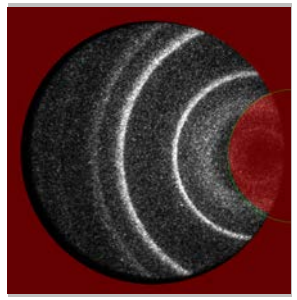
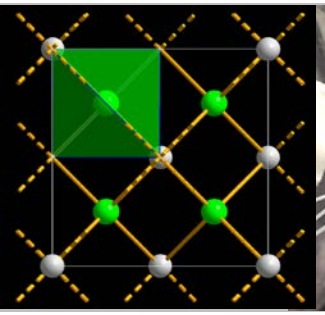
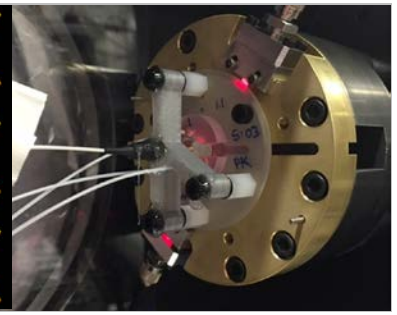
SAND2017-7121C

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# Dynamic XRD, Shock and Static Compression of $CaF_2$

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U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

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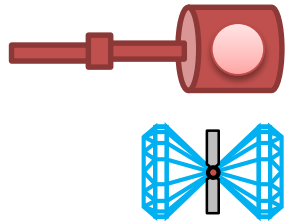
# Overview

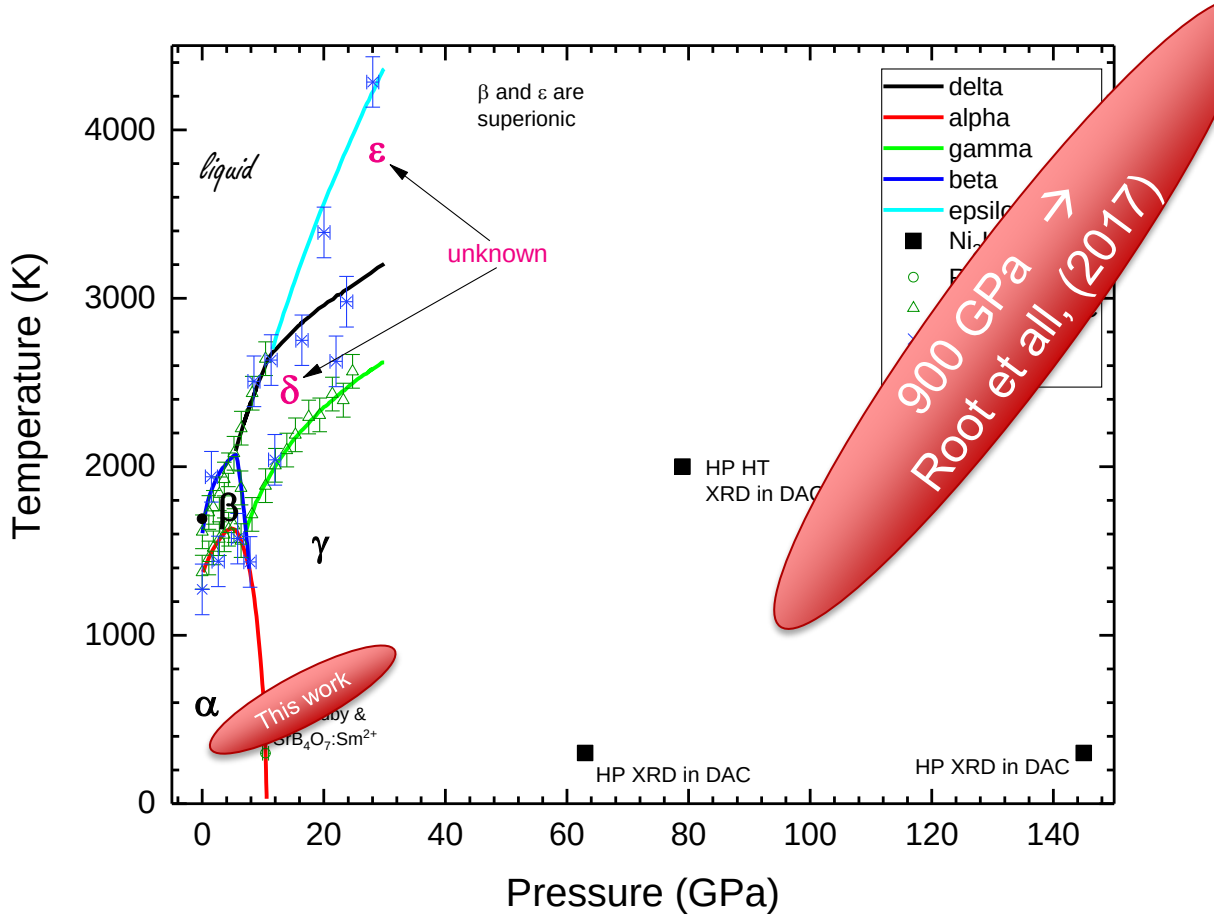
- Why $CaF_2$?
- APS-ANL Sector 35 DCS: **dynamic compression** and in situ XRD
- APS-ANL Sector 16 HPCAT: **static compression** and in situ XRD
- Hugoniot equation of state for 75% dense porous $CaF_2$
- Dynamically-driven phase transition
- Dynamic vs static compression
- Summary



# 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)*

# Advanced Photon Source at Argonne National Lab

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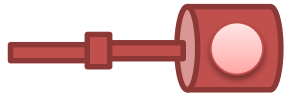

