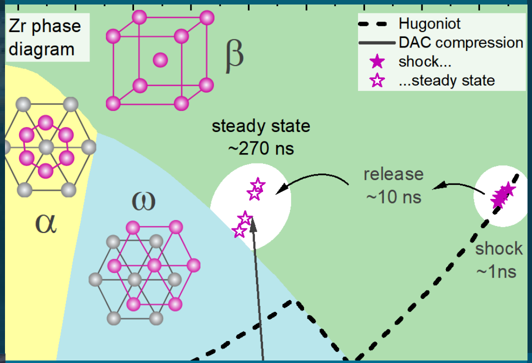
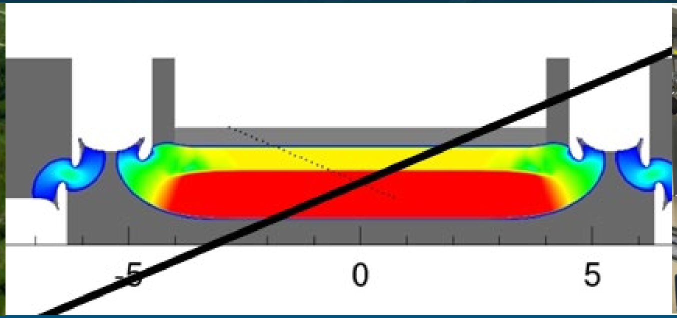
SAND2022-5056C

Sandia National Laboratories

Hurry up or take your time: kinetics of shock-driven phase transitions and dynamic x-ray diffraction





PRESENTED BY

Patricia Kalita, SNL

Argonne NATIONAL LABORATORY

UNLV

APS March 2020 Meeting – Invited Talk
Session L03: Materials in Extremes: Phase Transitions
03-04-20 - 9:12 am-9:48 am

U.S. DEPARTMENT OF ENERGY NNSA

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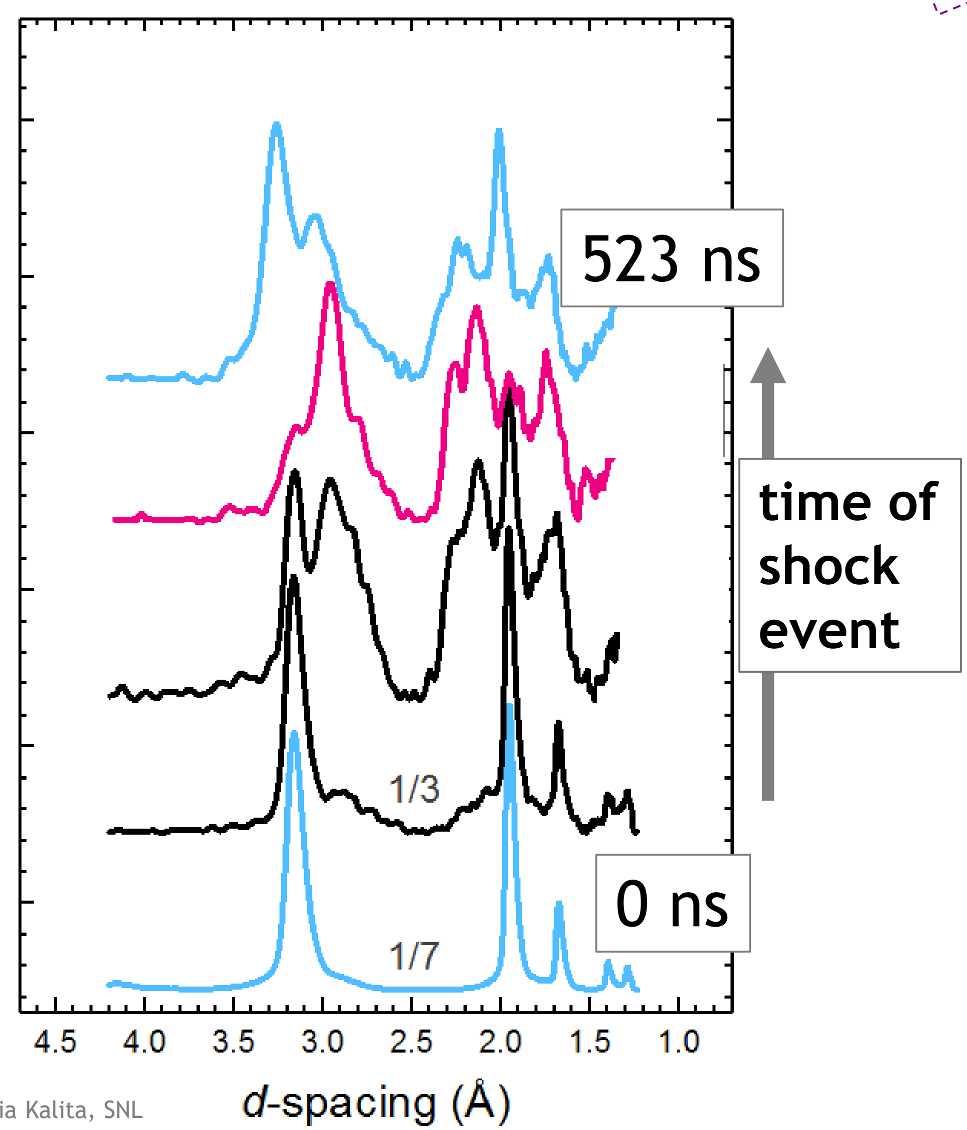
In collaboration with the following awesome scientists:

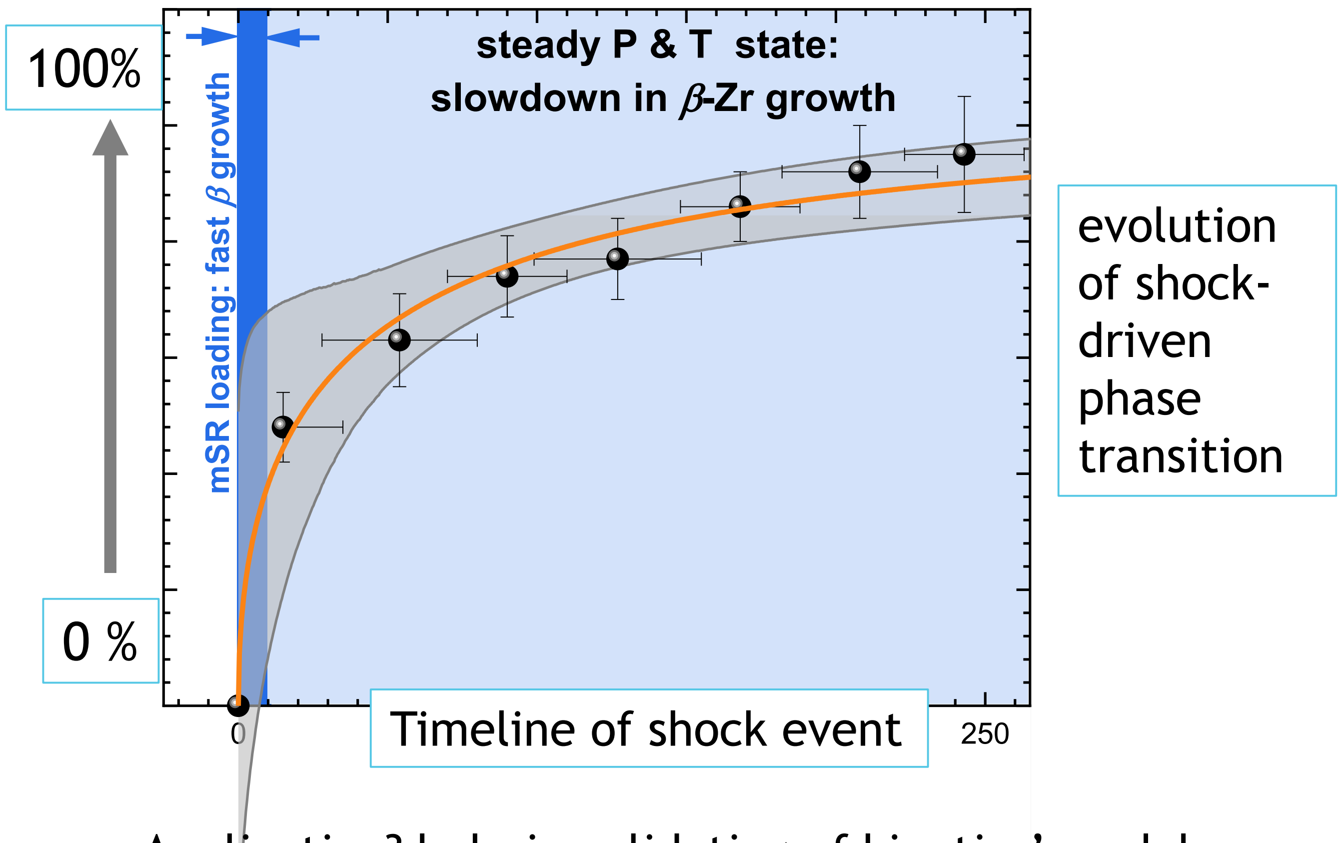
- Justin Brown, Paul Specht, and Seth Root, SNL
- Melanie White, Andrew Cornelius, UNLV
- Jesse S. Smith, HPCAT, APS – ANL
- Nicholas Sinclair, Adam Schuman, Paulo Rigg, DCS, WSU & APS – ANL

Preview…

DXRD

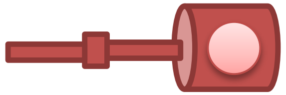
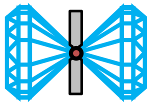
- with dynamic XRD (DXRD), we get a microscopic insight into shock processes,
- we can quantify the kinetics of shock-driven phase transition at nanosecond scales





Application? help in validating of kinetics' models for phase transitions in shock processes

Outline

1. DXRD & Shock compression at DCS, APS - ANL 
2. XRD & Static compression at HPCAT, APS - ANL 
3. CaF_2 structures and phase diagram
4. Real-time DXRD probe of a **single-step shock event** in CaF_2
5. Kinetics of formation of tetragonal CaF_2 under shock compression
6. Zirconium structures and phase diagram
7. Real-time DXRD probe of a **multi-step shock/release** process in Zr
8. Kinetics of formation of β-Zirconium under shock compression
9. Summary & Takeaways

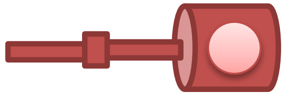
All about experiments (items 1–2)

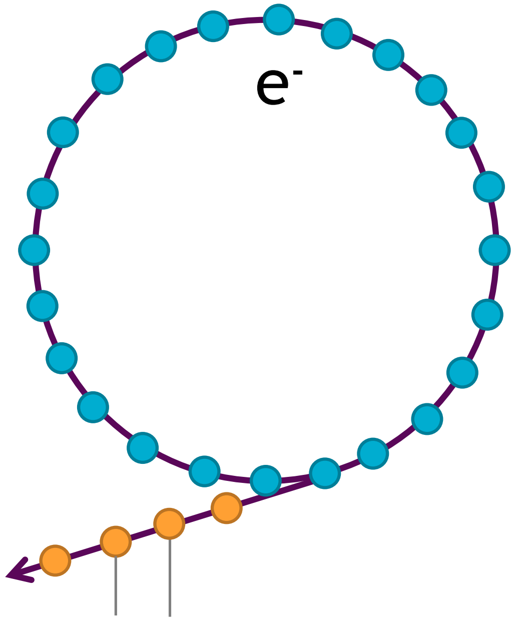
Phase transition kinetics in a simple ionic solid (items 3–5)

