto, Canada

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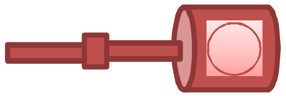
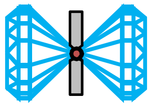
Overview

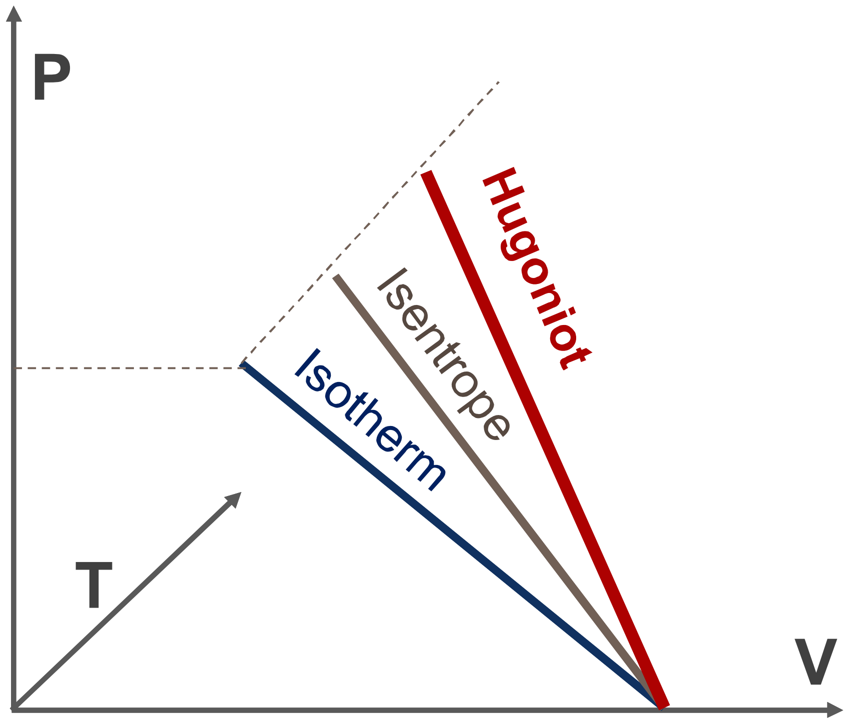
- Why shock compression?
- APS-ANL Sector 35 DCS: **dynamic compression** and in situ XRD
- APS-ANL Sector 16 HPCAT: **static compression** and in situ XRD
- Hugoniot equation of state of CaF_2
- Dynamically-driven phase transition: DXRD
- Dynamic vs static compression
- Summary

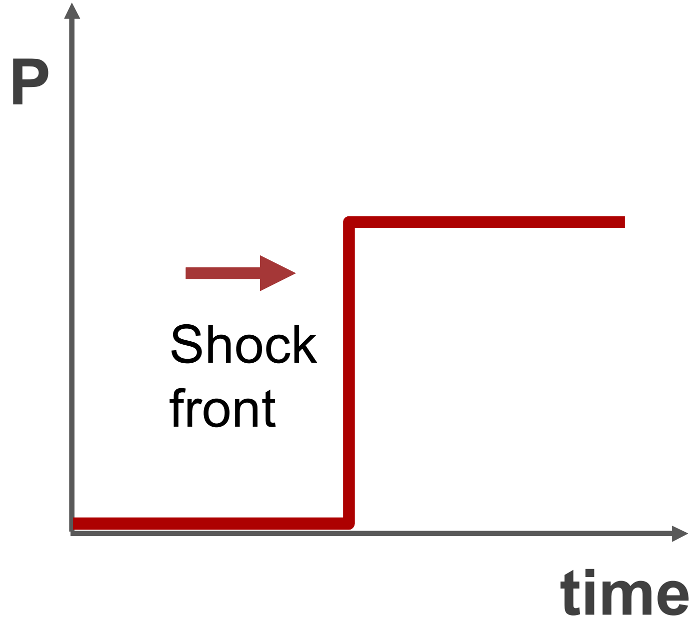




1D Shock Compression Wave

- High strain rate
- Energy scattering
- Shear forces
- Instantaneous
- Puts energy into atoms and molecules
- Creates defects in material (increases entropy)

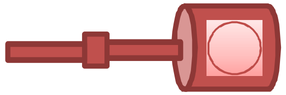


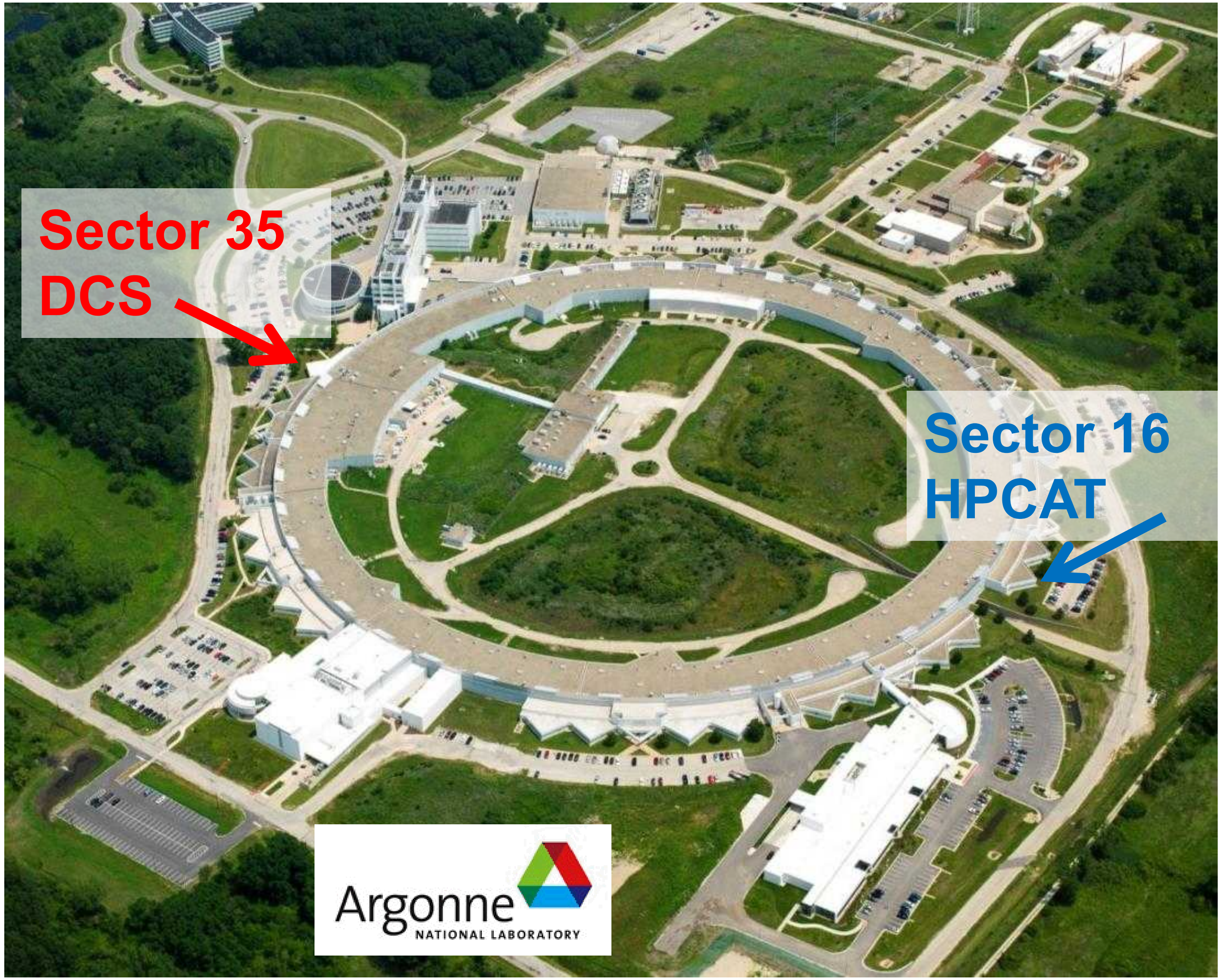


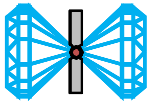
What do we get?

- very high pressure thermodynamic P-v curve – Hugoniot EOS
- test of accuracy of molecular potentials over large compression
- **with dynamic XRD, we get a microscopic insight into shock processes, kinetics of phase transitions…**