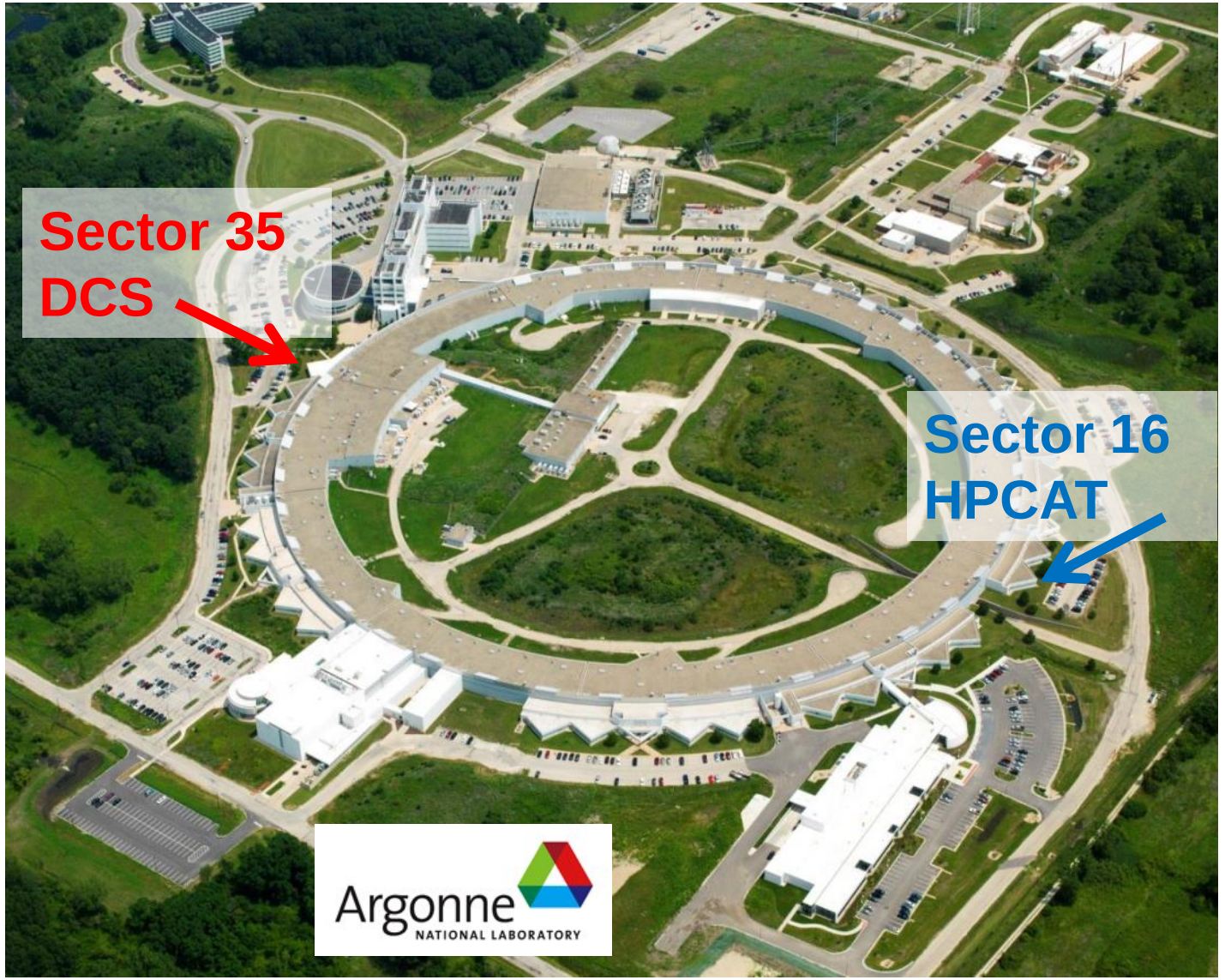


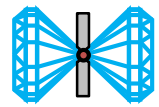

- 3rd generation synchrotron source
- 1,104m = 3,622 ft.
- X-rays ON 24h/day
- 6 days/week

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

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

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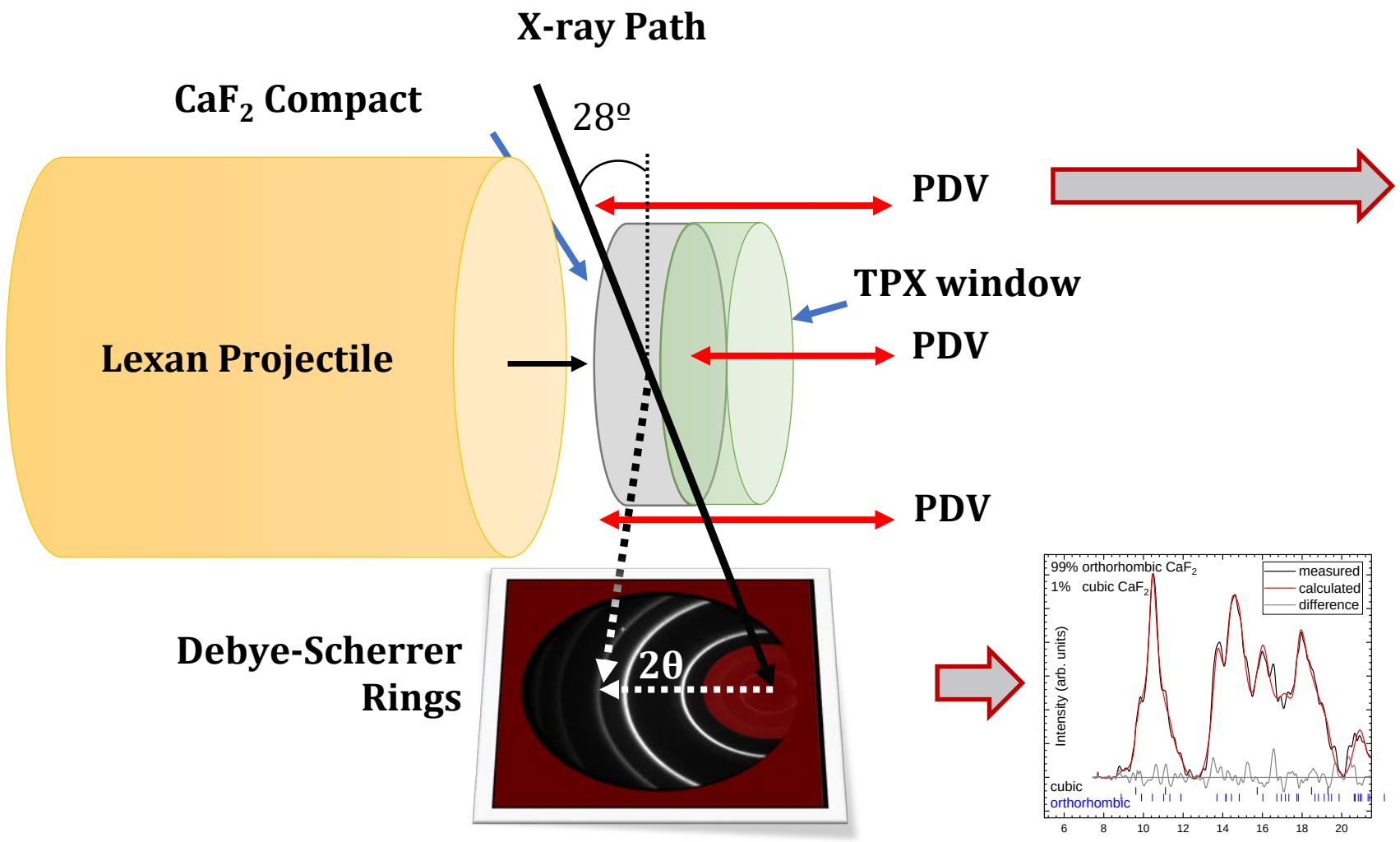