Phase transition kinetics in a metal (items 6–8)

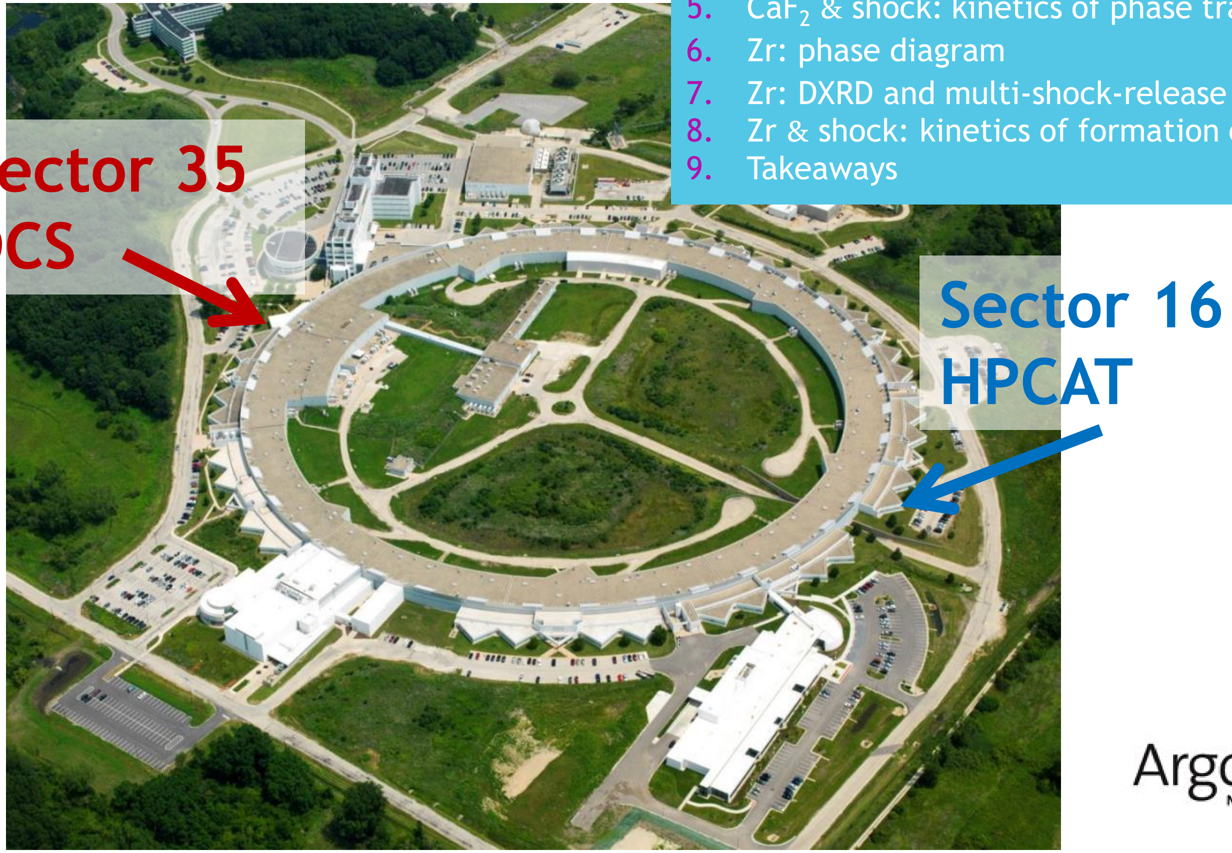
Advanced Photon Source, ANL: DCS and HPCAT

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

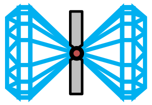




X-rays every 154 ns that last for ~100ps



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



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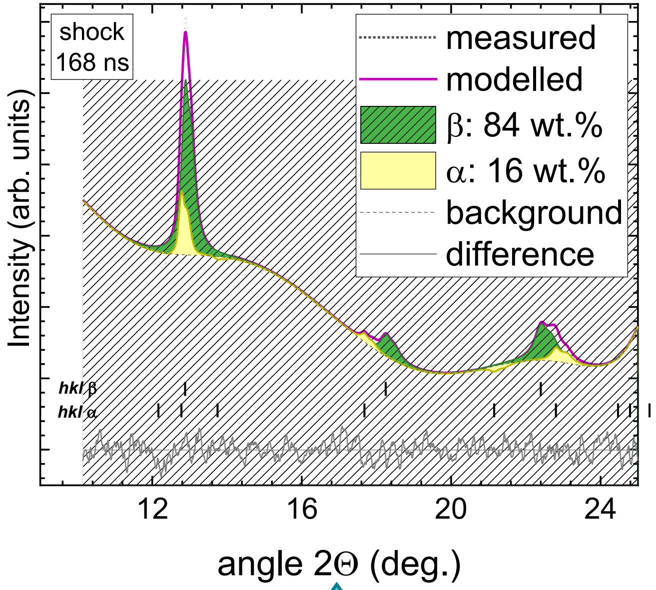
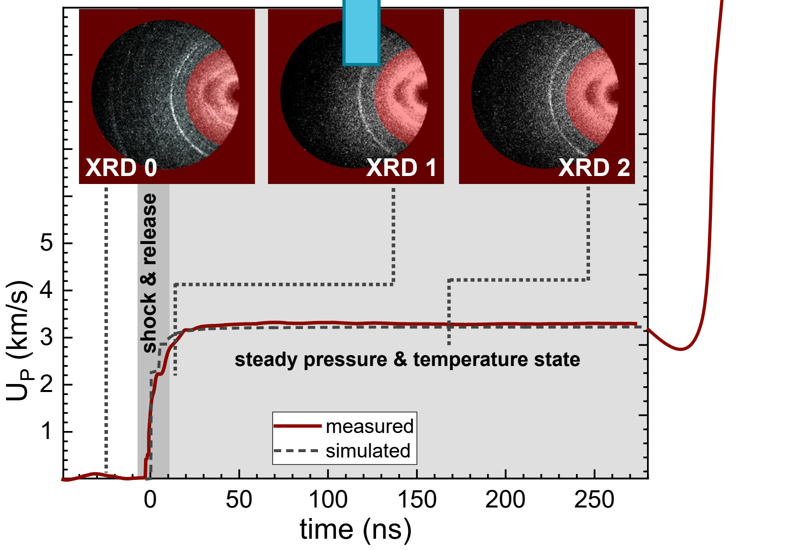
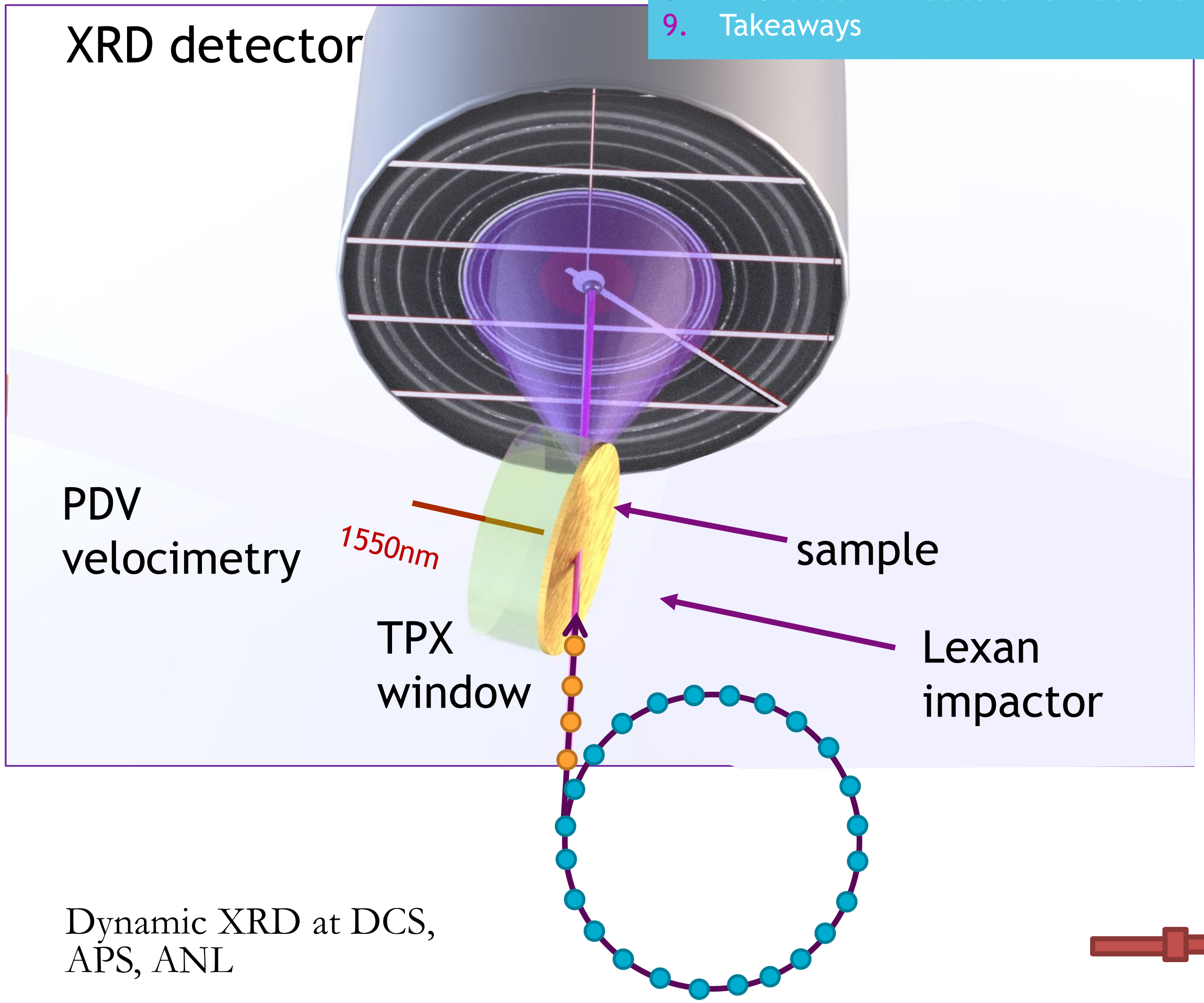
DXRD: dynamic x-ray diffraction
DAC: diamond anvil cell

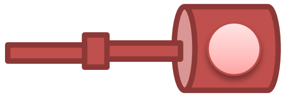
Dynamic XRD and Shock compression experiments