Advanced Photon Source at Argonne National Lab





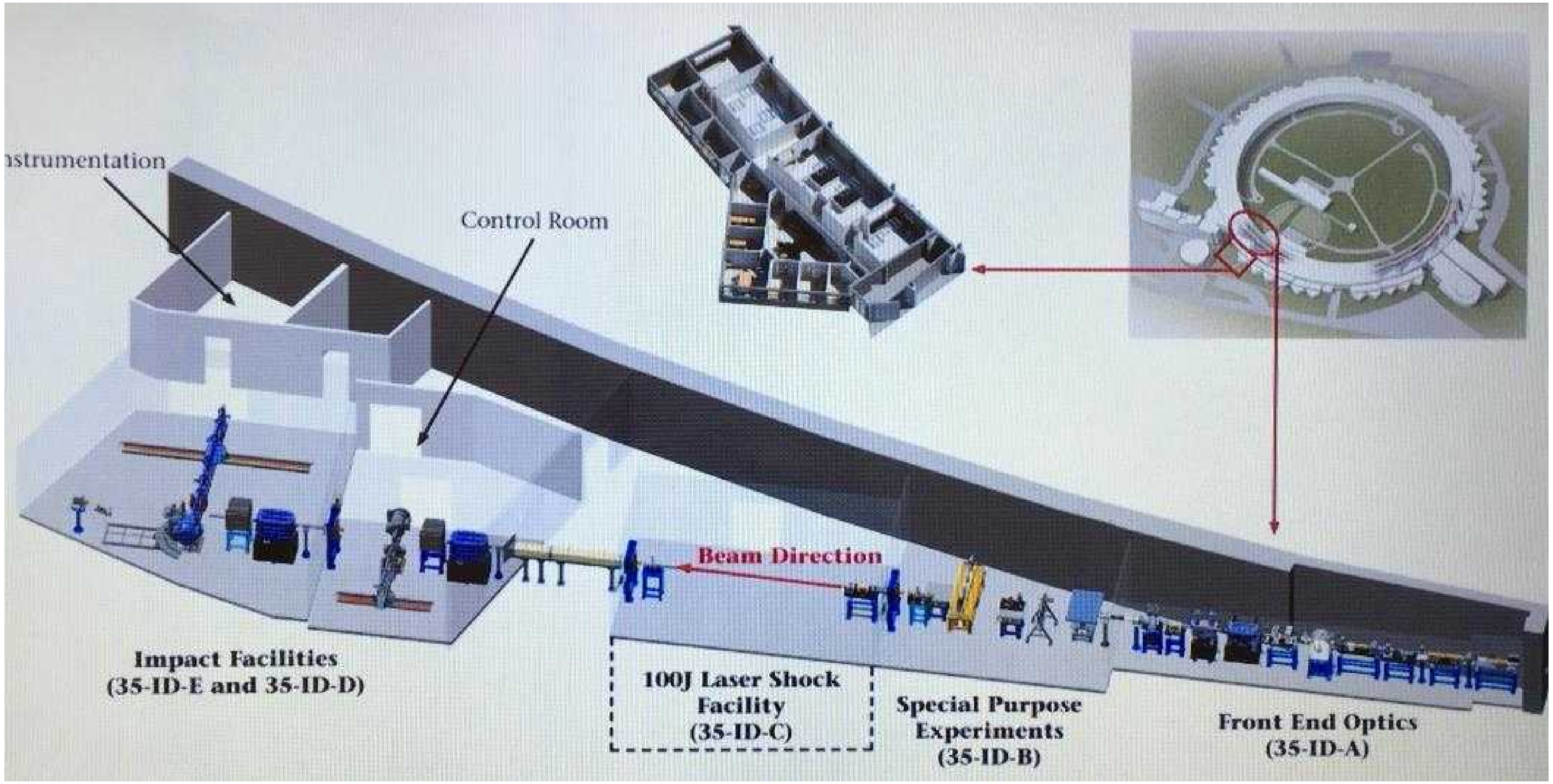


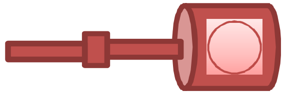
- 3^{rd} generation synchrotron source
- 1,104m = 3,622 ft.
- X-rays ON 24h/day
- 6 days/week

Advanced Photon Source Image Bank (aps.anl.gov)