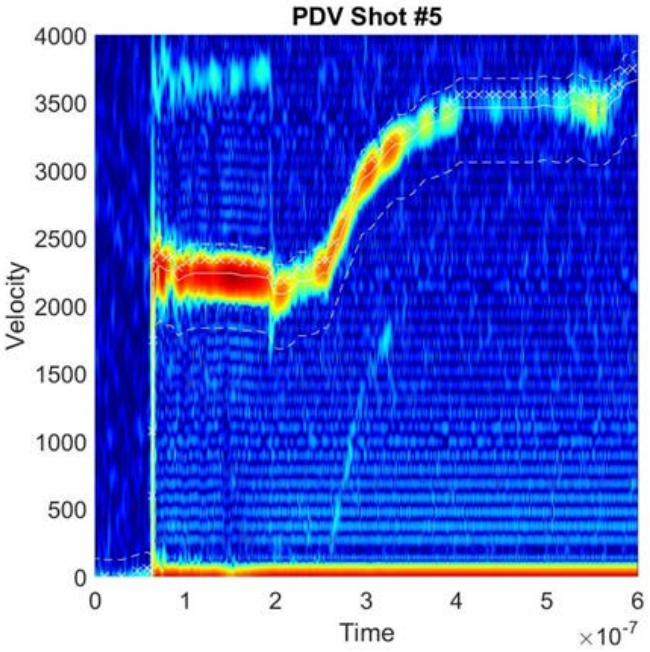





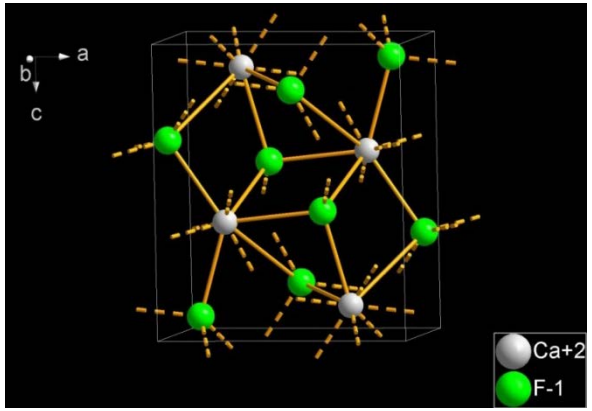

# APS Sector 16 – HPCAT: **Static** Compression & XRD

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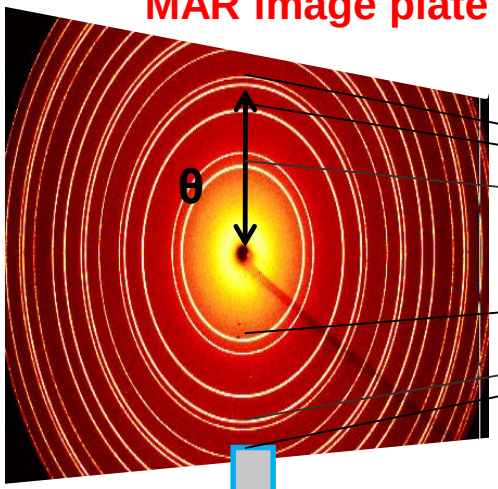
## Diamond Anvil Cell