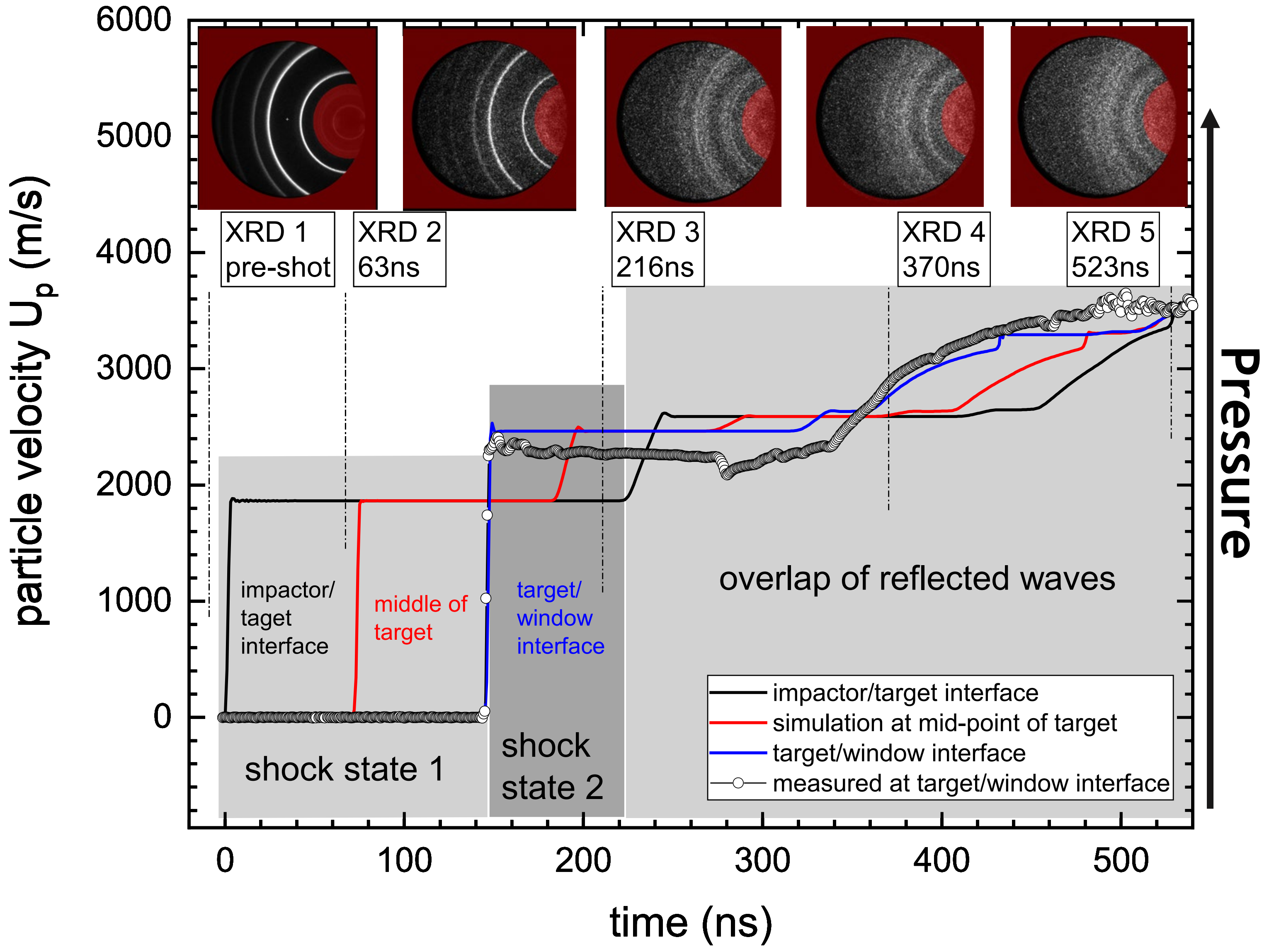


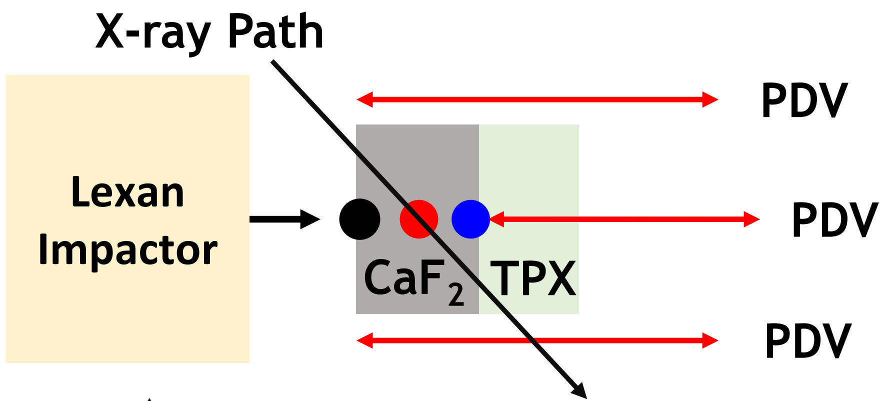


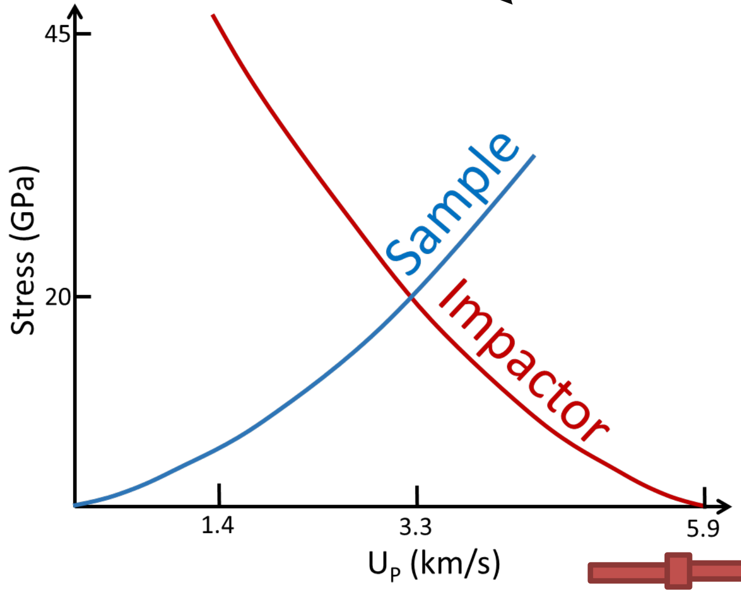
Dynamic XRD at DCS, APS, ANL



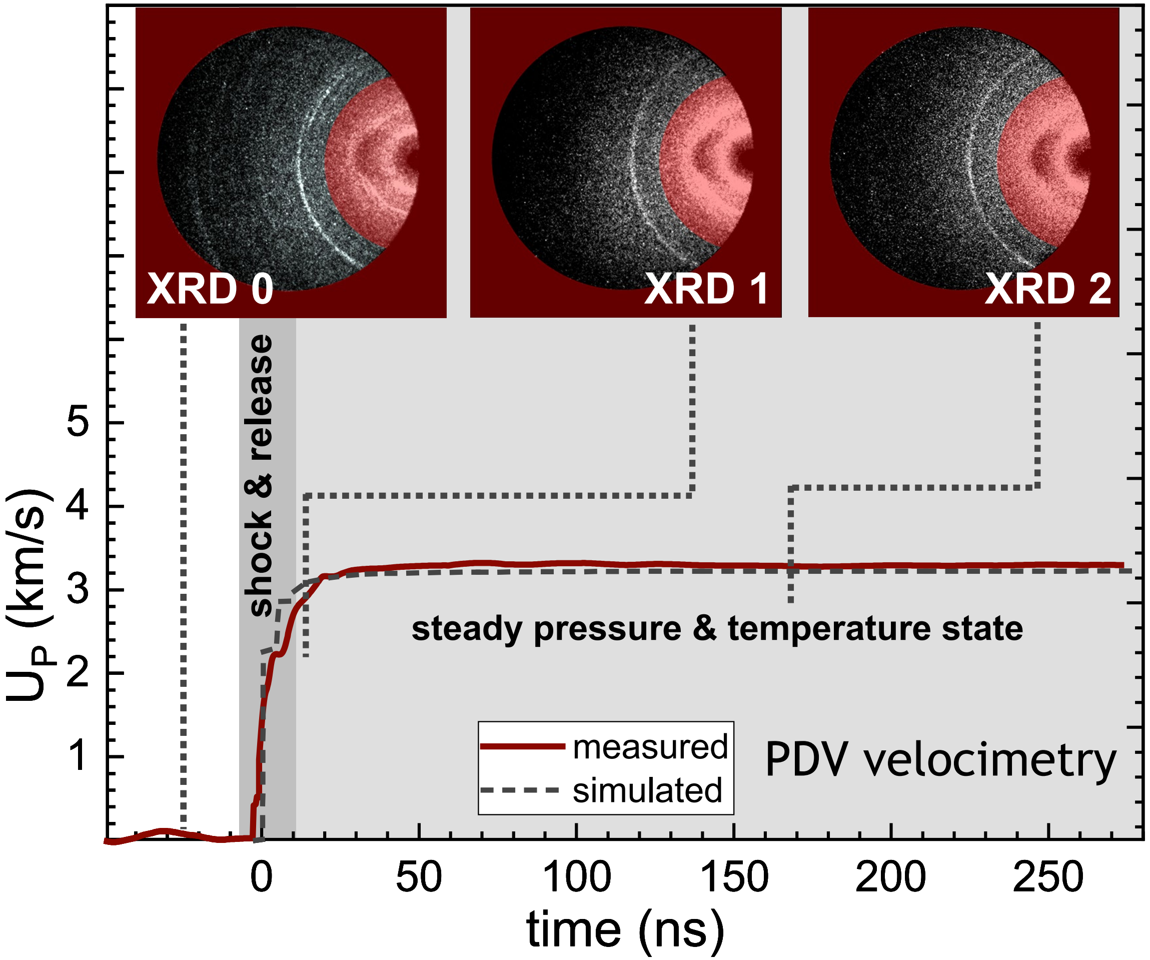
A steady stress state & kinetics of phase transitions: DXRD & single-step shock event