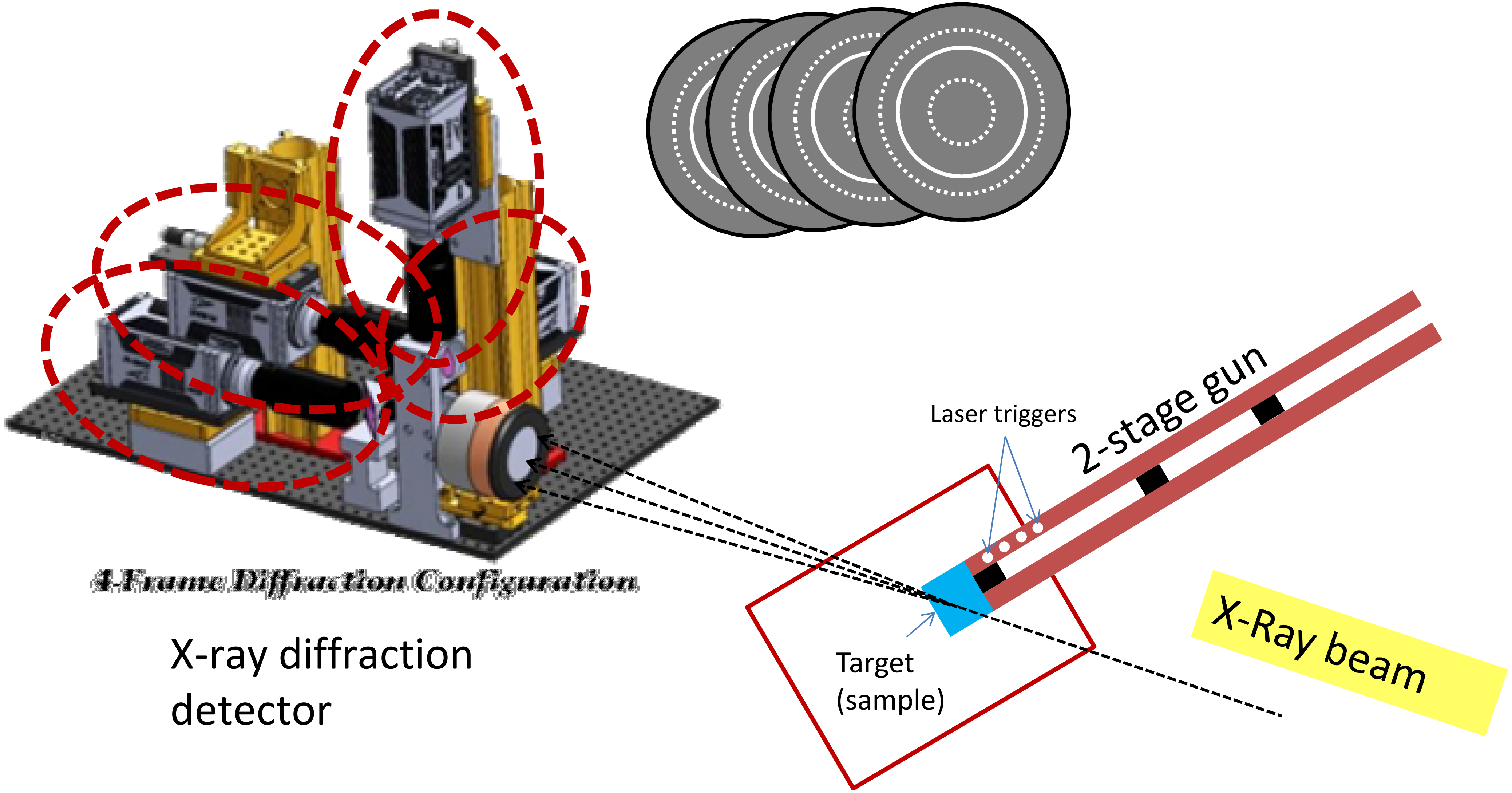
APS Sector 35 – DCS - Layout

Shock Compression and *in situ* X-Ray Diffraction

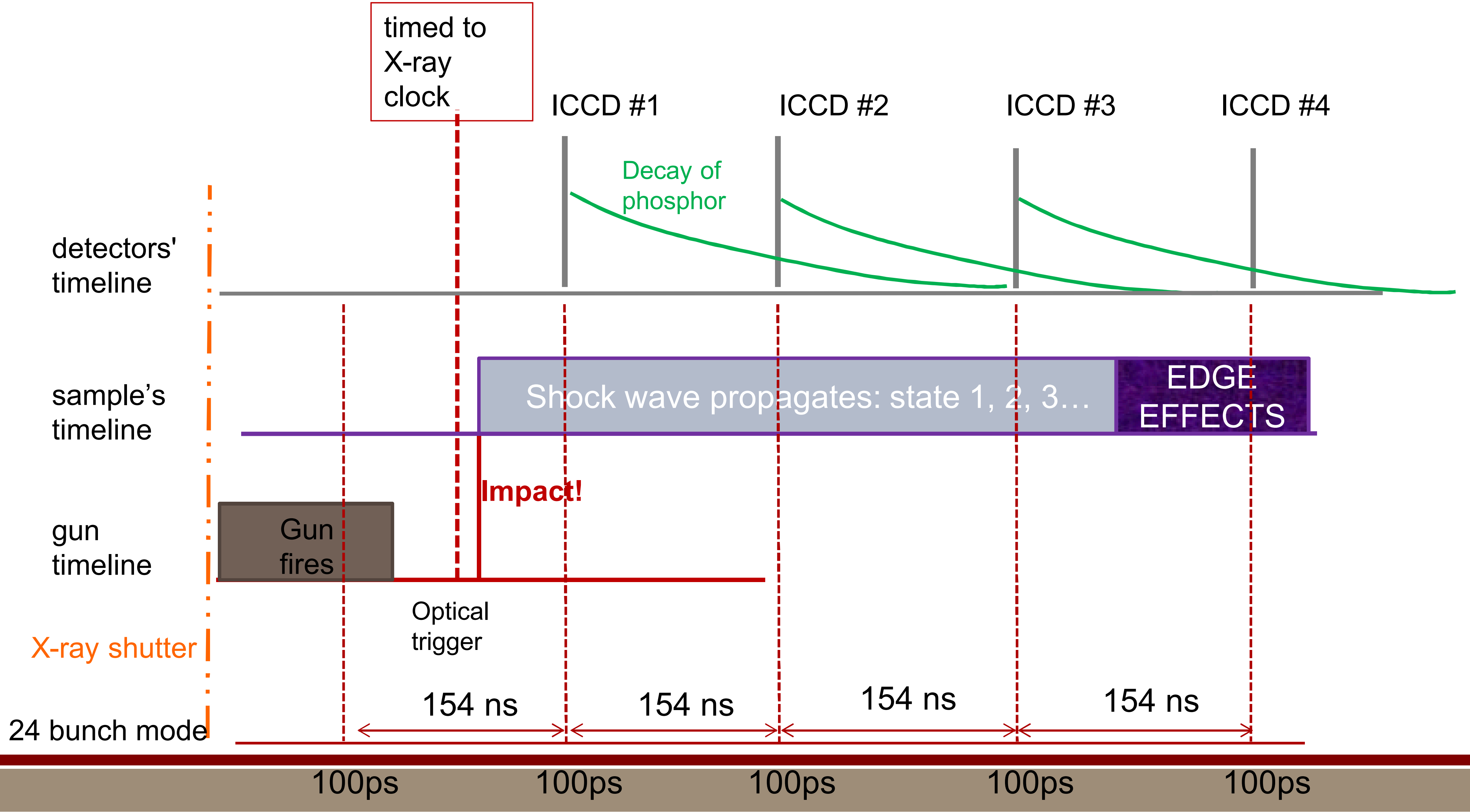




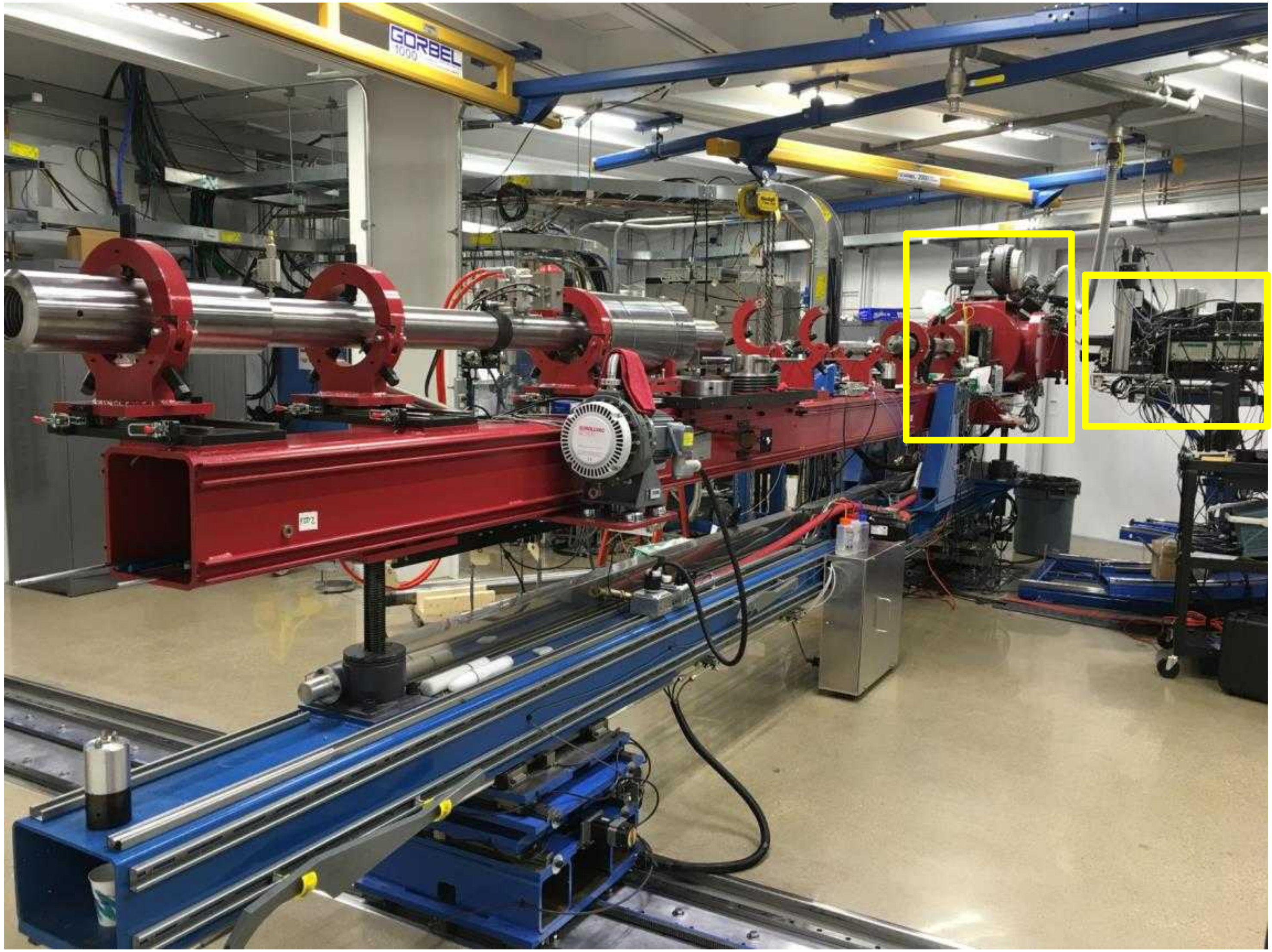
DCS End-station ID-E



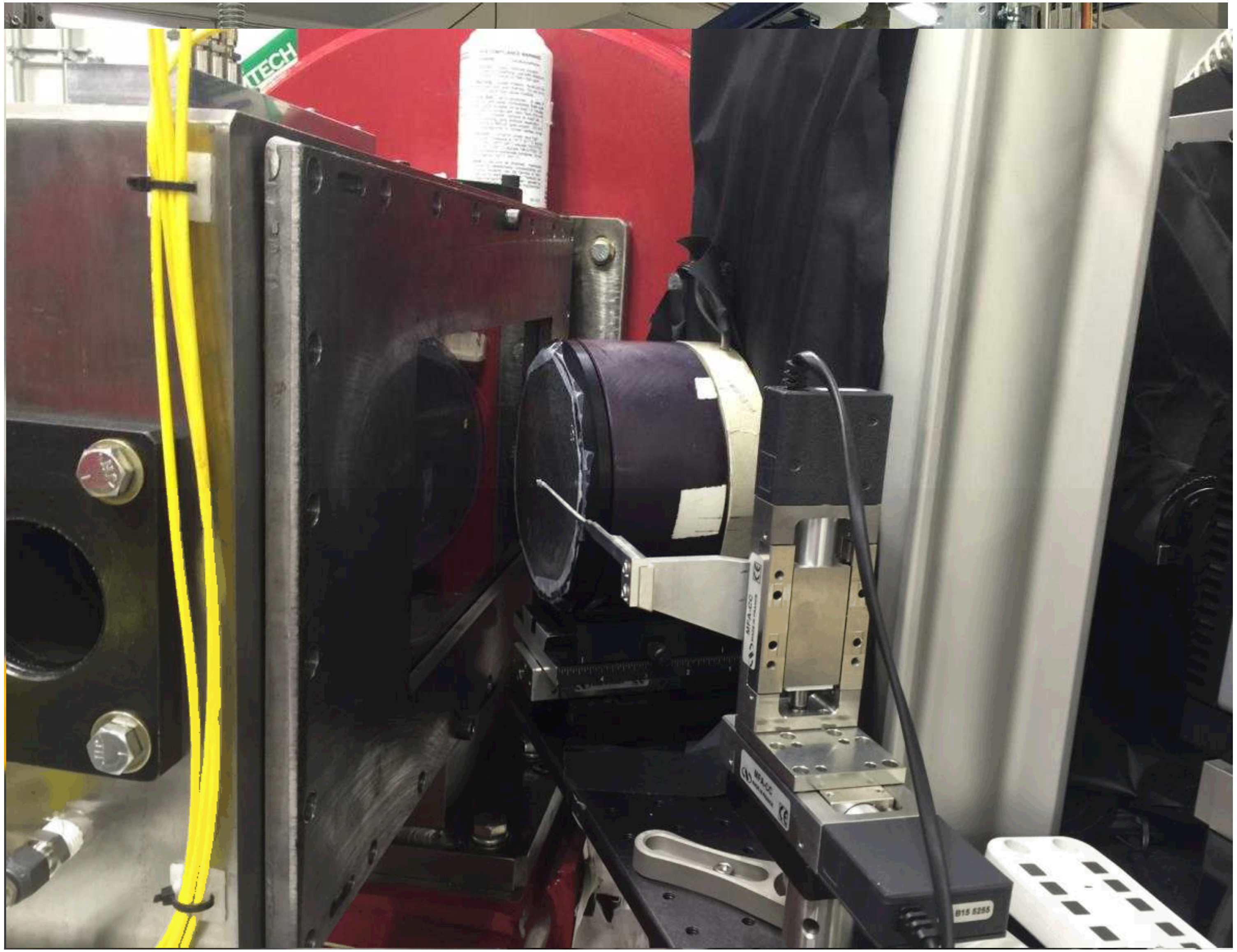
DCS End-Station IDE: Timing of events



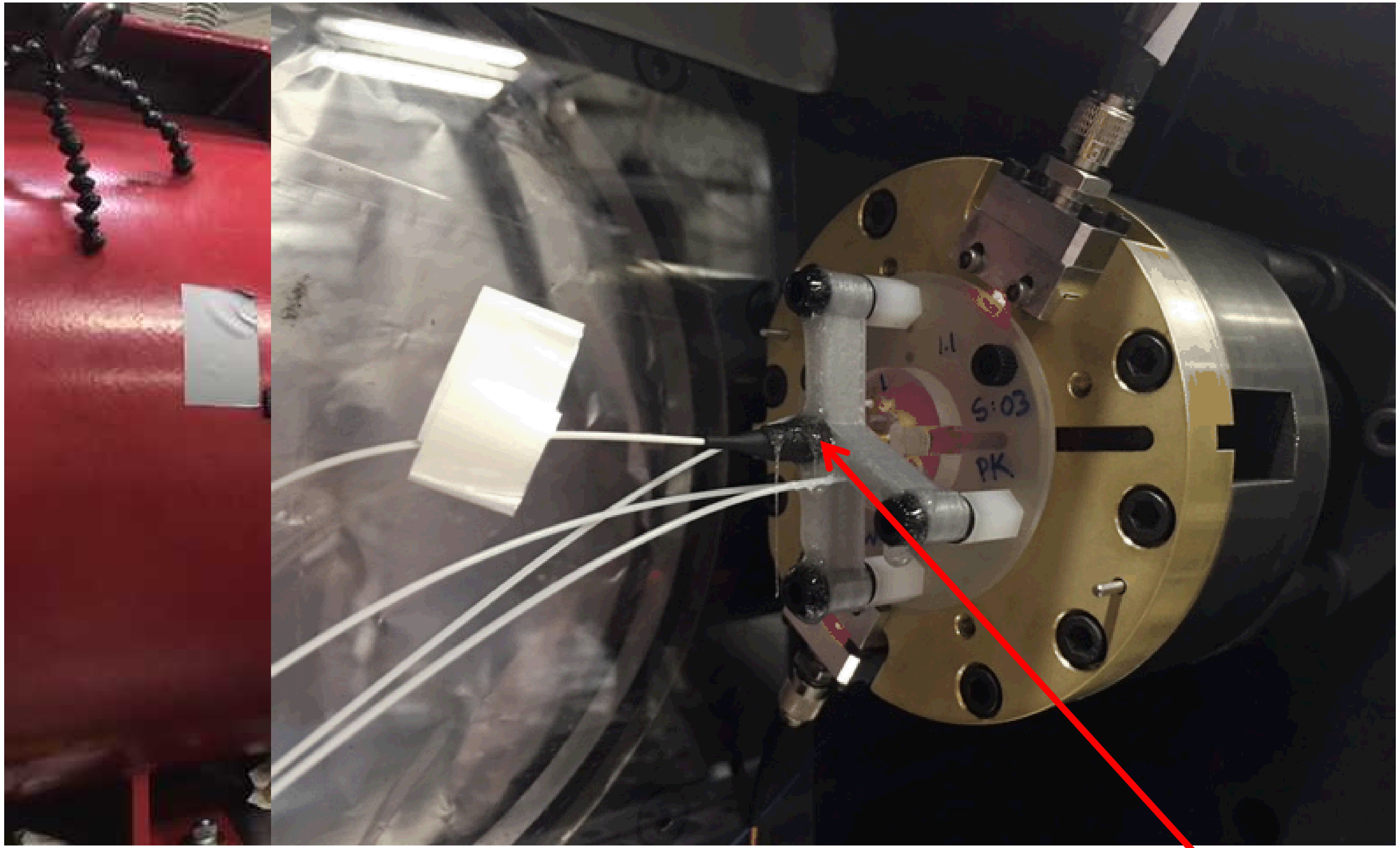
DCS End-station ID-E



XRD: target chamber with all shielding mounted



XRD: SNL-designed powder-sample holder mounted inside DCS gun