**Area Detector:**
**MAR image plate**




beam stop

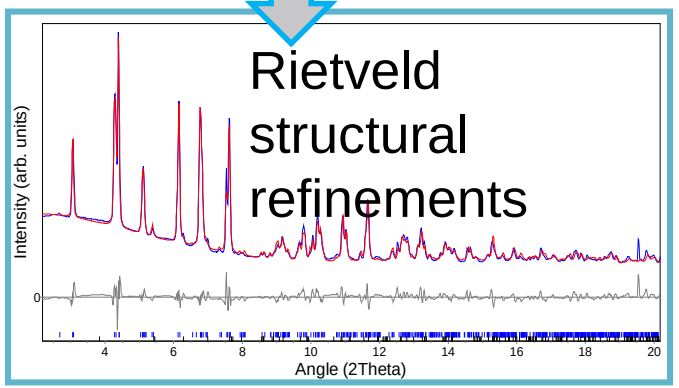
**SAMPLE**

Synchrotron x-ray beam micro-focusing optics

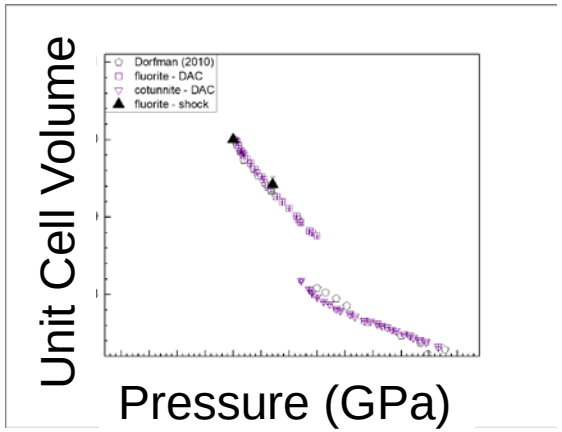
monochromatic synchrotron x-ray beam

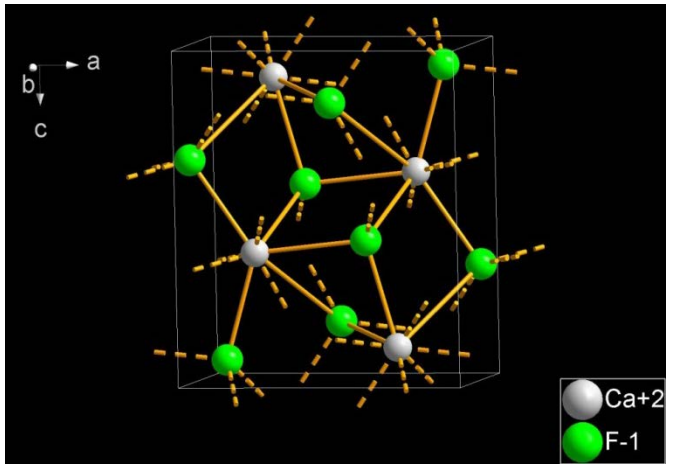