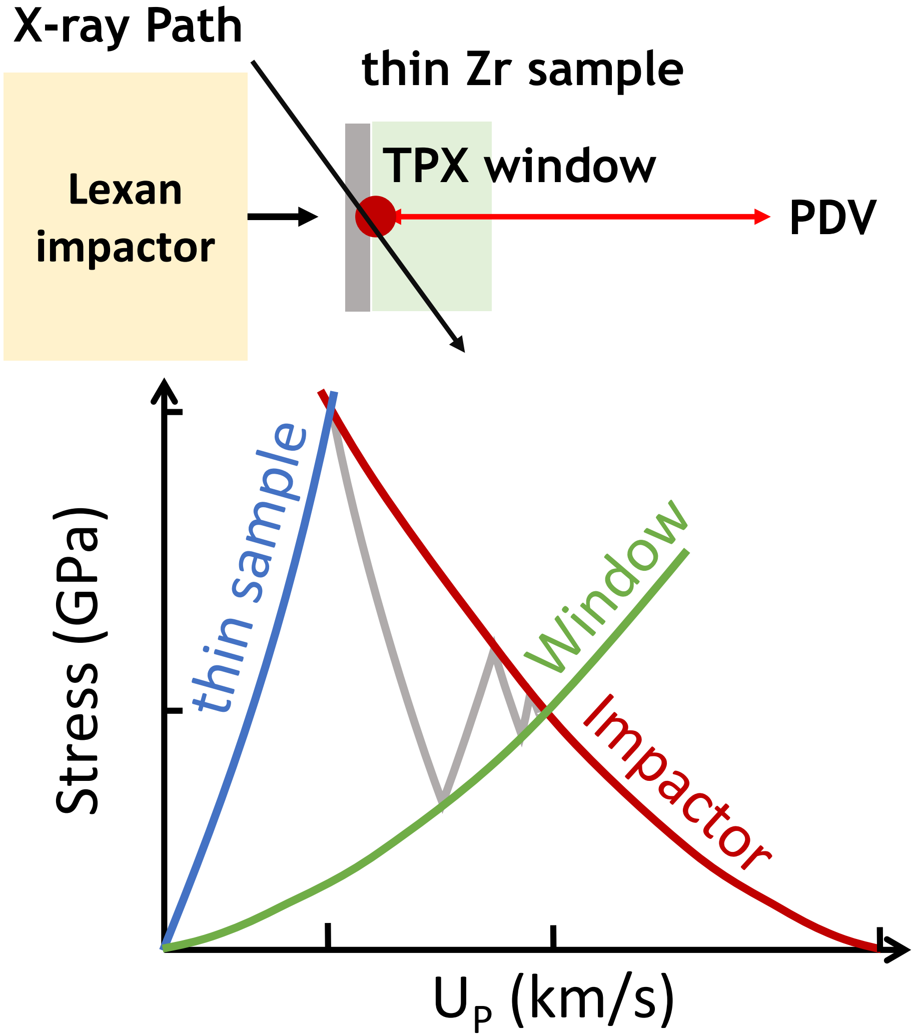






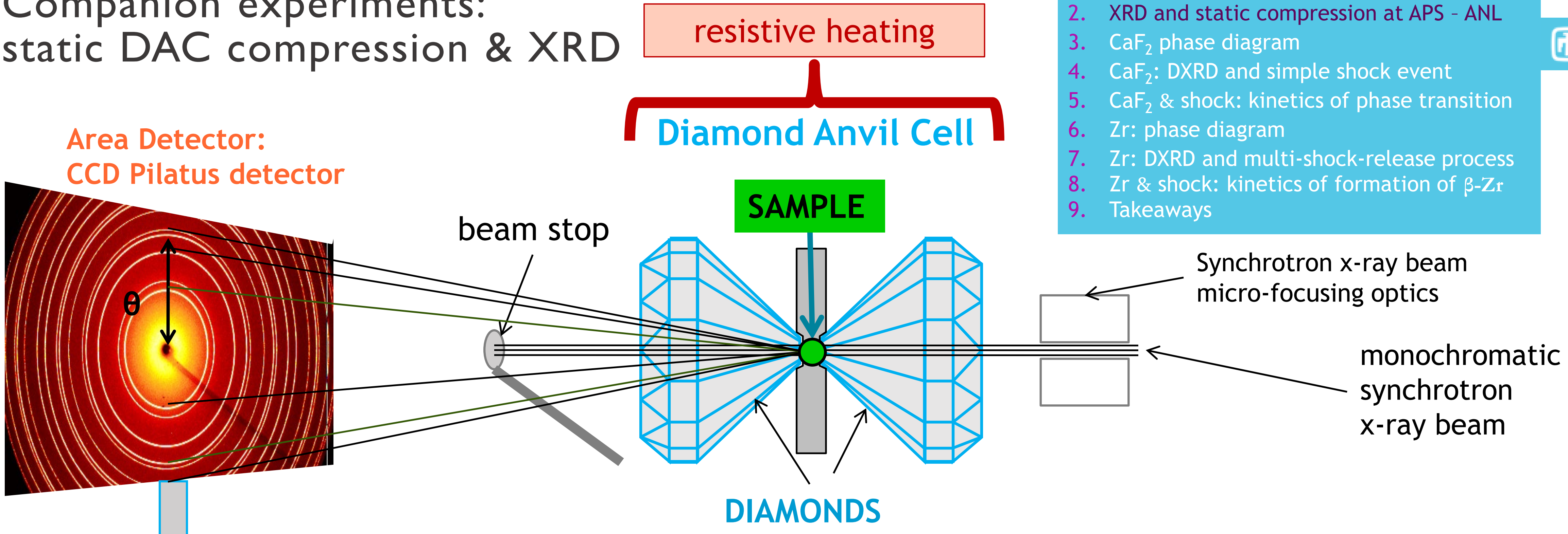
A steady stress state & kinetics of phase transitions: DXRD & a multi-shock-release process

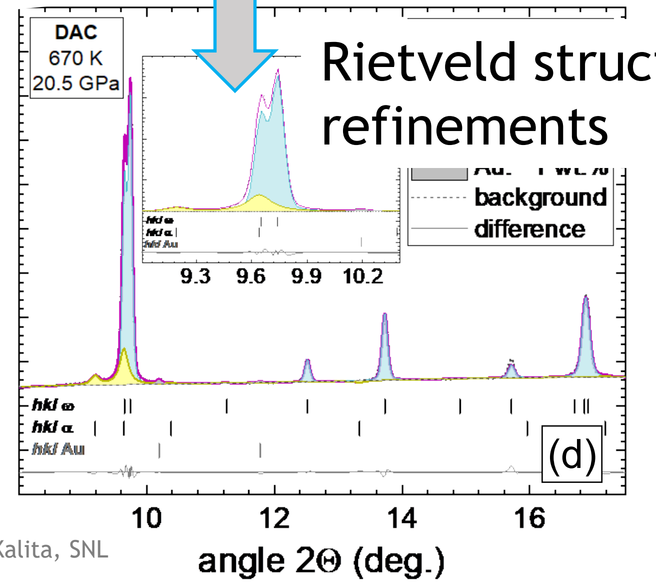


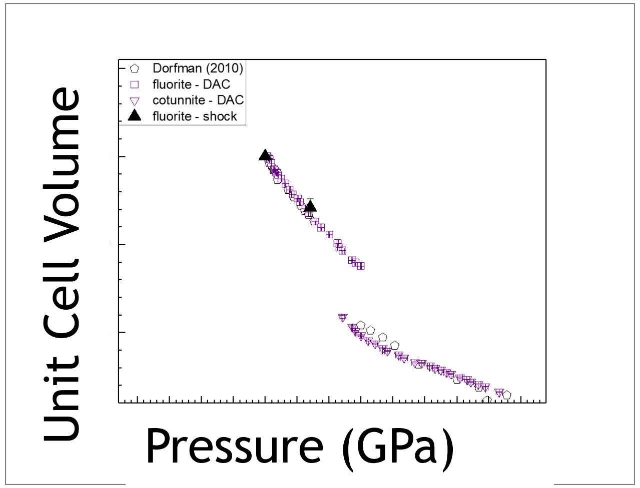


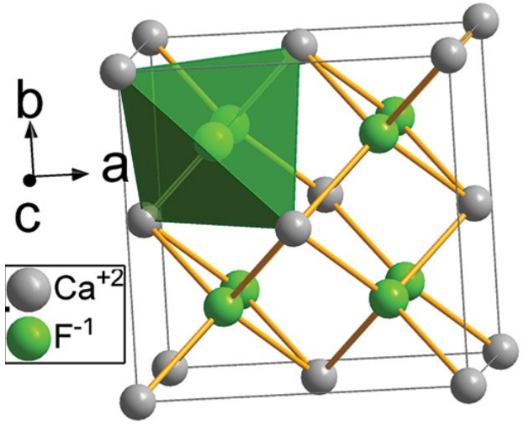
- Steady, well defined P & T state
- Great for quantitative XRD analysis

Companion experiments: static DAC compression & XRD

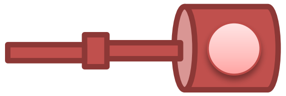
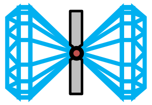








Outline

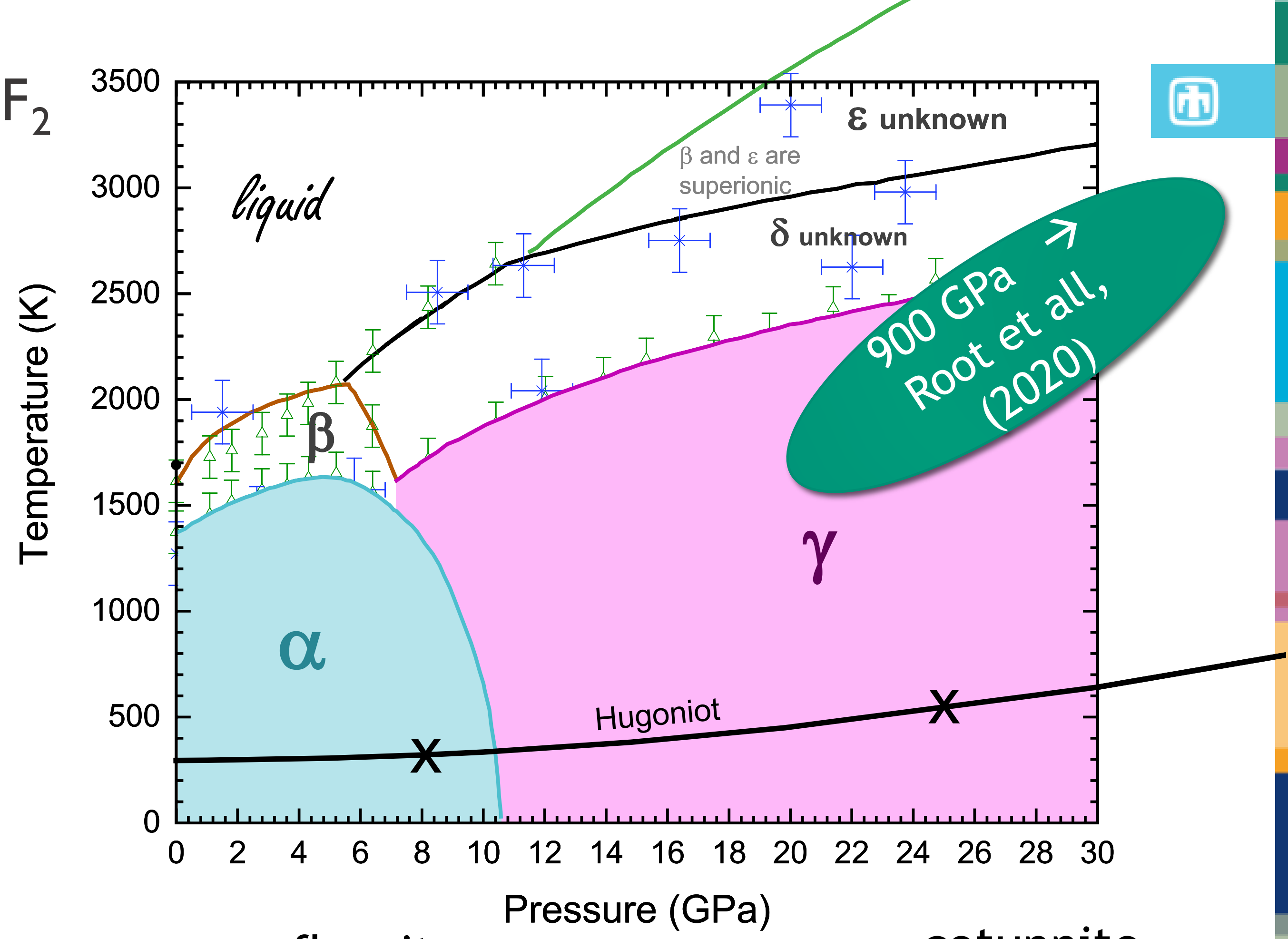
1. DXRD & Shock compression at APS – ANL 
2. XRD & Static compression at APS – ANL 
3. CaF_2 structures and phase diagram
4. Real-time DXRD probe of a **single-step shock event** in CaF_2
5. Kinetics of formation of tetragonal CaF_2 under shock compression