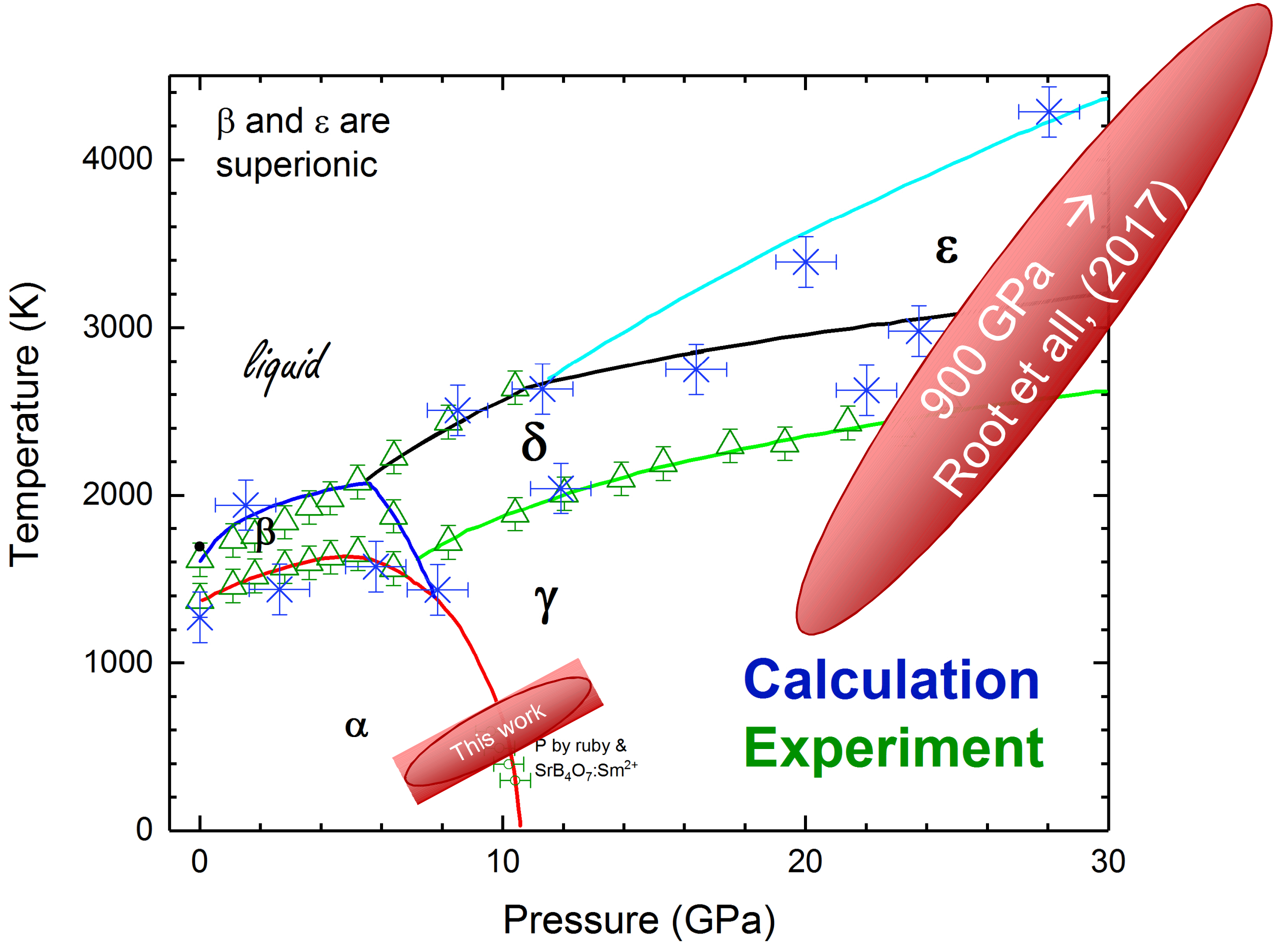


Sample probe

Shock compression of CaF_2

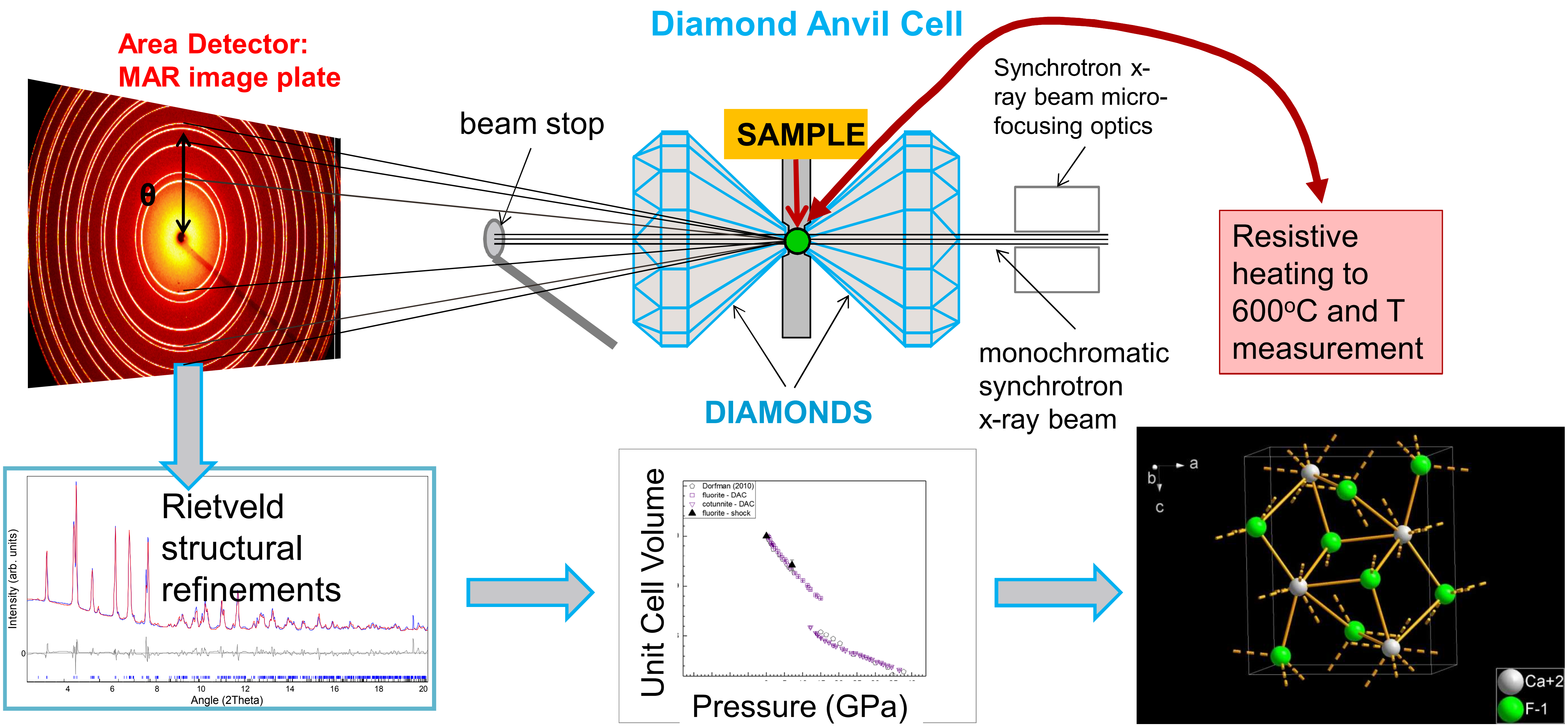
- part of a larger project on shock/ramp/static loading behavior of CaF_2

- limited Hugoniot data above 30 GPa
- high pressure Hugoniot phase (solid or melt) undetermined
- extended phase diagram undetermined
- **previous shock compression**: continuum scale velocimetry & inferred phase transition
- **static compression**: at least 2 solid → solid pressure-driven phase transitions