**DIAMONDS**

Resistive heating to 600°C and T measurement

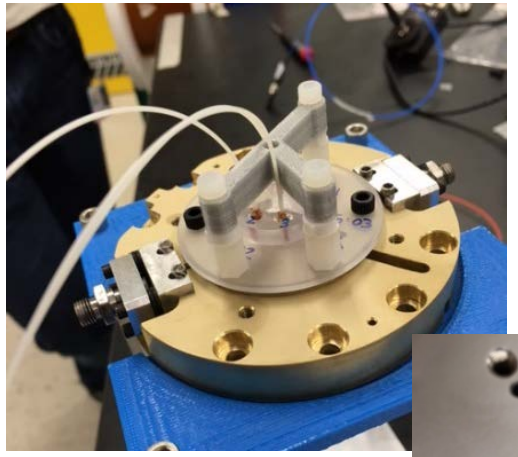


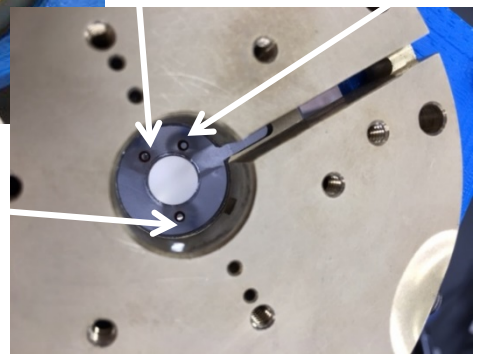

Rietveld structural refinements

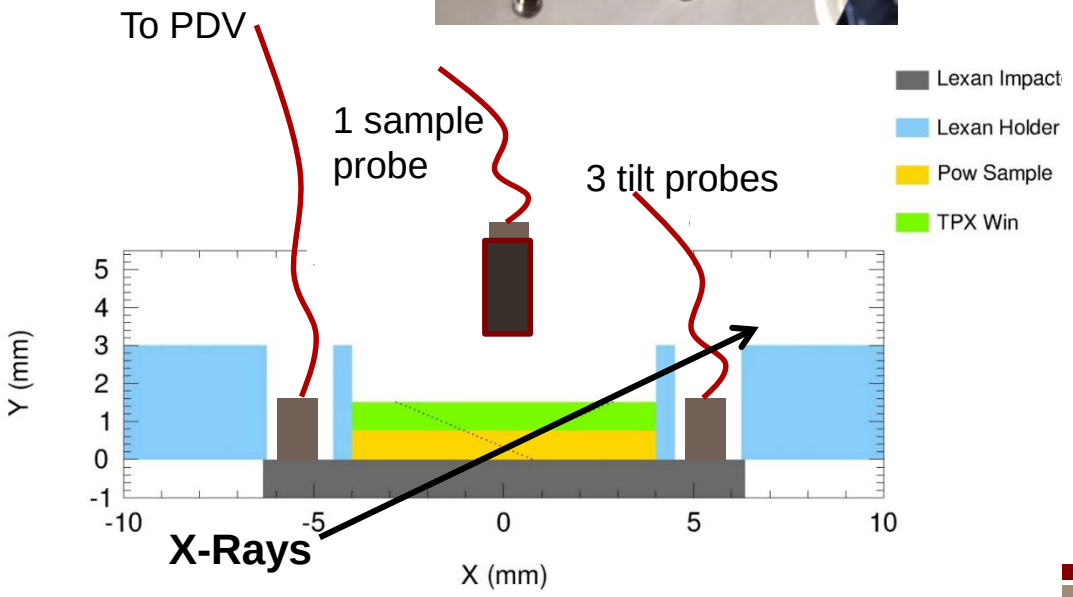


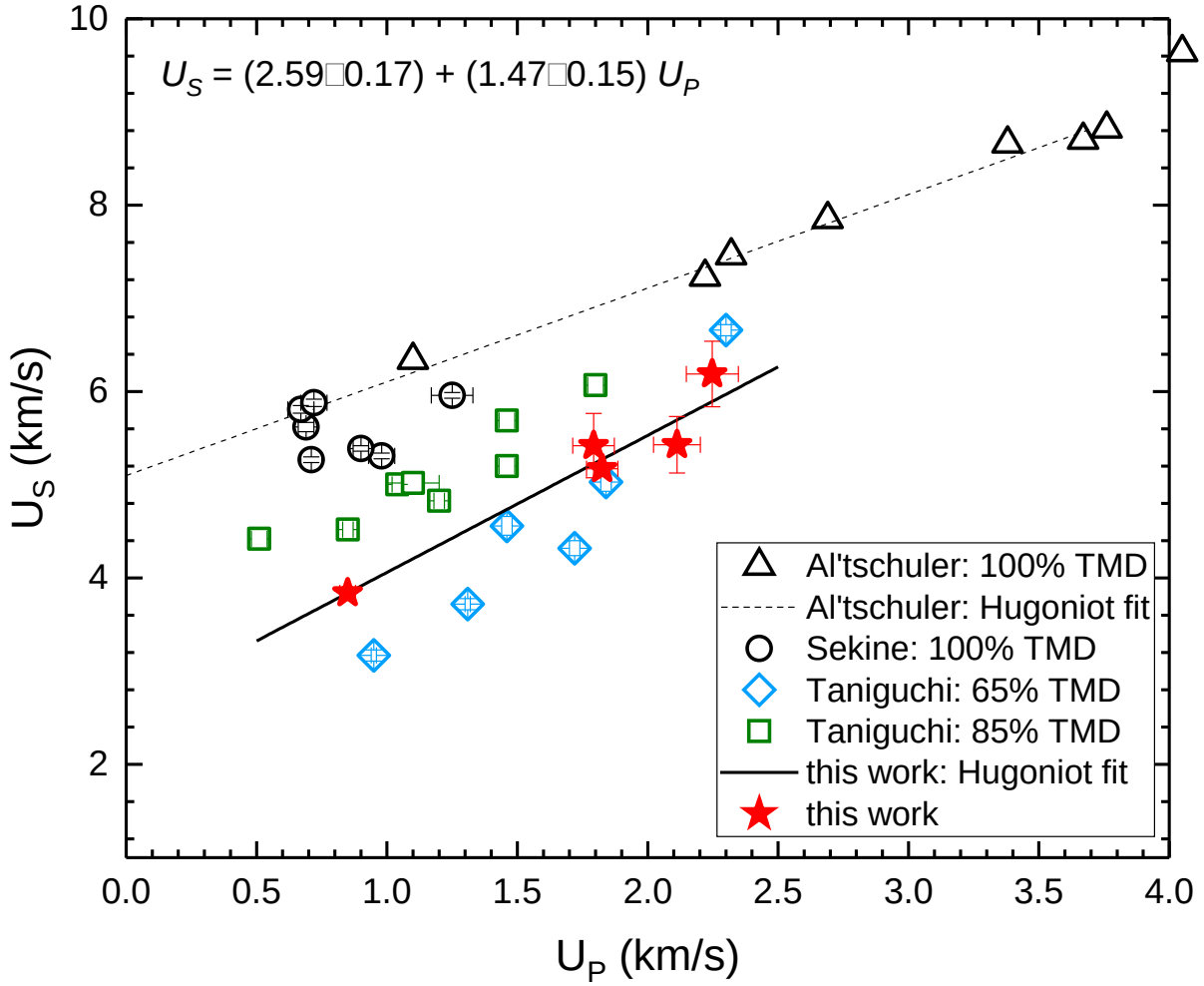



# Hugoniot of 75% dense $CaF_2$



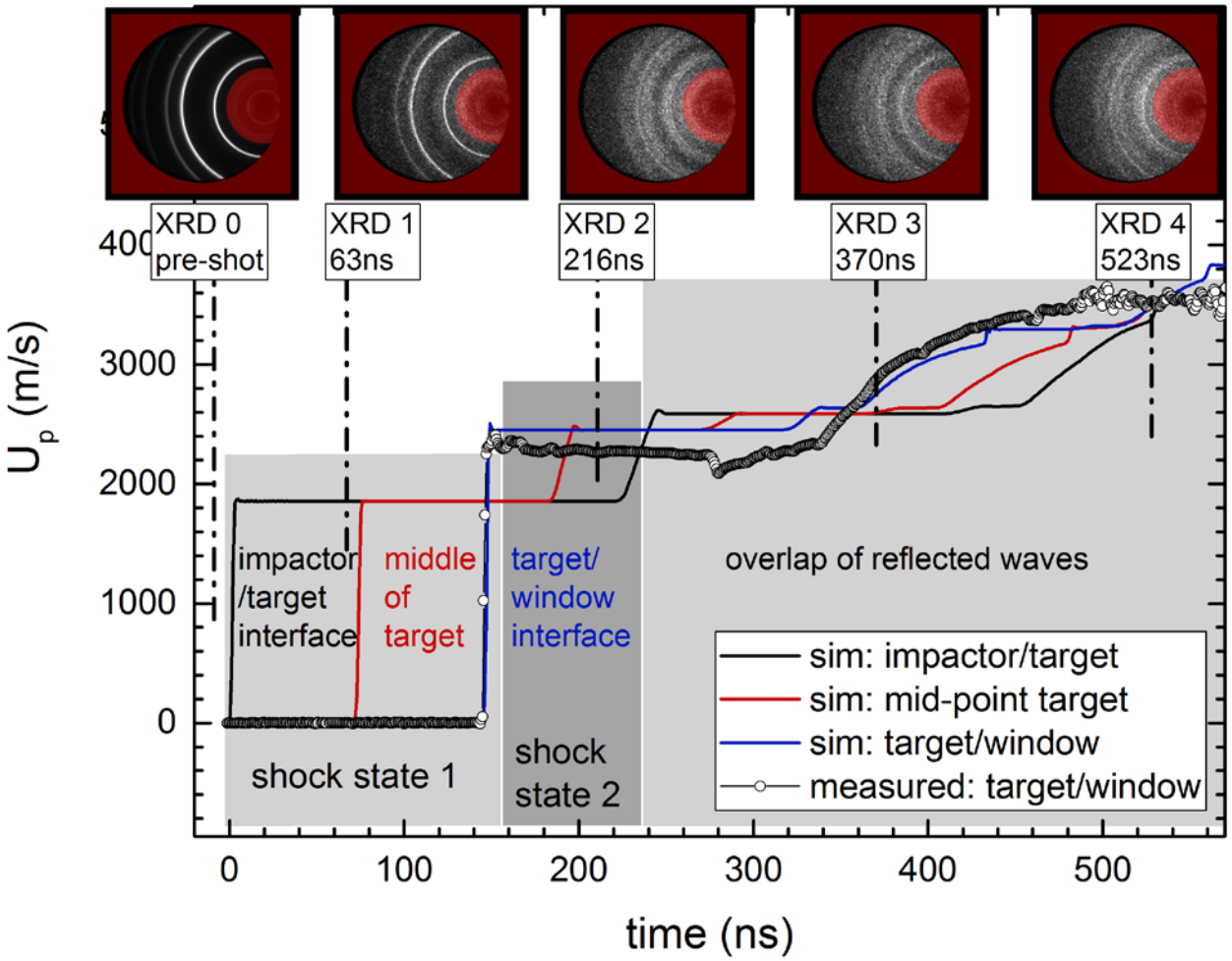