Phase transition kinetics in a simple ionic solid

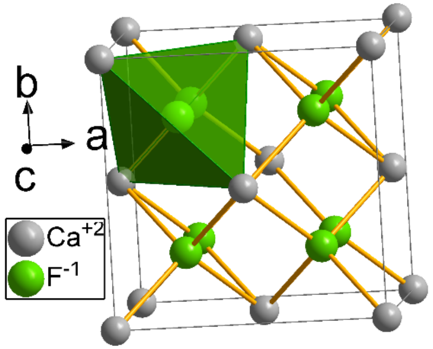
Single-step shock compression of CaF_2

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

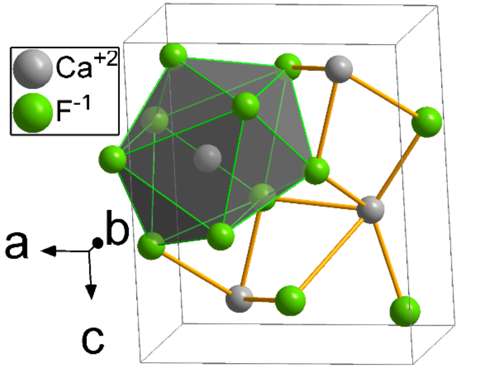
- limited Hugoniot data above 30 GPa
- high pressure Hugoniot phase (solid or melt) undetermined
- extended phase diagram undetermined
- **previous shock compression**: continuum scale velocimetry & inferred phase transition
- **static compression**: at least 2 solid → solid pressure-driven phase transitions



α - fluorite

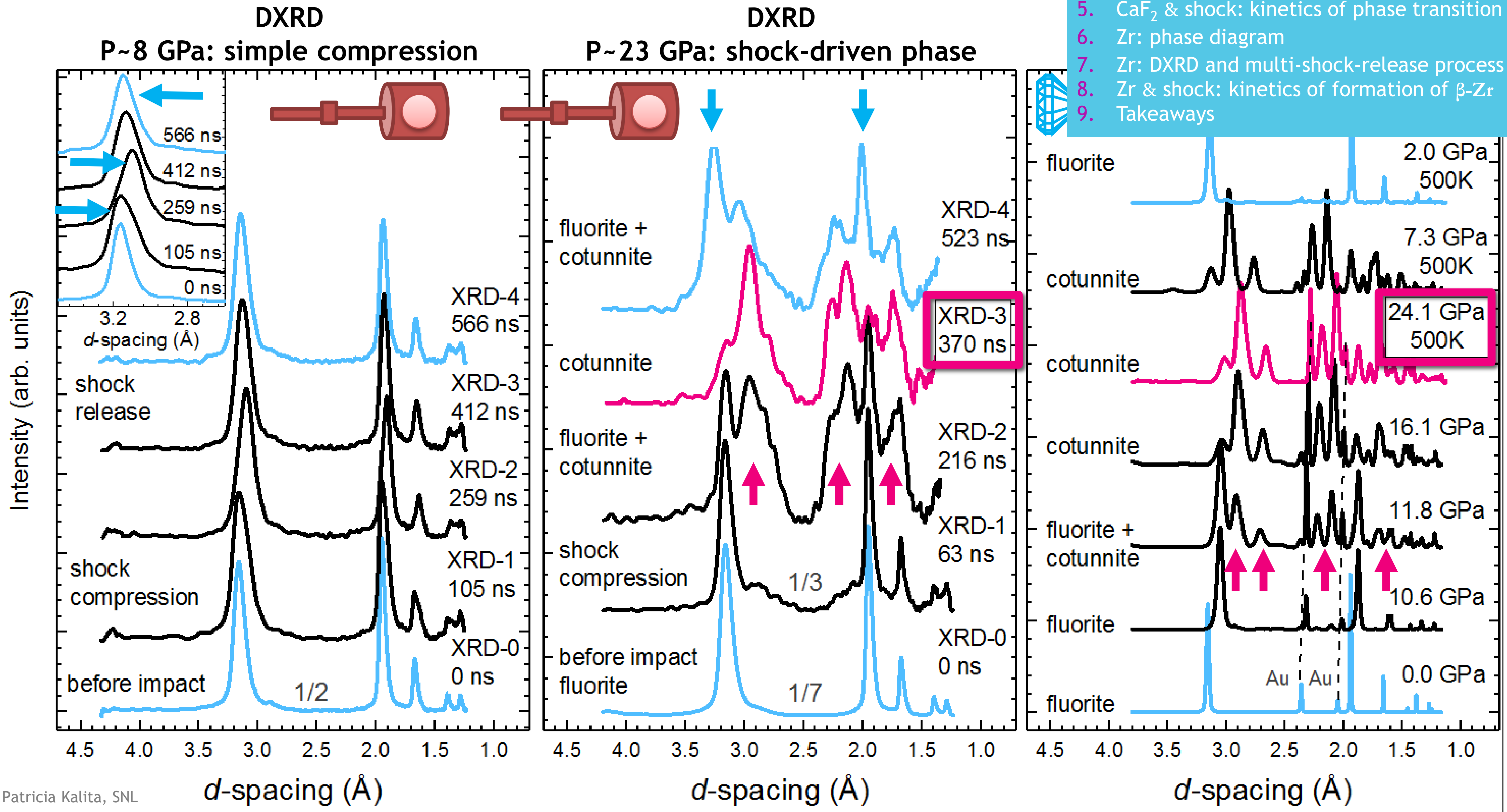


γ - cotunnite



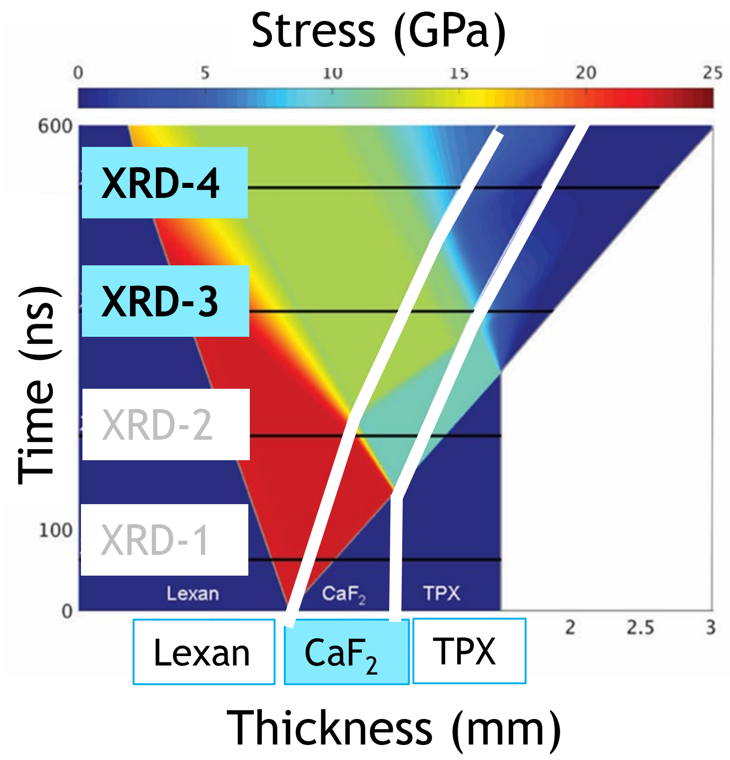
Errandonea, PRL 113, 235902 (2014)
Cazorla, PRL 113, 235902 (2014)
Dorfman et al., Phys. Rev. B 81, 174121 (2010)

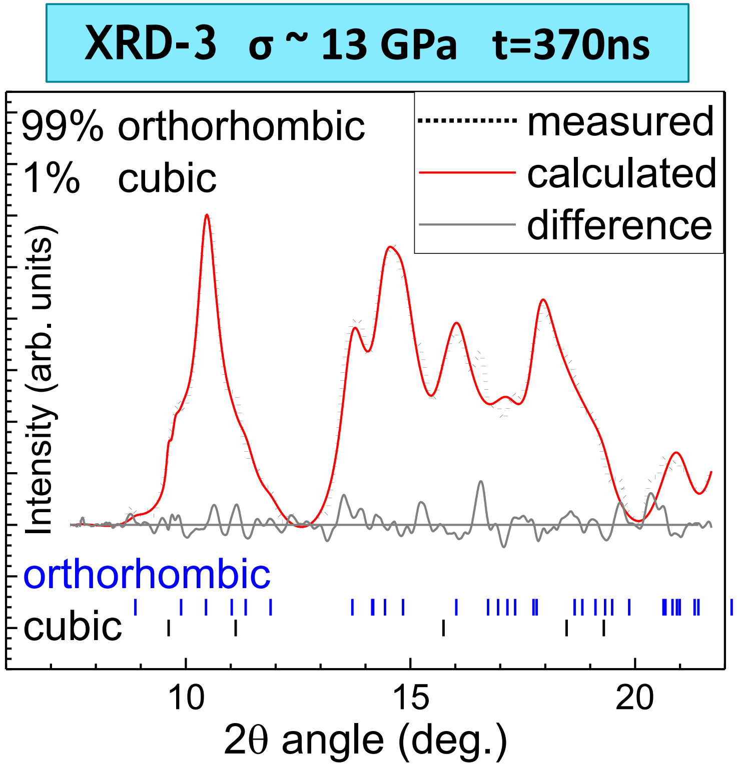
Shock-driven phase transition at atomic and nanosecond scales in CaF_2