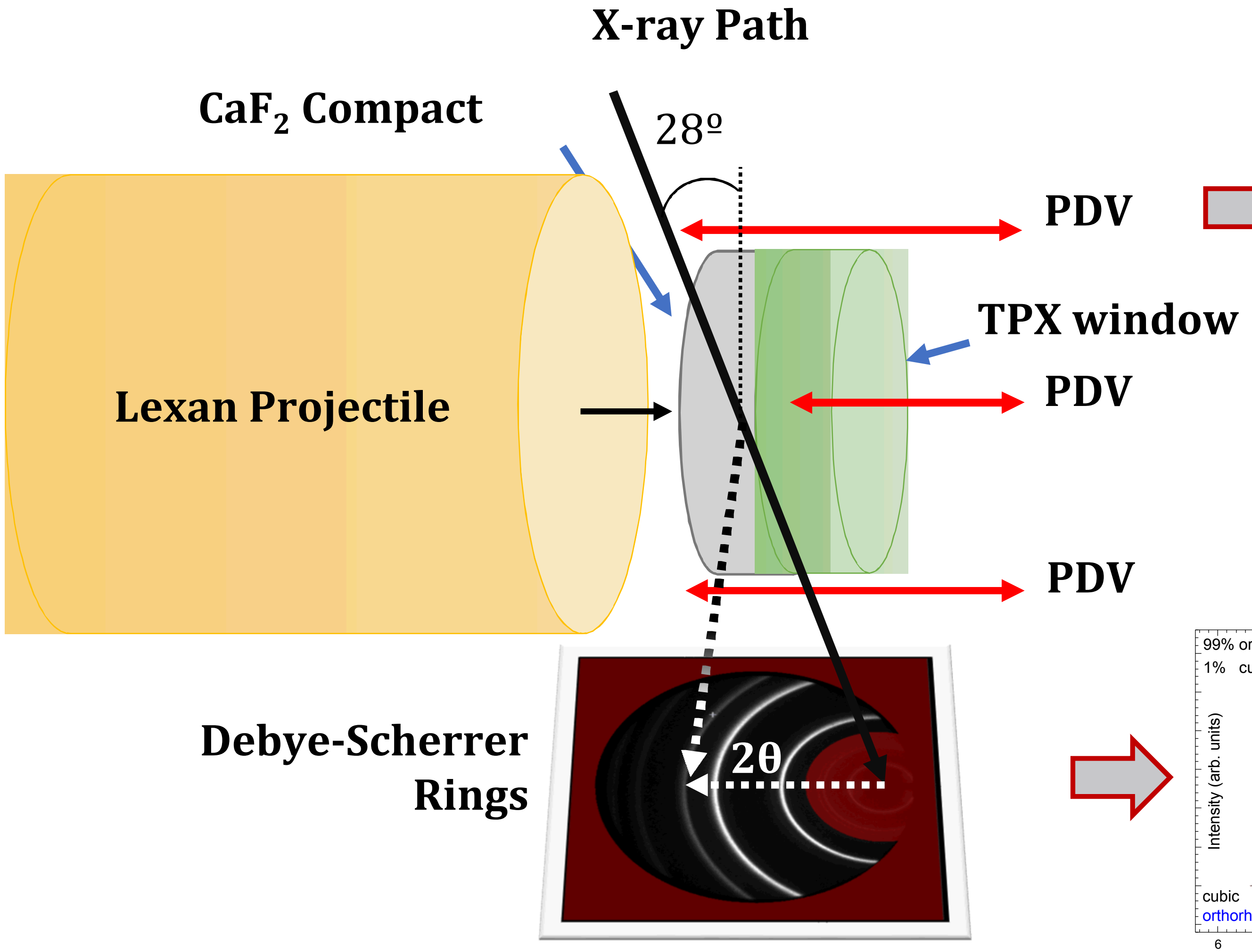


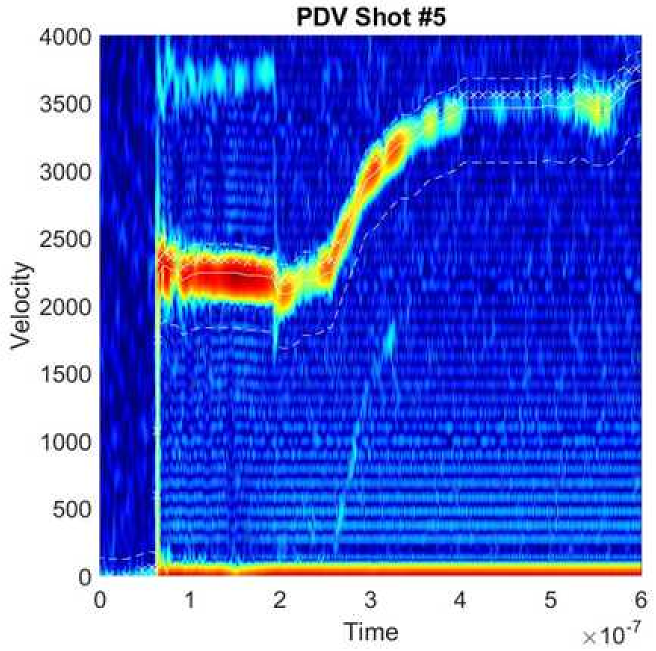
Cazorla, PRL 113, 235902 (2014)
Dorfman et al., Phys. Rev. B 81, 174121 (2010)

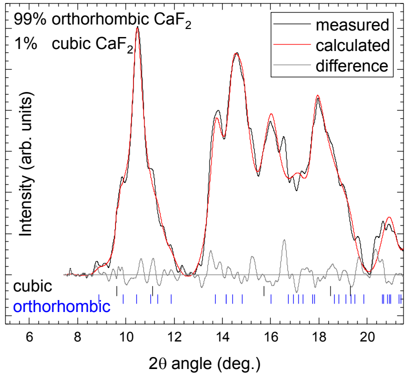
APS Sector 16 – HPCAT: Static Compression & XRD