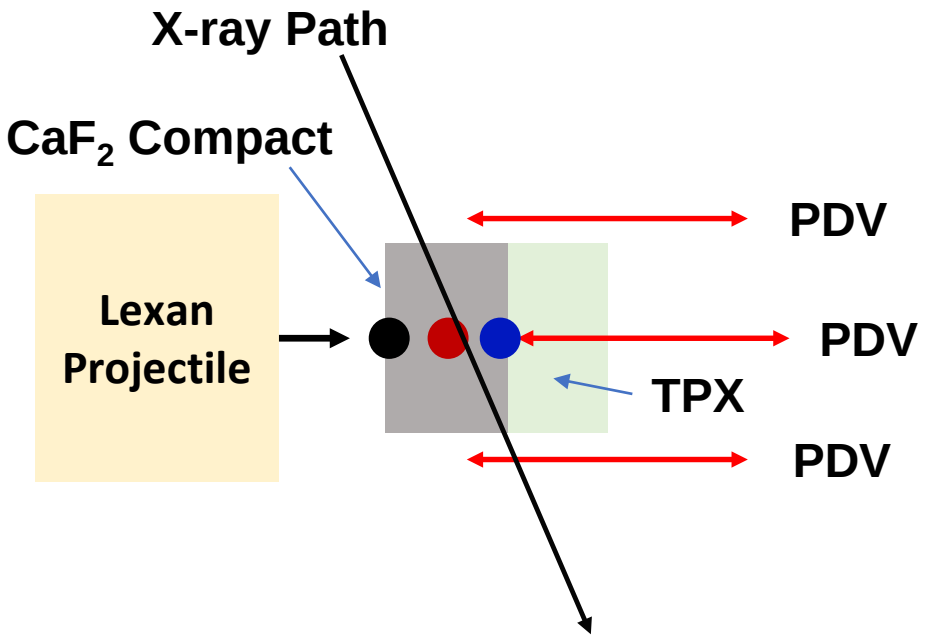



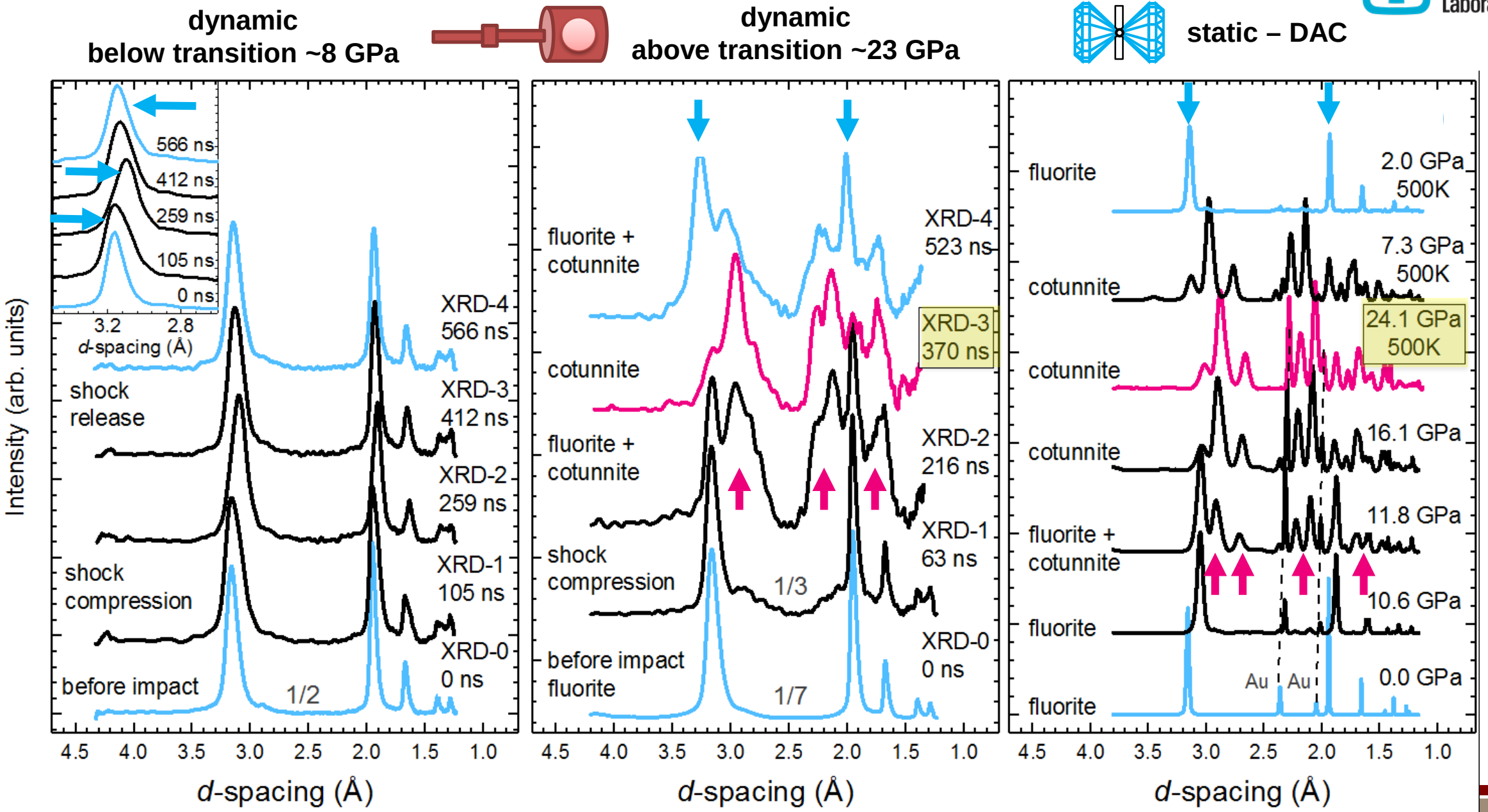

*Al'tshuler et all, Sov. Phys. Solid State 15, 969 (1973)*
*Sekine et all, Phys Chem Miner 38, 305 377 (2011)*
*Taniguchi, et all, J. Appl. Phys. 384 61, 196 (1987)*