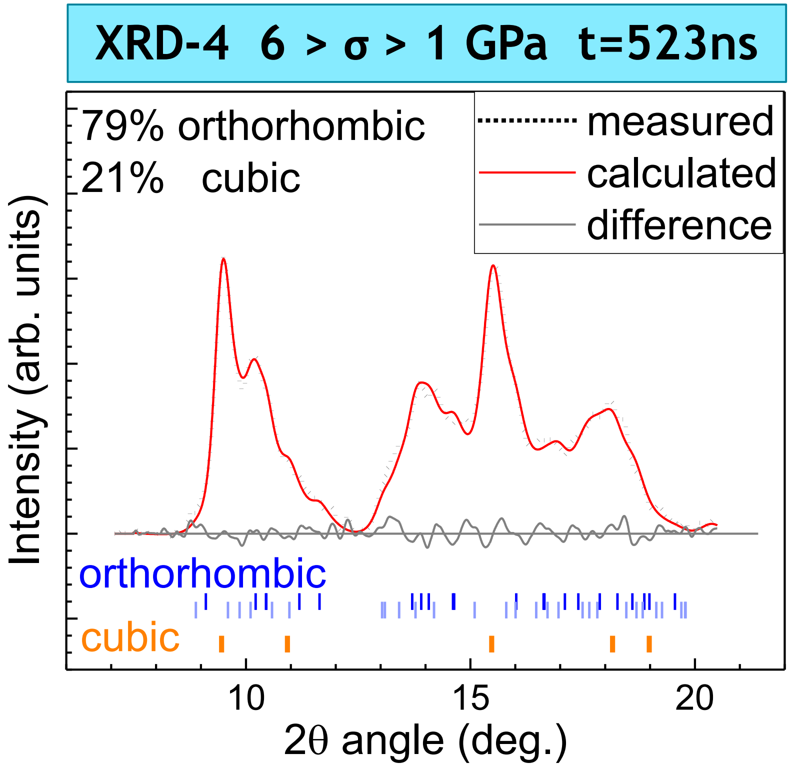


DXRD analysis

at late times > 140 ns material is subjected to distribution of pressures



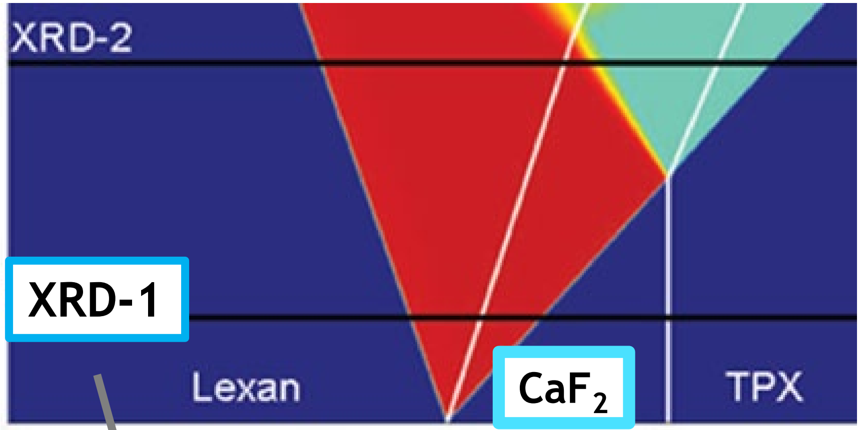


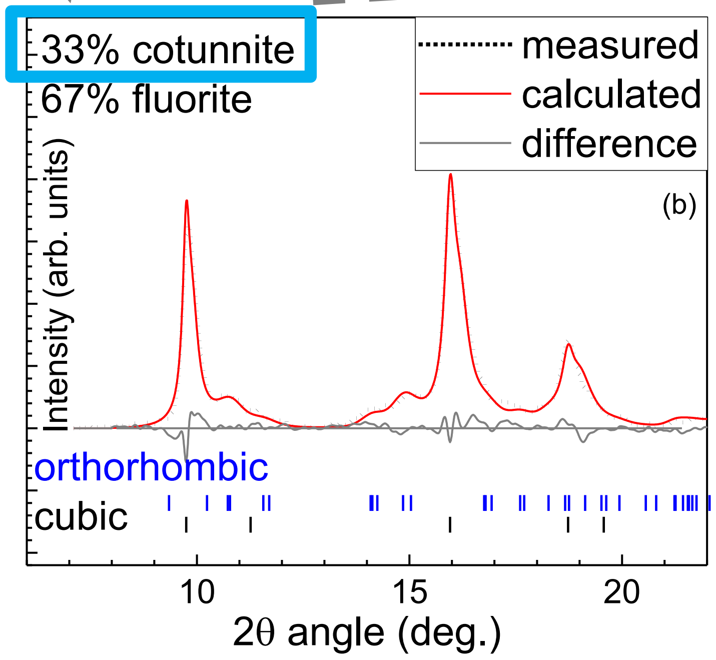


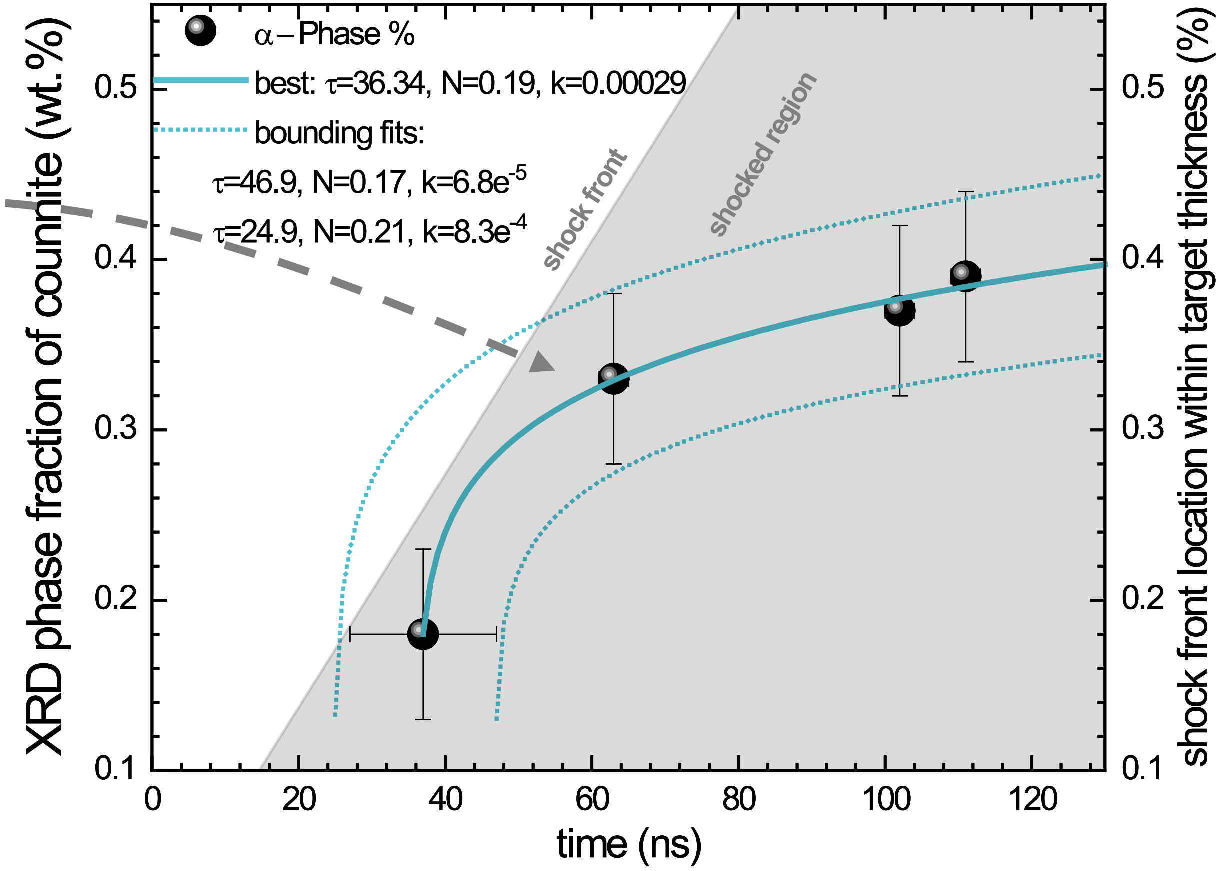
- complete phase transition fluorite → cotunnite

- reversible transition
- hysteresis on stress release

Quantitative DXRD analysis: kinetics of shock-driven phase transition







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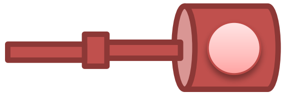
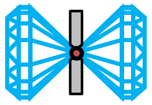
1. DXRD & Shock compression at APS – ANL 
2. XRD & Static compression at APS – ANL 

Phase transition kinetics in a simple ionic solid:

3. CaF_2 structures and phase diagram
4. Real-time DXRD probe of a simple shock event in CaF_2
5. Kinetics of formation of tetragonal CaF_2 under shock compression

Phase transition kinetics in a metal:

6. Zirconium structures and phase diagram
7. Real-time DXRD probe of a multi-shock-release process in Zr
8. Kinetics of formation of β-Zirconium under shock compression

Multiple shock-and-release experiment in Zr

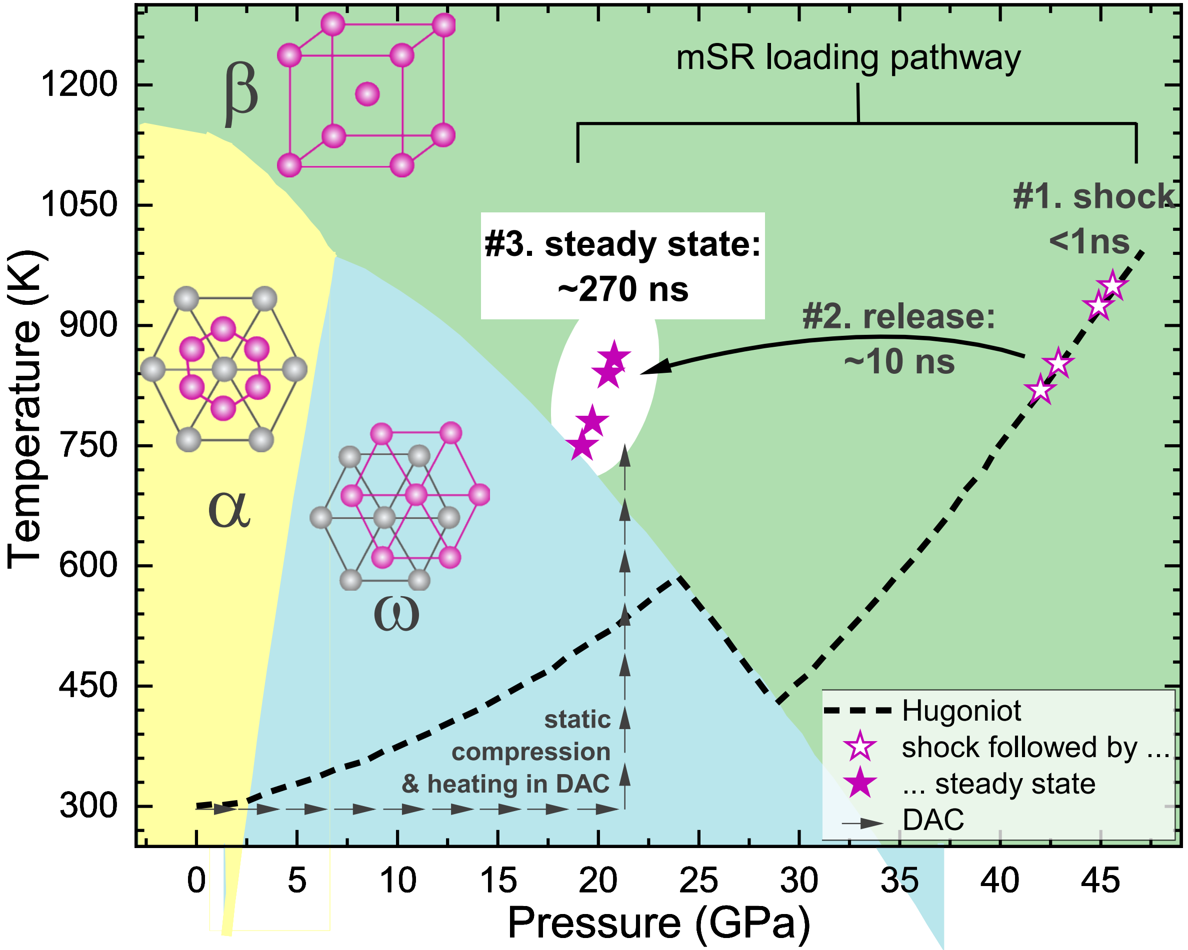
- Bridgman discovered the ω phase in 1952 [1]
- a lot of studies on α (hcp) → ω (hexagonal)
- ω (hexagonal) → β (cubic) transition discovered in 1990 [2]
- β phase is less studied

this work:

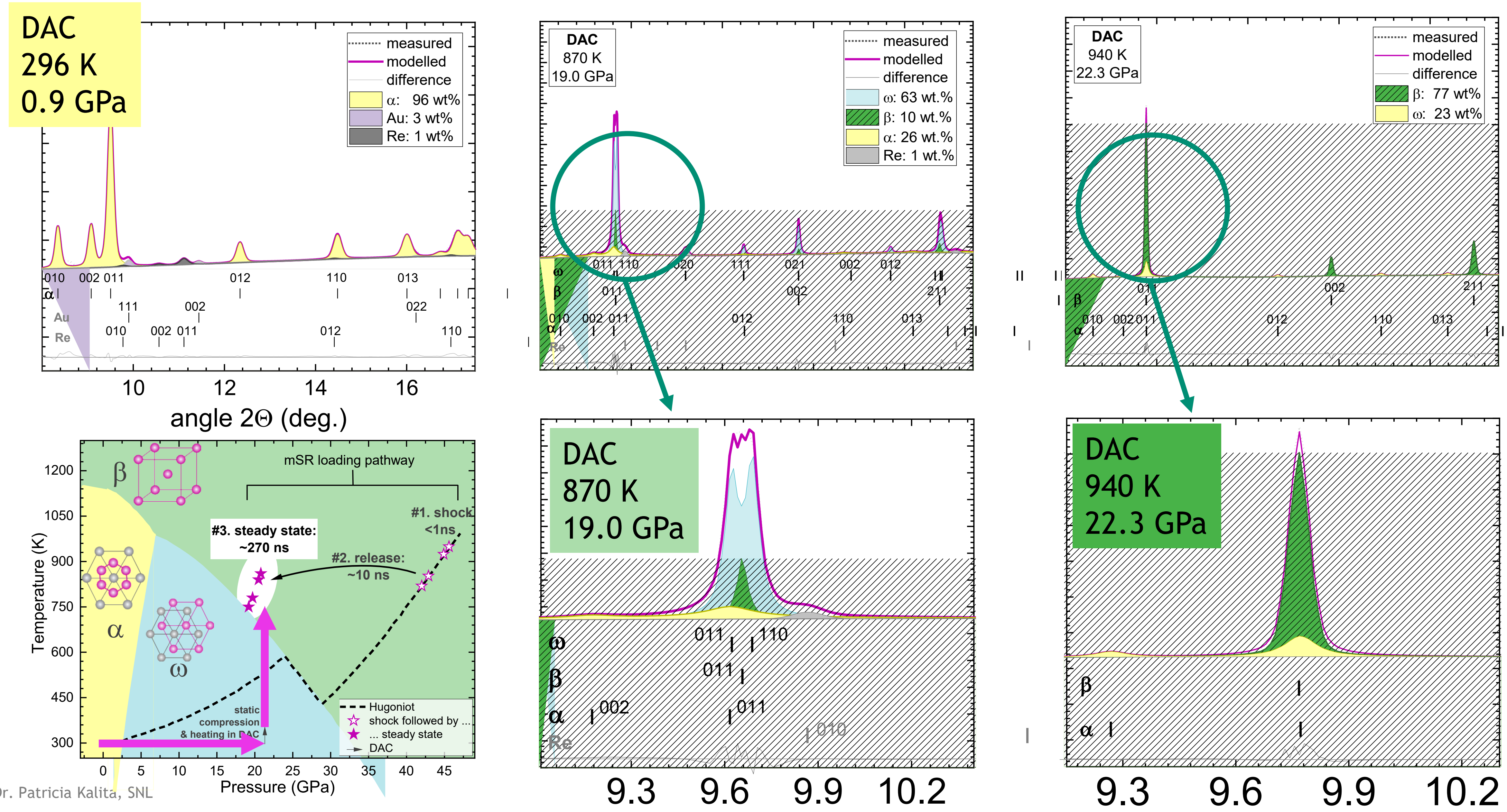
→ quantify the kinetics of formation of the β-Zr phase under shock compression

[1] P. W. Bridgman, PNAAS 81, 165 (1952).
[2] H. Xia, S. J. Duclos, A. L. Ruoff, and Y. K. Vohra, PRL 64, 204 (1990).

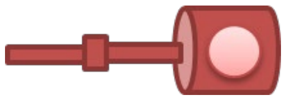
phase diagram after: C. W. Greeff, Modelling and Simulation in Materials Sci. & Engi. 13, 1015 (2005).