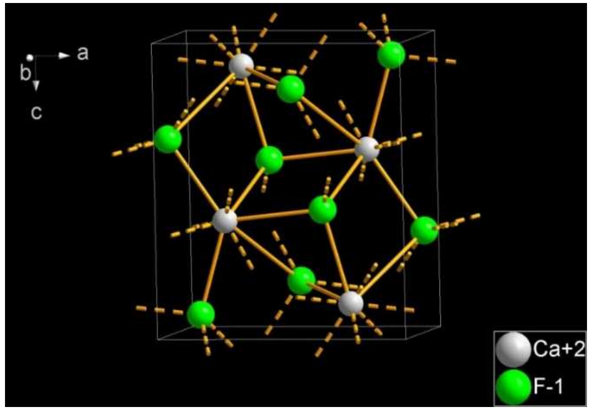


APS Sector 35, DCS: **Dynamic** Compression & XRD

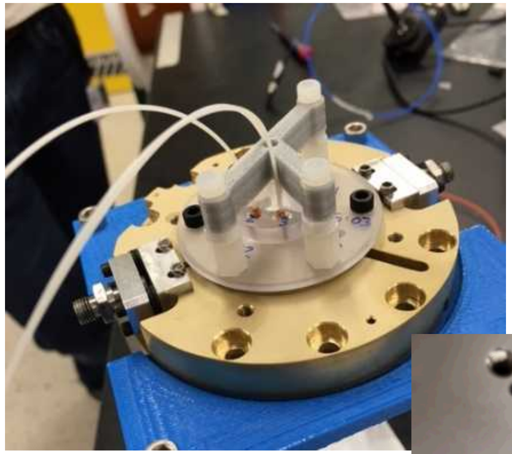


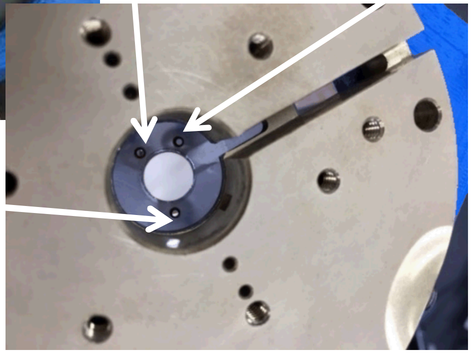


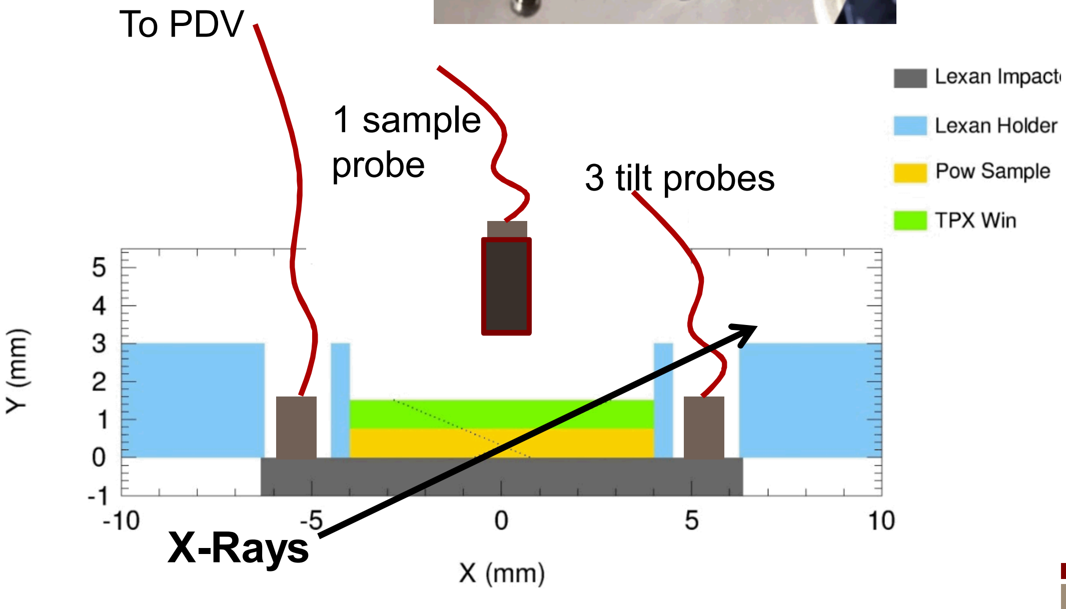


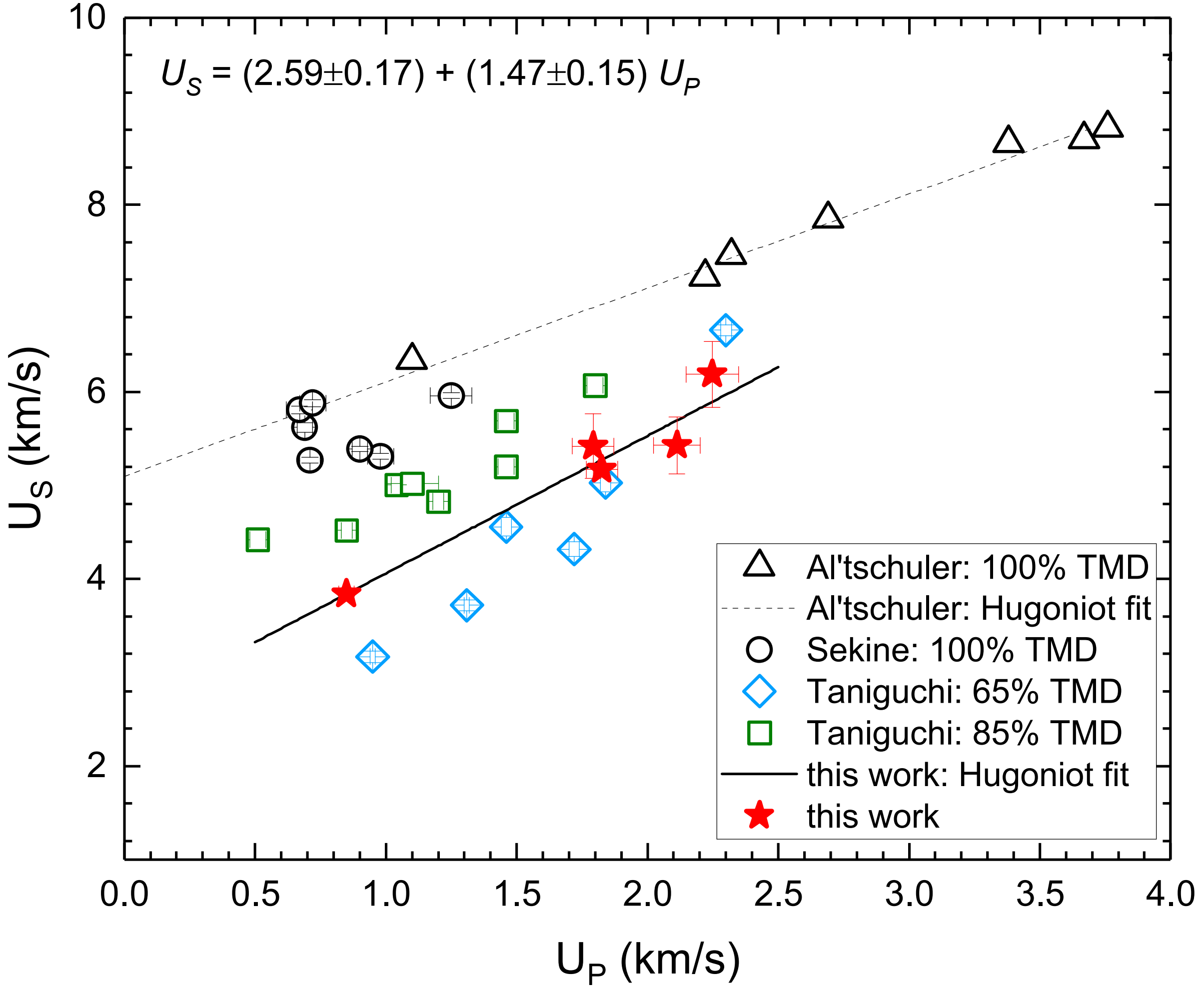


Hugoniot of 75% dense CaF_2



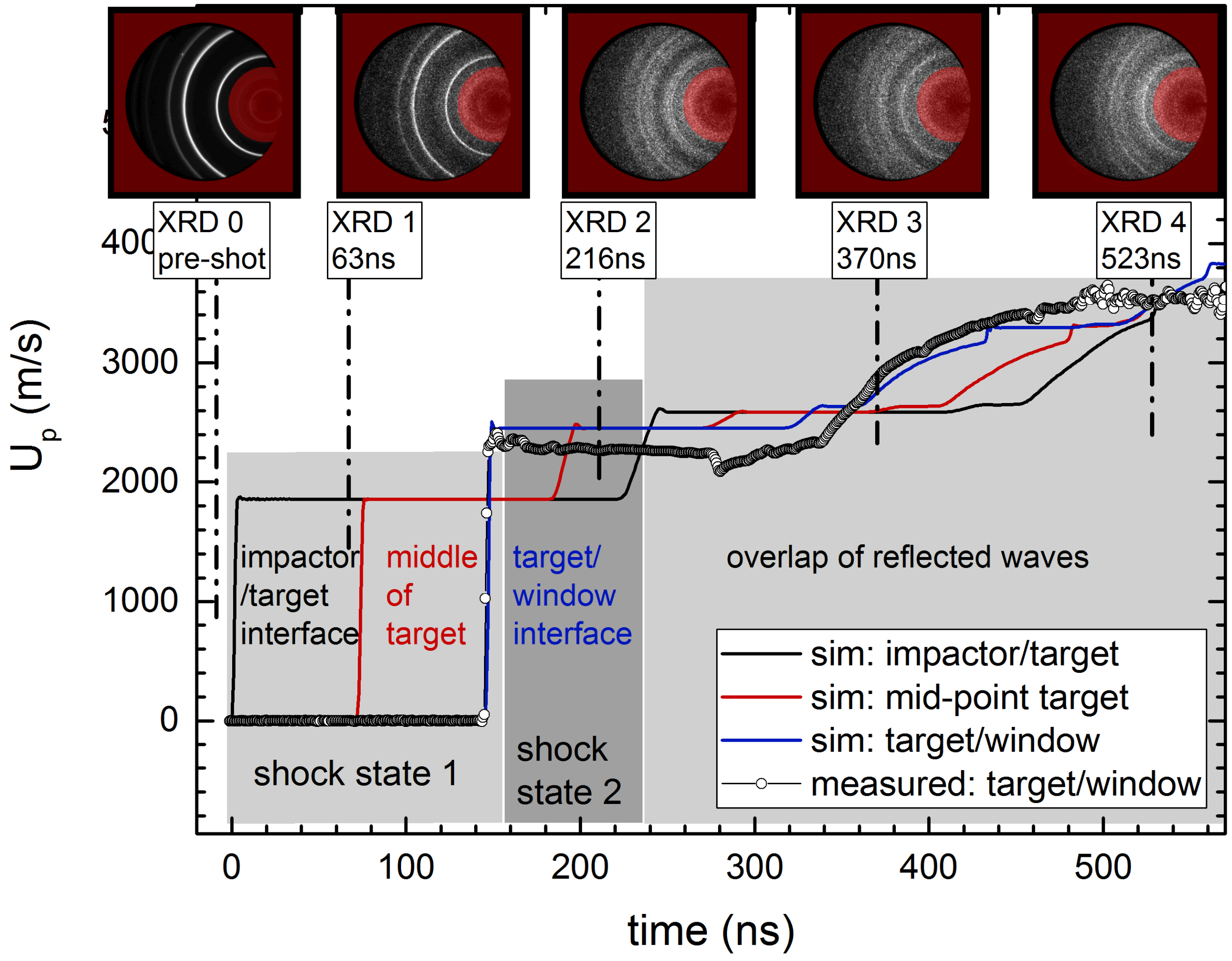


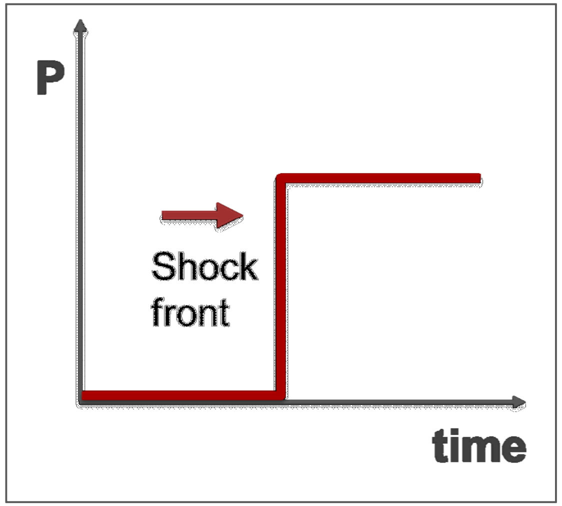


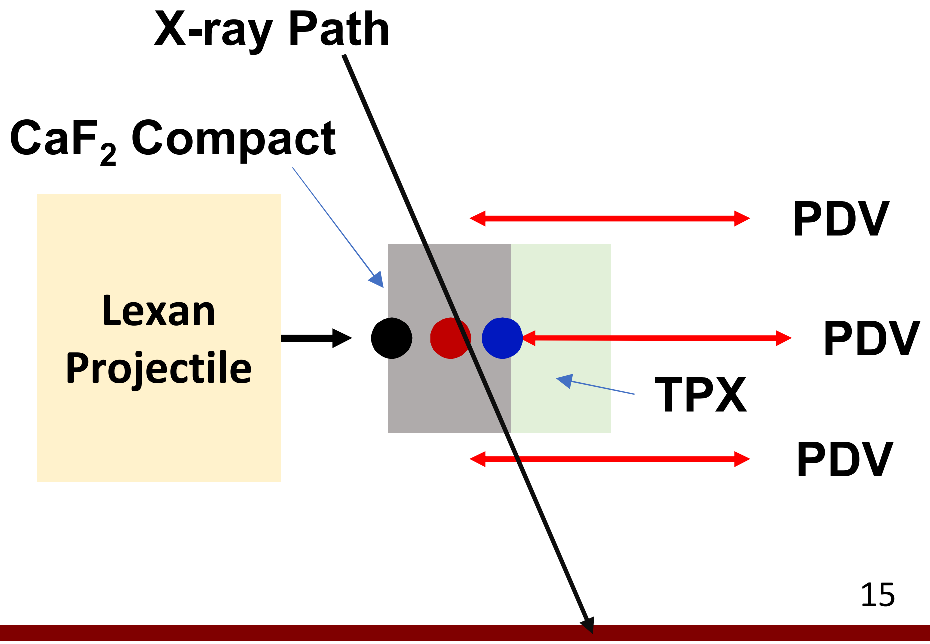


Al'tshuler et all, Sov. Phys. Solid State 15, 969 (1973)
Sekine et all, Phys Chem Miner 38, 305 377 (2011)
Taniguchi, et all, J. Appl. Phys. 384 61, 196 (1987)

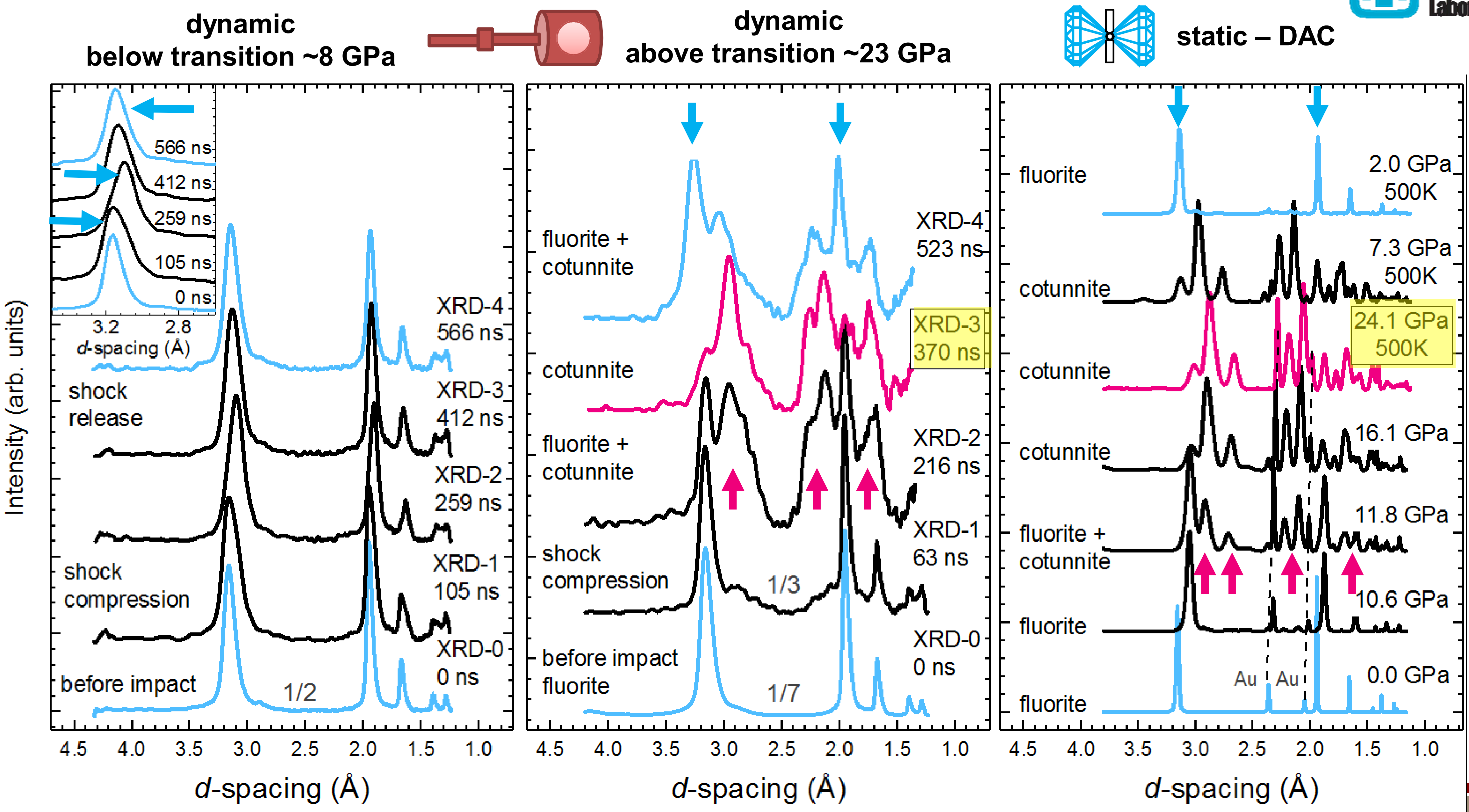
Dynamic XRD and Shock: WHEN?