# Dynamic XRD and Shock: WHEN?



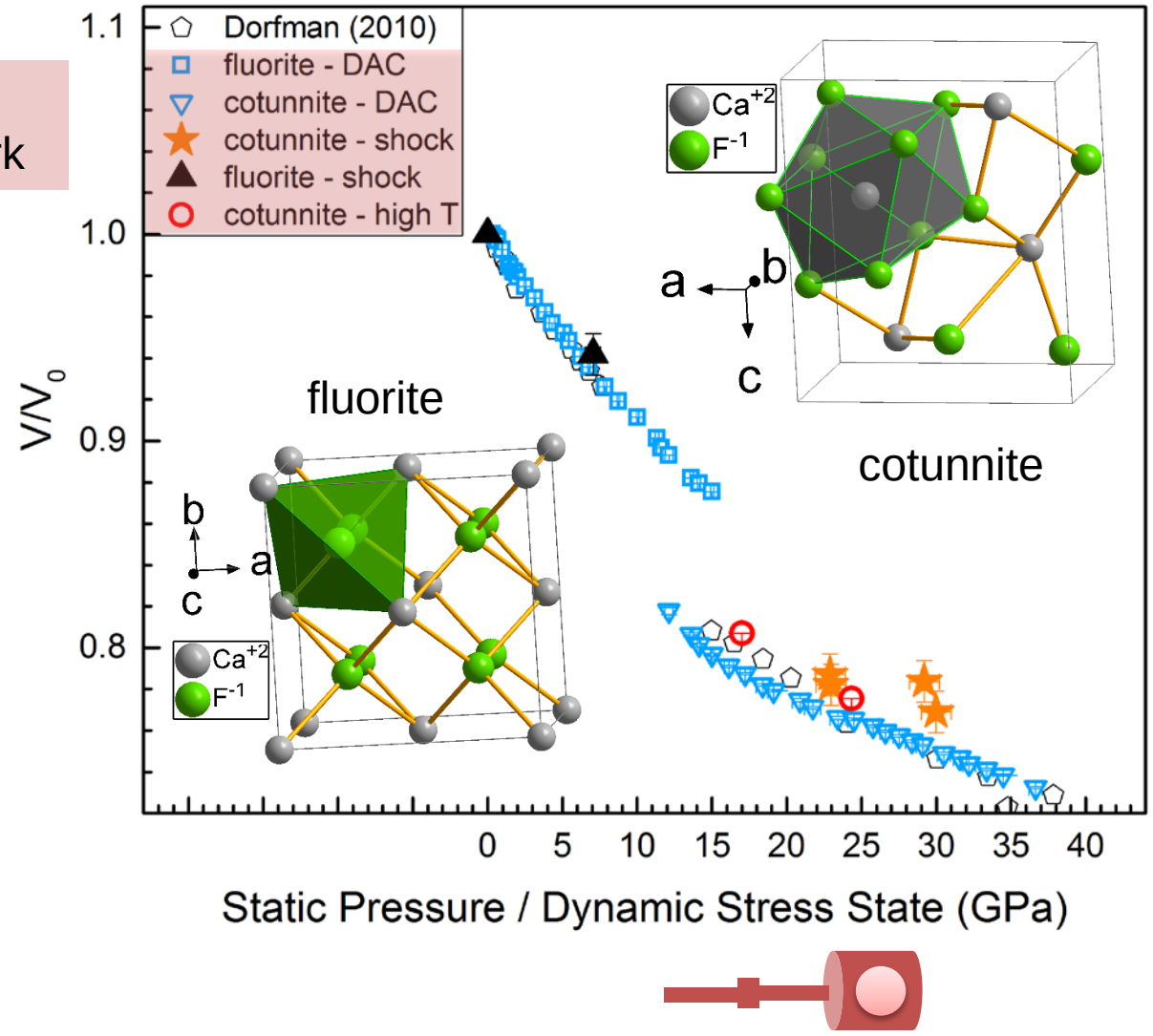



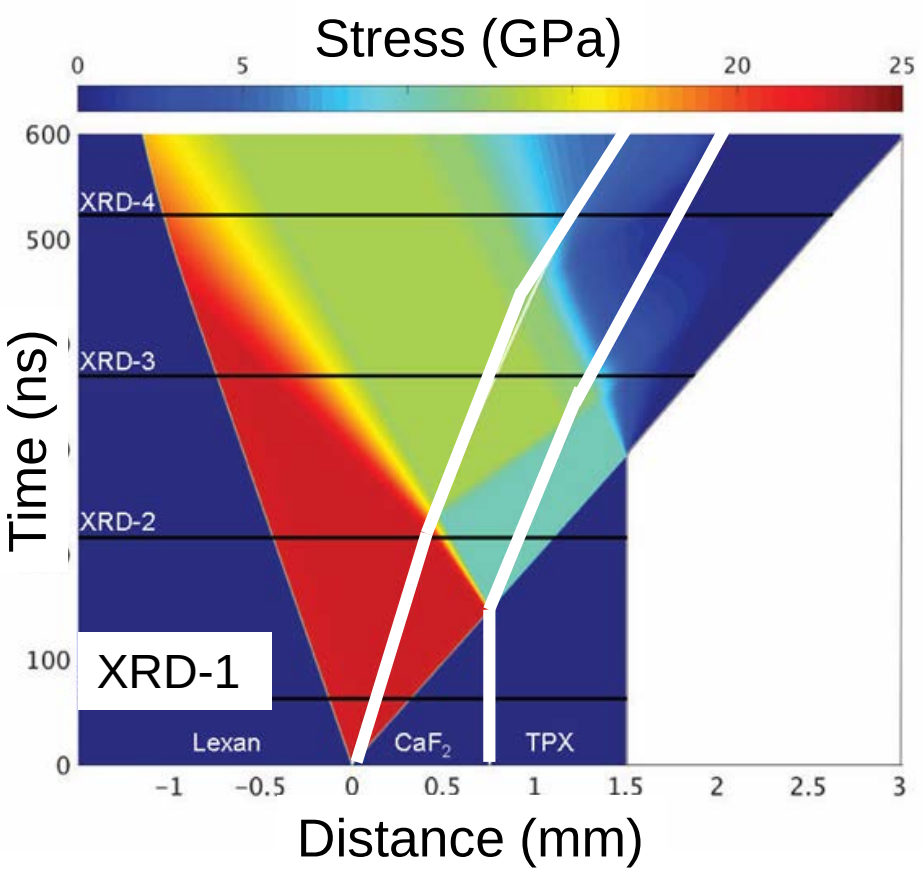
# Dynamic vs Static XRD and Phase Transition



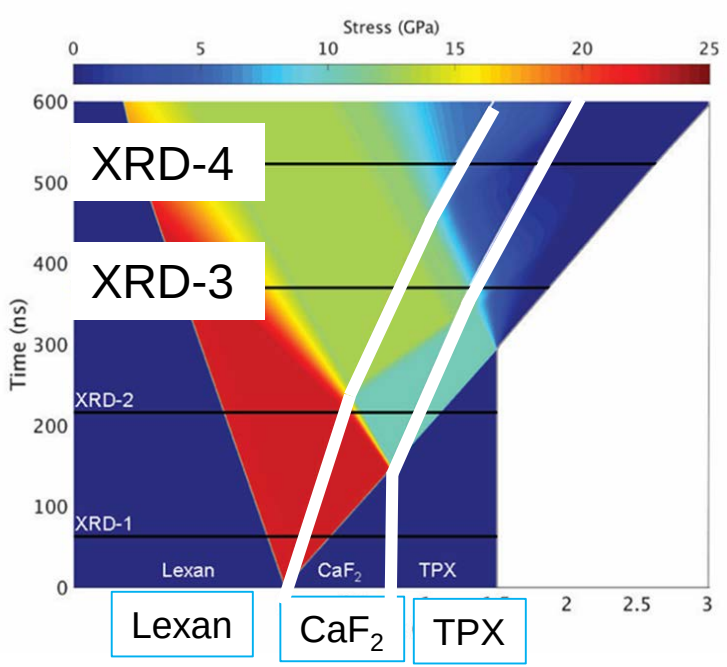
# Dynamic vs Static Compression: Evolution of Unit Cell Volume