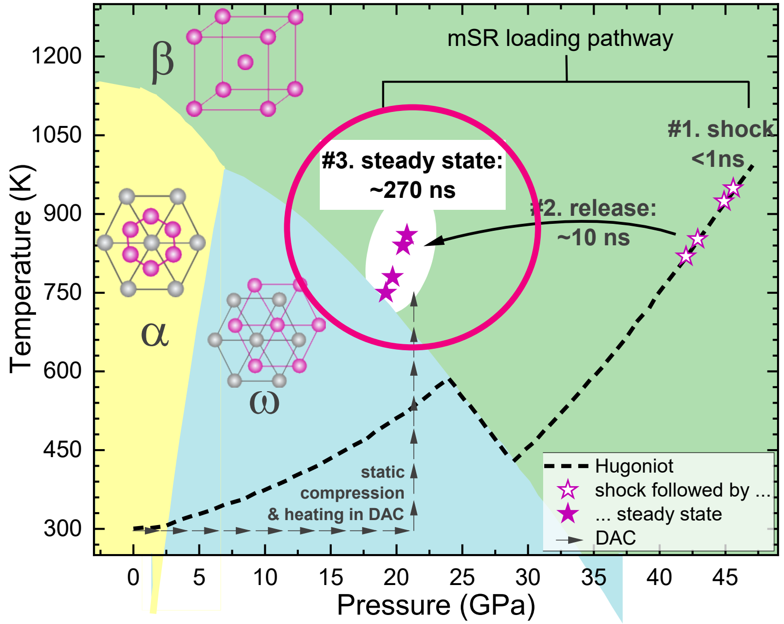


Zr: Static Compression XRD in DAC at high T



Zr: multi shock-release process: DXRD at nanosecond scale



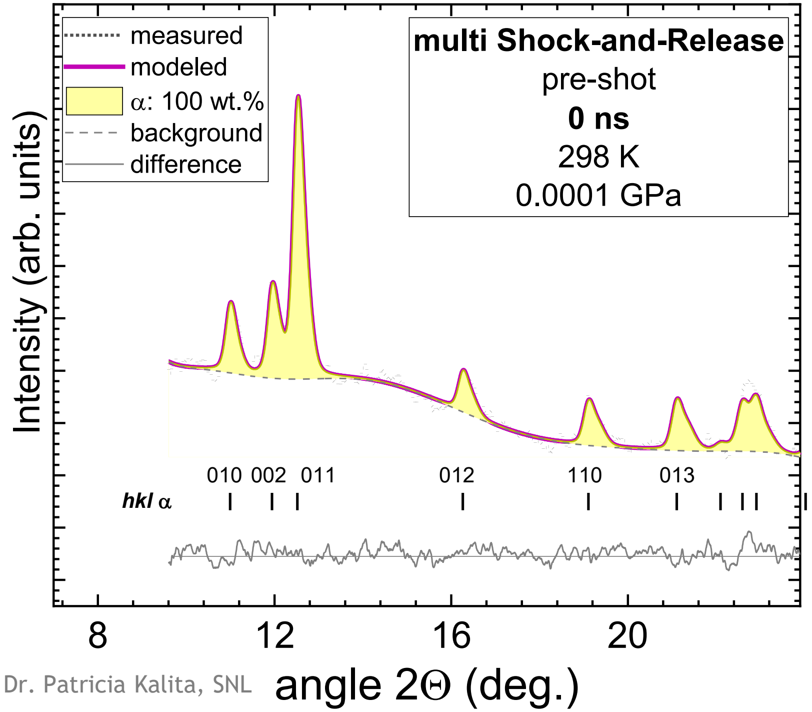


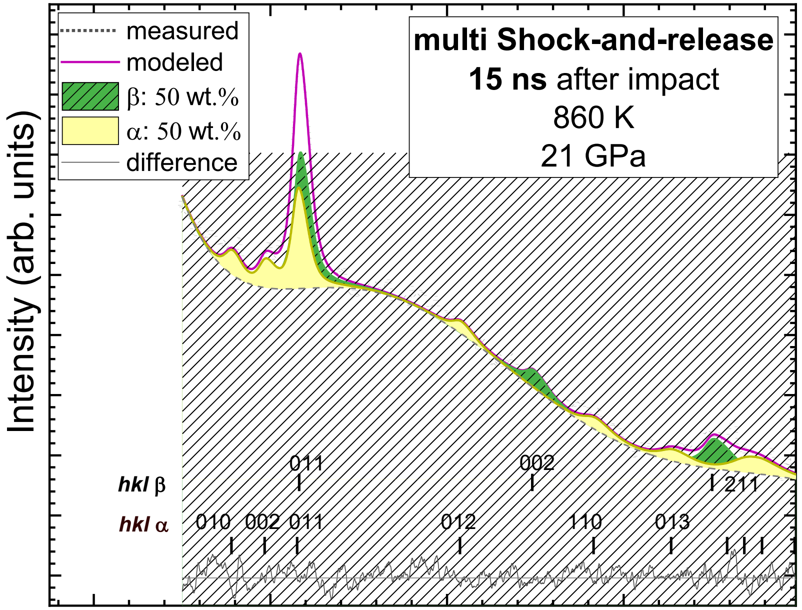
times with respect to impact

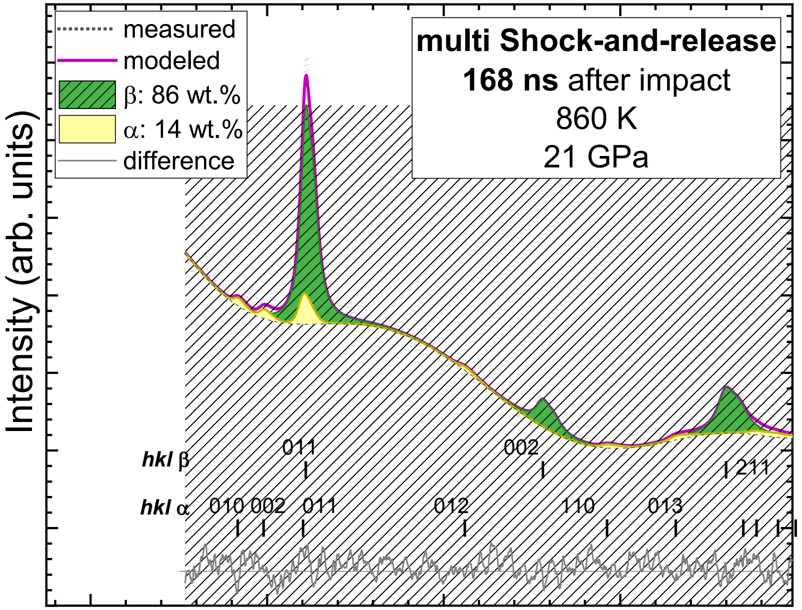
0 ns

15 ns

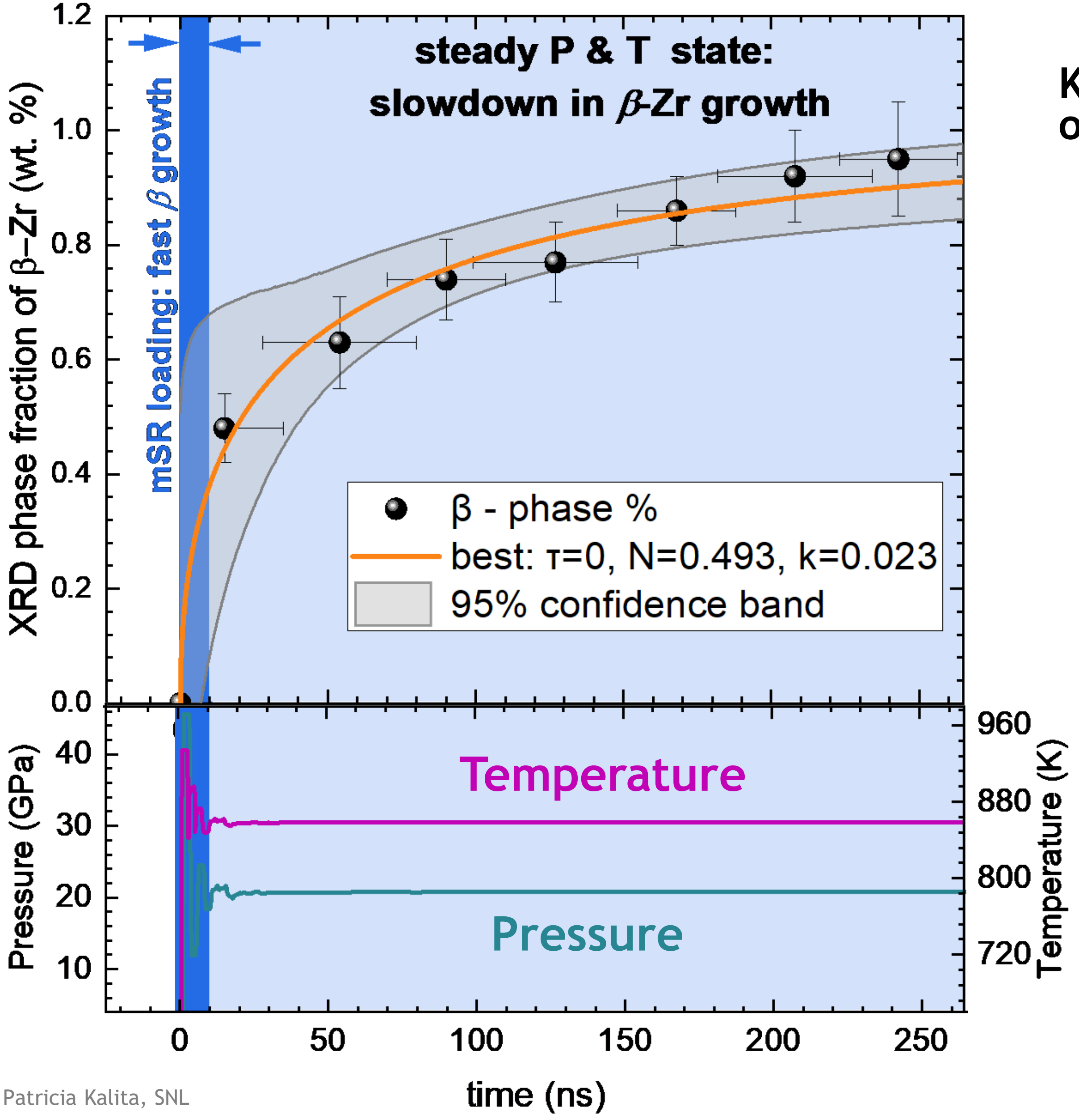
168 ns







Quantifying the kinetics of β-Zr under shock compression



KJMA Model of kinetics

- short incubation time τ~0 ns and ~250 ns needed to complete the transition
- atomic displacement during transition requires tens of ns to complete the process

- the applicability of the KJMA formalism for describing of polymorphic transitions under shock compression must be approached carefully, since it was developed for transformations between isotropic phases with a small volume jump and a zero shear modulus.

$$\beta(t) = 1 - \exp(-(k(t-\tau))^N)$$

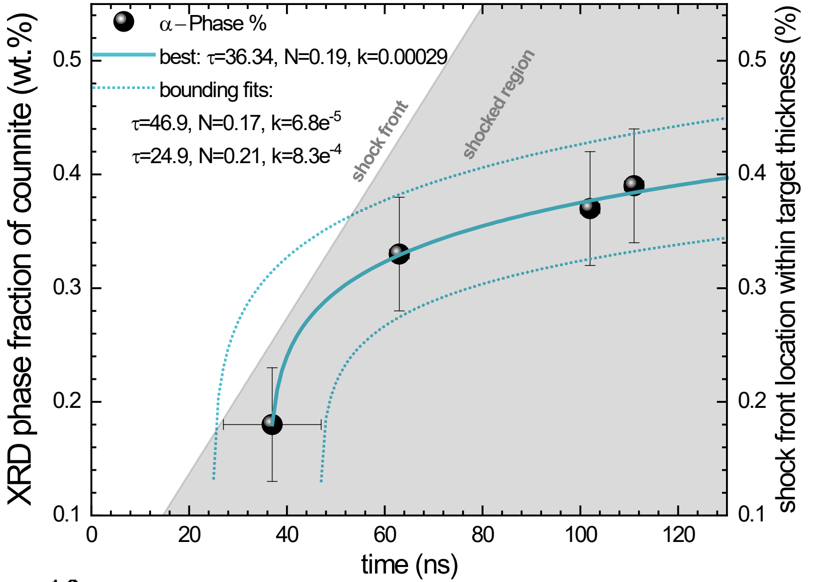
incubation time

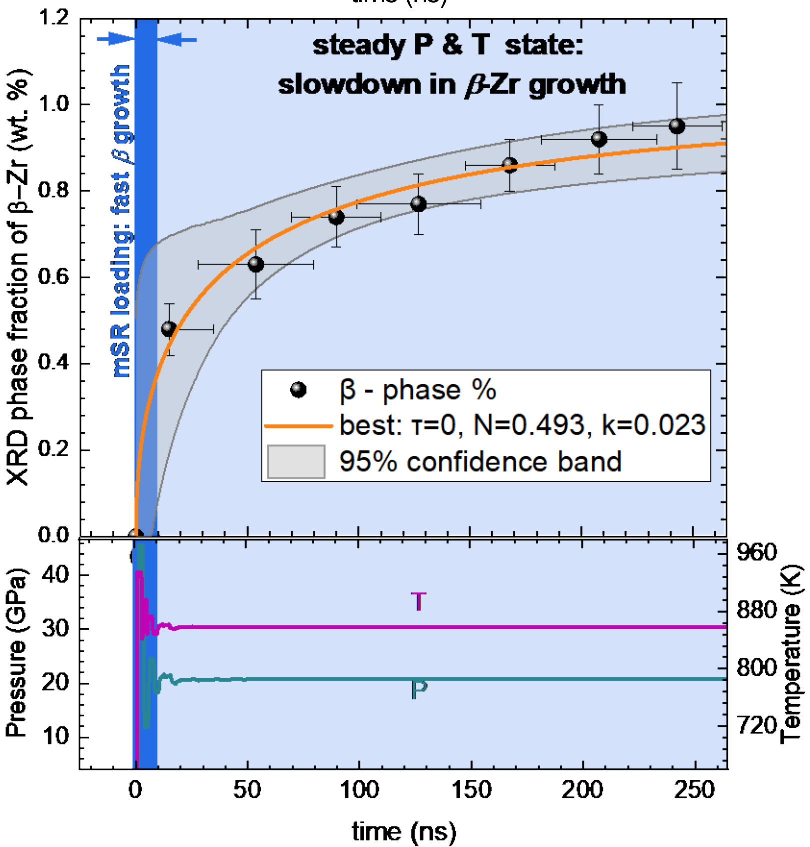
crystallization rate

Avrami parameter

Takeaways

- both projects show that we can use DXRD to follow the unfolding of phase transitions during different shock events
- both projects show that we can use quantitative analysis of DXRD patterns to put numbers on how fast a phase transition unfolds during a shock event
- first experimental evidence that, at tens of nanoseconds, **intermediate states are irrelevant in shock compression**: the **Hugoniot truly is a locus of end states**, which only depend on the initial state and the shock strength
- Outlook: there is a need to develop models of kinetics of phase transition specifically for shock processes
- Outlook: now we are able to use DXRD to generate atomic-scale time-resolved experimental data to validate such models





Acknowledgements!

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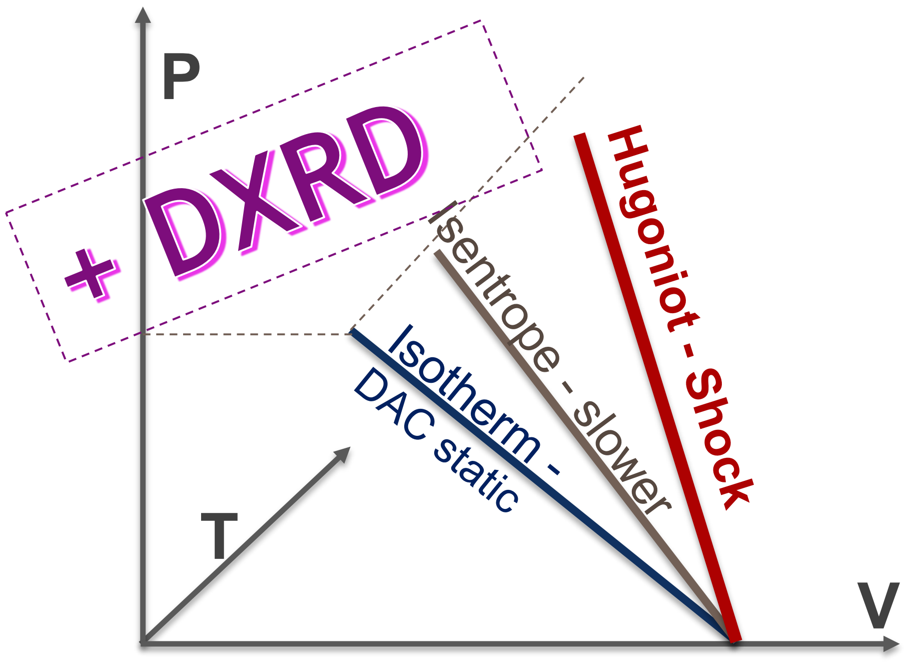
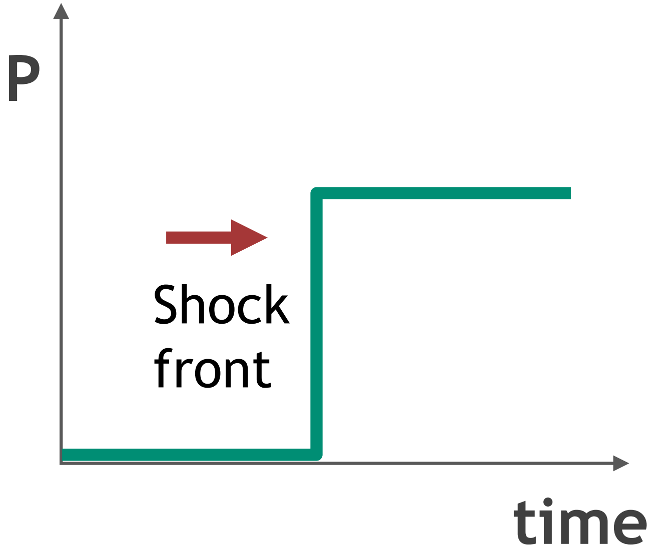
- Portions of this work were performed at the **Dynamic Compression Sector**, which is operated by Washington State University under the U.S. Department of Energy (DOE)/National Nuclear Security Administration Award No. DE-NA0002442.
- Portions of this work were performed at **HPCAT (Sector 16), Advanced Photon Source (APS),** Argonne National Laboratory. HPCAT operations are supported by DOE-NNSA's Office of Experimental Sciences. 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.
- P. Rigg, N. Sinclair, A. Schuman and the DCS team as well as E. Rod, C. Benson and the HPCAT team.
- **Sheri Payne of MSTS** and **Lena Pacheco, Nicole Cofer, Josh Usher, Keith Hodge** and **Randy Hickman** of SNL for invaluable assistance with preparing the experiments.
- **Carrie Blada** and **Dr. Marius Schollmeier** of SNL created the fabulous! rendering of the DXRD setup.

Dr. Patricia Kalita, SNL

1-D Shock Compression Wave

- Instantaneous discontinuity in **P**, **E**, **ρ**
- High strain rate
- Energy scattering
- Shear forces
- Puts energy into atoms and molecules
- Creates defects (increases entropy)





What do we get out?

- very high pressure thermodynamic P-v curve – Hugoniot EOS
- test of accuracy of molecular potentials over large compression

+ DXRD

- **with dynamic XRD, we get a microscopic insight into shock processes,**
- **We can quantify the kinetics of shock-driven phase transition at nanosecond scales**