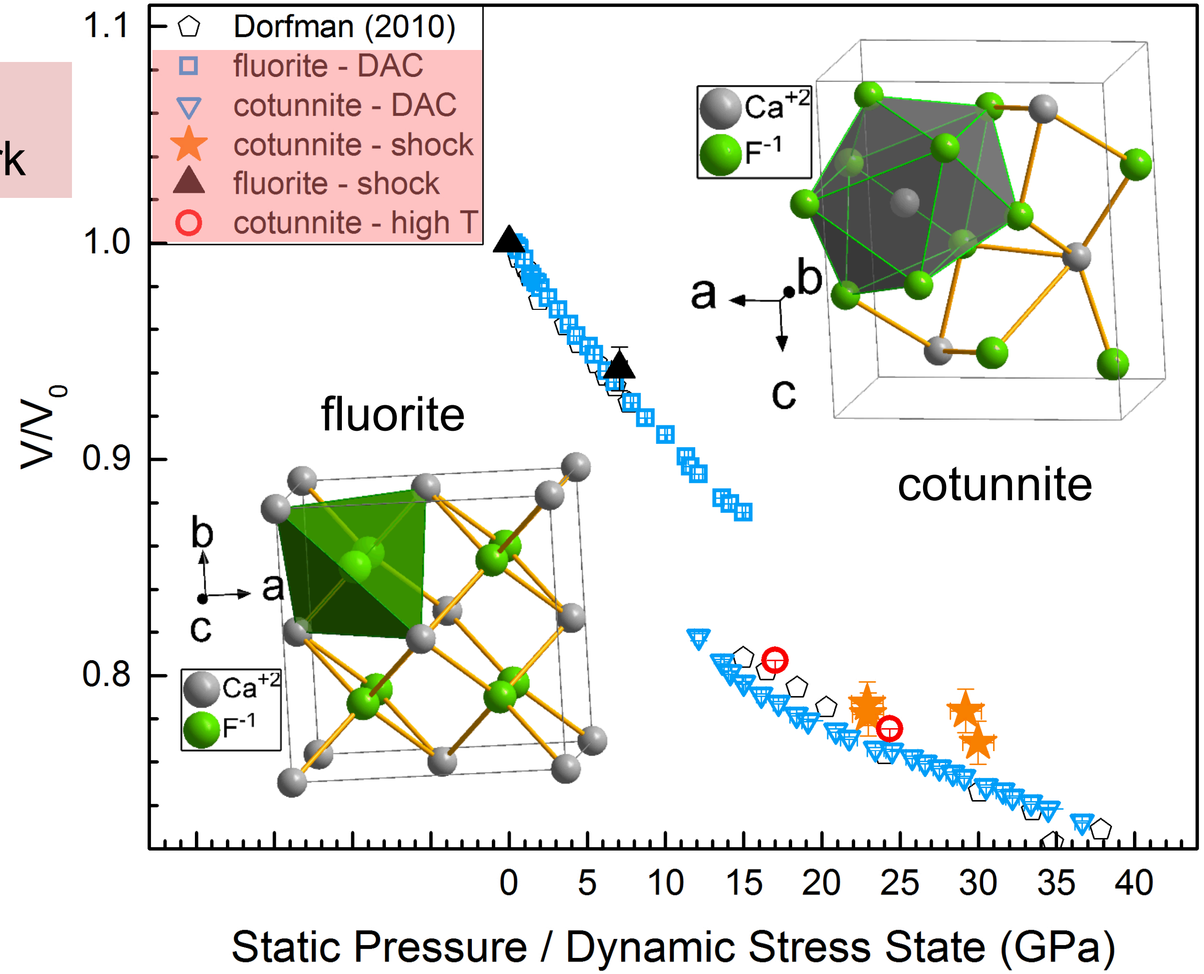


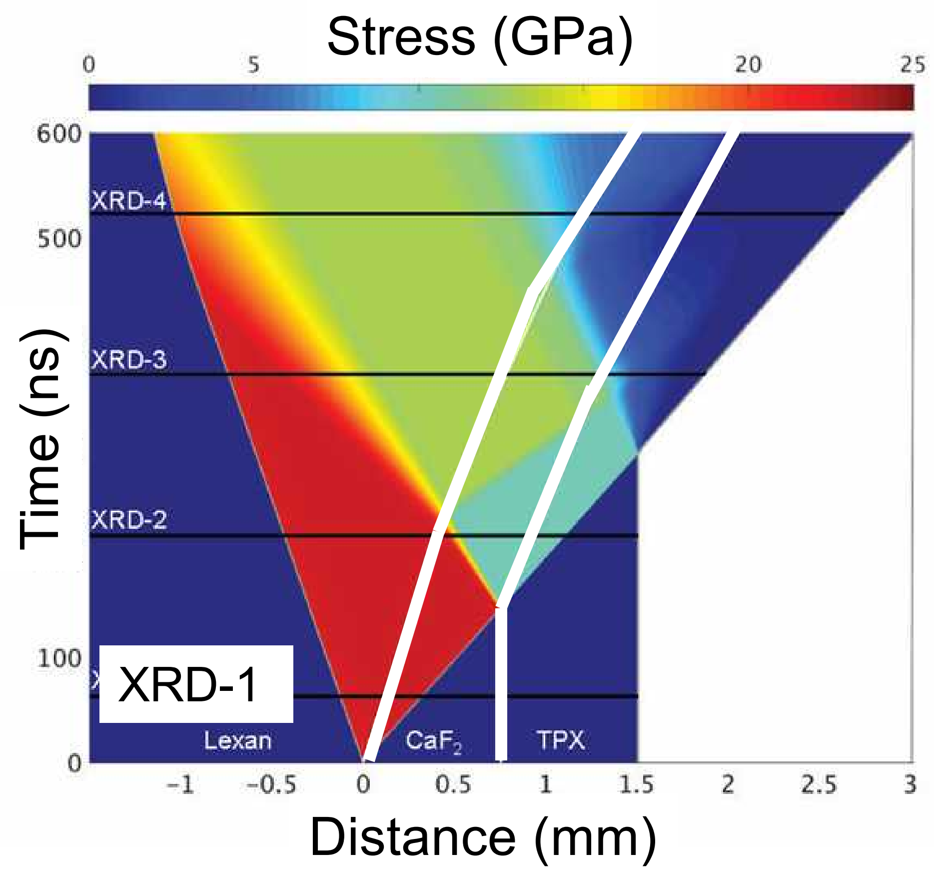
Dynamic vs Static XRD and Phase Transition