this work

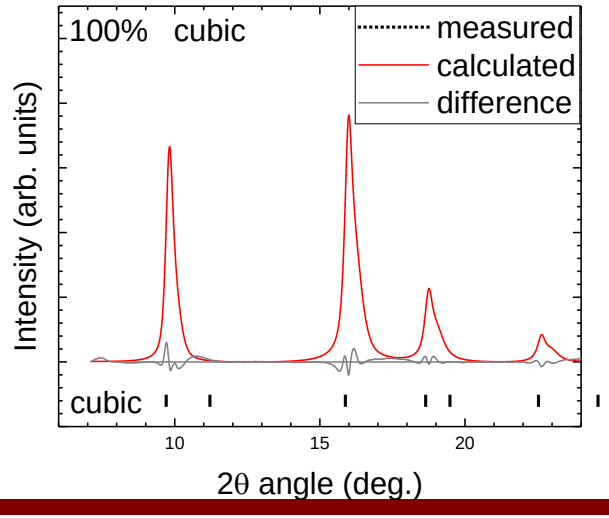


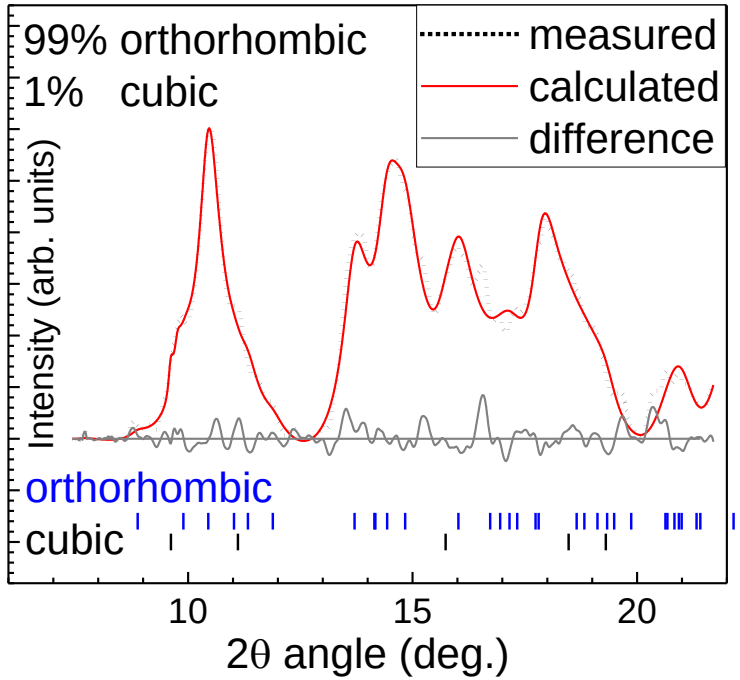
# Quantitative Shock XRD Analysis




**XRD-0 σ = 0 GPa**

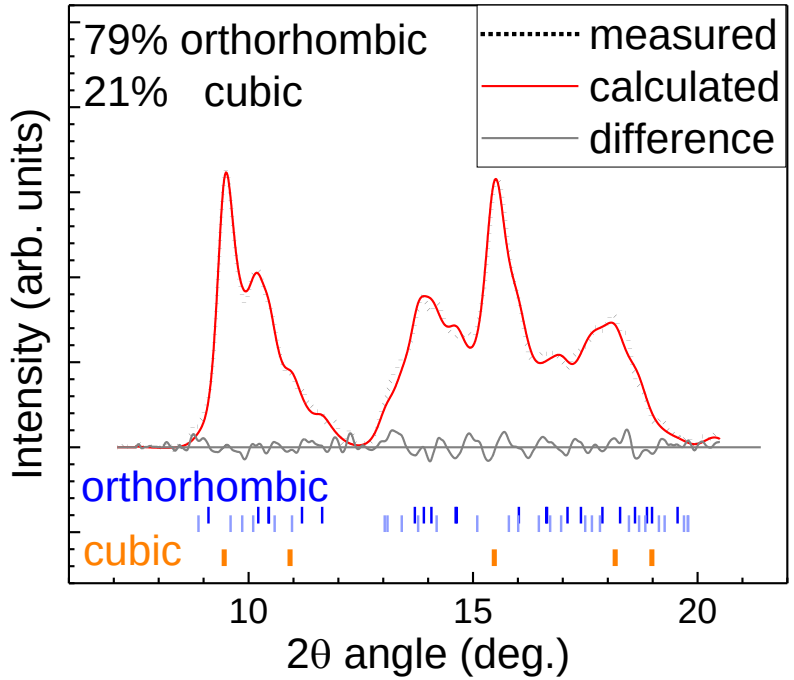



**XRD-3**
**σ ~ 13 GPa**



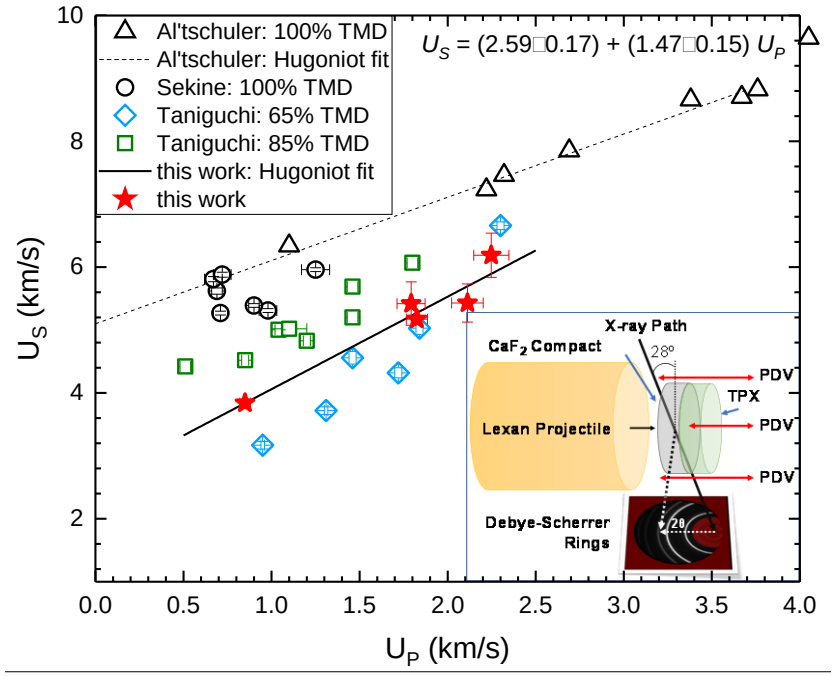

- complete phase transition fluorite → cotunnite

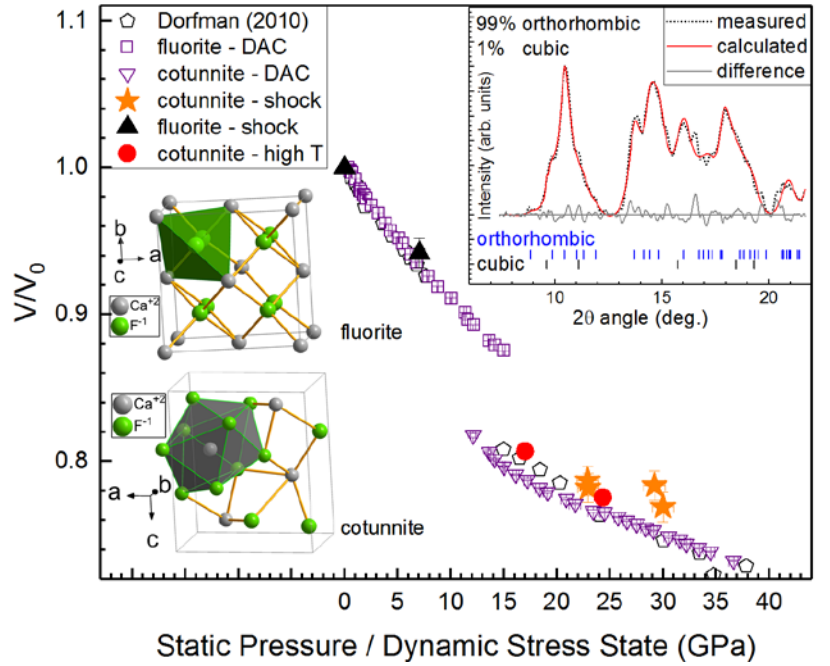
**XRD-4**
**6 > σ > 1 GPa**




- reversible transition
- hysteresis on stress release

# Summary




- **DXRD** enabled 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.

**Session V6: Equation of State VI**
3:45 PM–5:15 PM, Thursday, July 13, 2017
Room: Regency Ballroom E

Chair: Travis Sjostrom, Los Alamos National Laboratory

**Abstract: V6.00005 : Shock Compression Response of Calcium Fluoride ($CaF_2$)**
5:00 PM–5:15 PM

Preview Abstract

**Author:**
Seth Root, Michael Desjarlais, Ray Lemke, Patricia Kalita, Scott Alexander
(Sandia National Laboratories)

# Acknowledgements


- The authors would like to acknowledge the large team that contributed to the design, fabrication, and fielding of the experiments at SNL, at DCS-APS and at HPCAT-APS.

- **Sandia National Laboratories** is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

- Portions of this work performed at the **Dynamic Compression Sector** supported by the Department of Energy, National Nuclear Security Administration, under Award Number DE-NA0002442 and operated by Washington State University.

- Portions of this work were performed at **HPCAT (Sector 16), Advanced Photon Source (APS),** Argonne National Laboratory. HPCAT operations are supported by DOE-NNSA under Award No. DE-NA0001974, with partial instrumentation funding by NSF.

- **J. Smith and S. Sinogeikin** acknowledge the support of DOE-BES/DMSE under Award DE-FG02-99ER45775 The Advanced Photon Source is a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357. Work at HiPSEC is supported by the National Nuclear Security Administration under the Stewardship Science Academic Alliances program through DOE Cooperative Agreement DE-NA0001982.