Dynamic vs Static Compression: Evolution of Unit Cell Volume

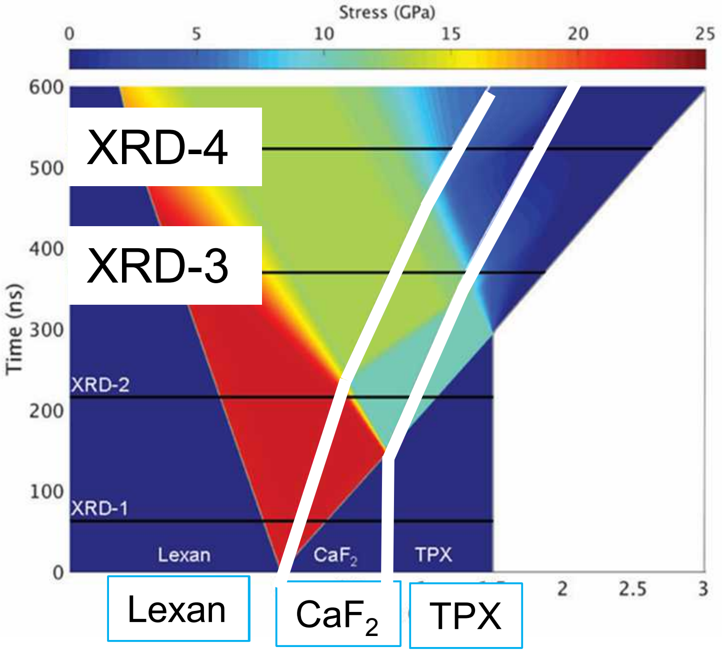
this work



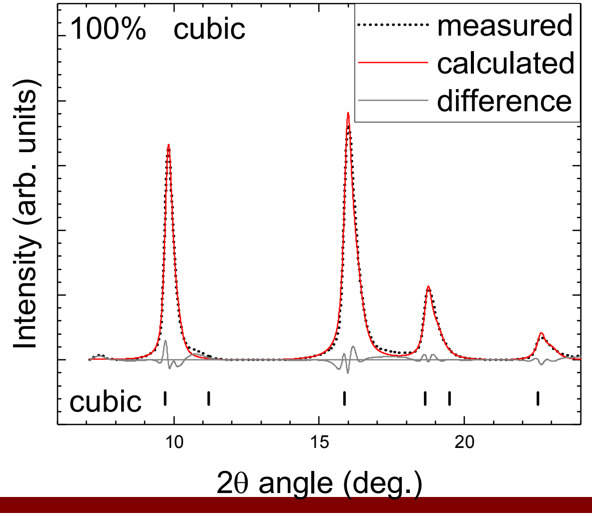


Quantitative Shock XRD Analysis

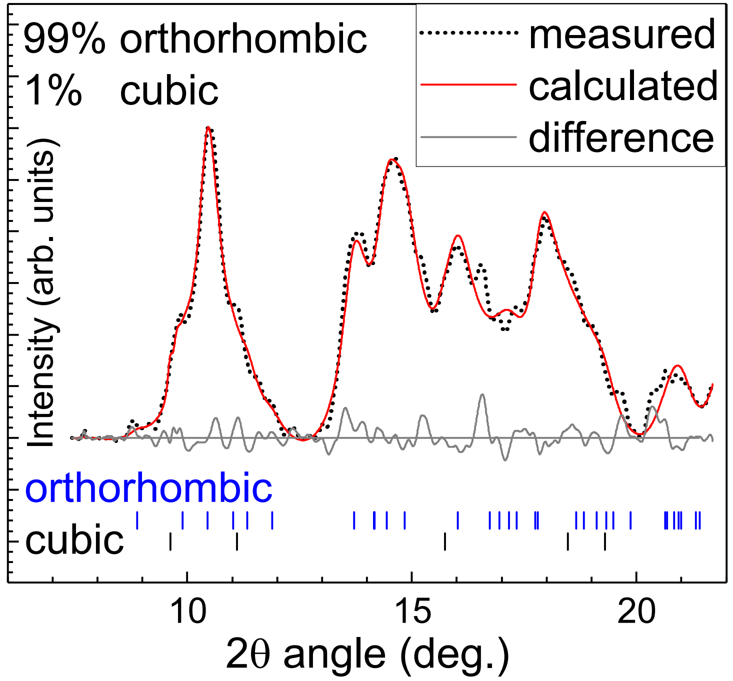
Sandia National Laboratories



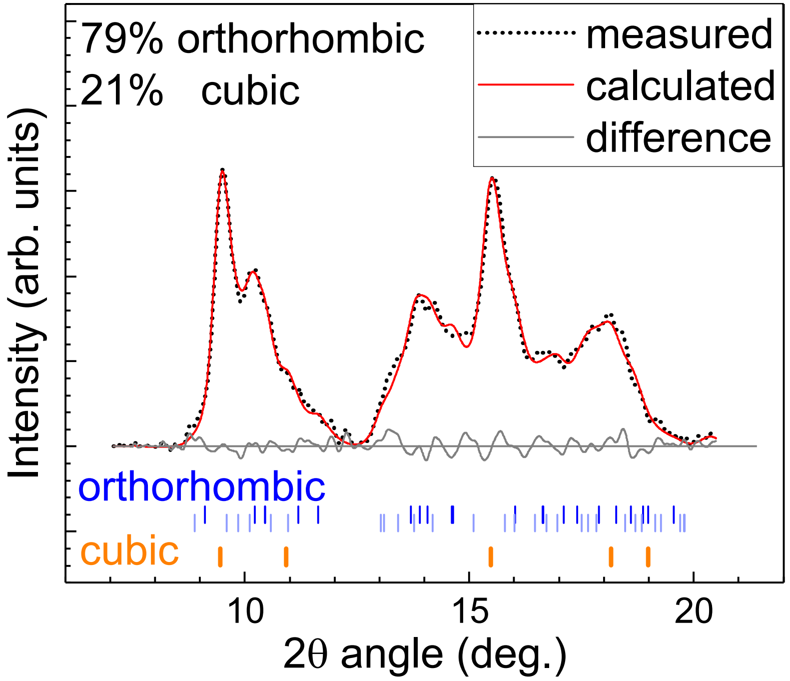
XRD-0 σ = 0 GPa



XRD-3
σ ~ 13 GPa



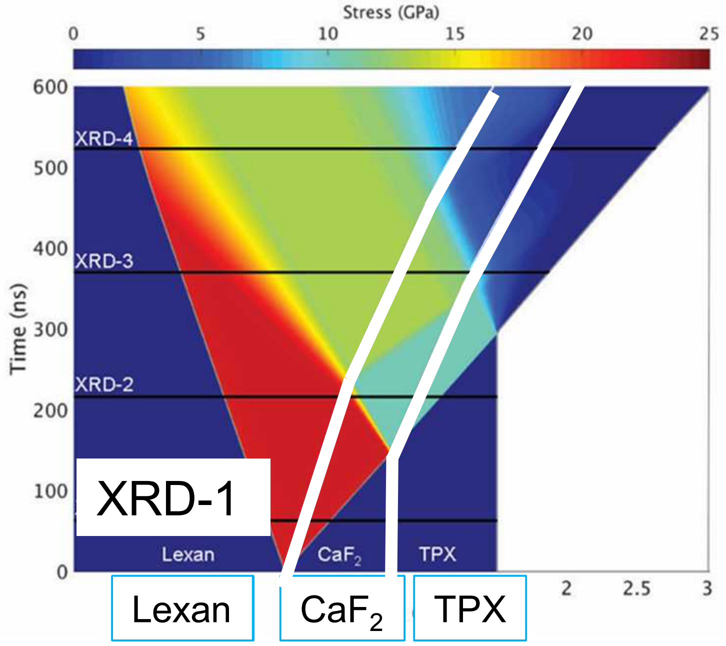
XRD-4
6 > σ > 1 GPa

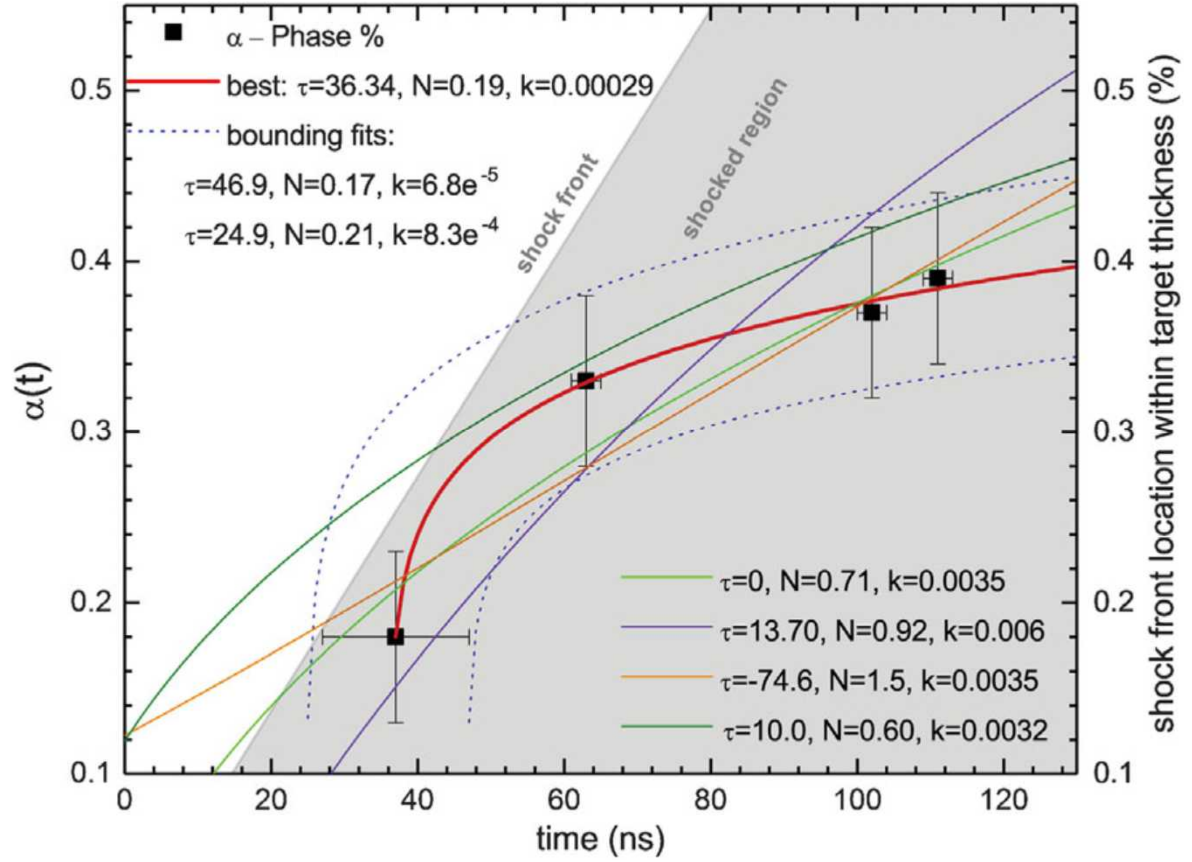


- complete phase transition fluorite → cotunnite

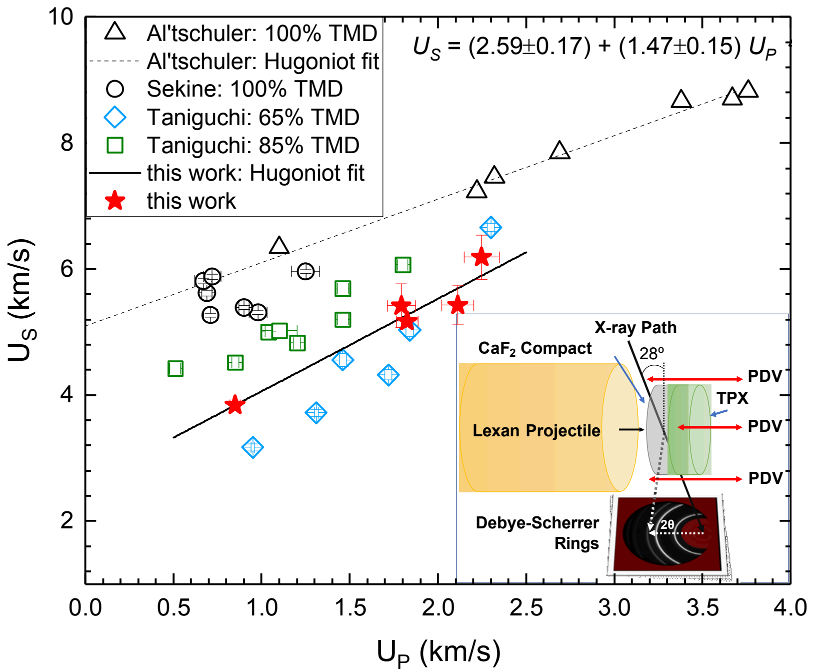
- reversible transition
- hysteresis on stress release

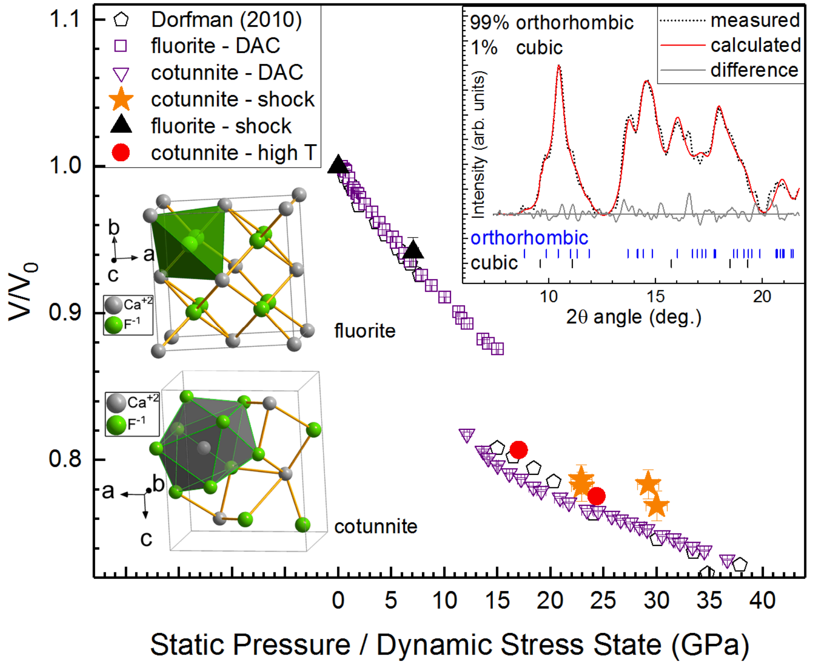
Kinetics of the Shock-Driven Transition





Summary





- **DXRD** enables a real-time observation of a shock-driven phase transition in a simple ionic crystal. We combine a **continuum scale diagnostic** with a **microstructural characterization technique** to understand a shock-driven process, which previously was only inferred from static compression.
- Work is part of a larger project on CaF_2 which combines different strain rates and timescales.
- These cross-platform comparisons provide understanding of phase transitions at different time scales and will improve our capability to simulate materials at extreme conditions.

Patricia Kalita, Paul Specht, Seth Root et. al. PRL, 119, 255701 (2017)

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