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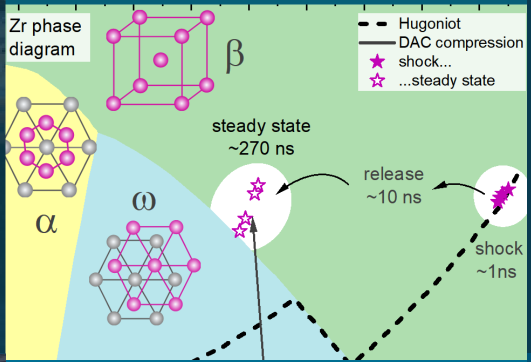
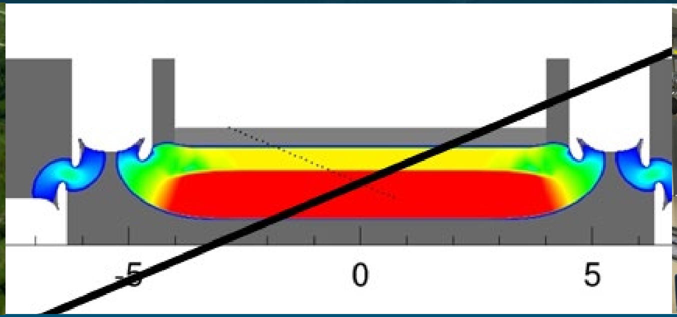
SAND2022-5055C

Off-Hugoniot shock compression of Zr probed at the microstructural and nanosecond scales with *in situ* XRD





PRESENTED BY

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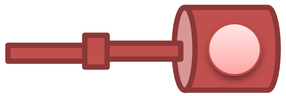
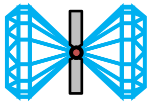
Outline

1. Zirconium structures and phase diagram
2. Shock and static compression at APS – ANL
3. Dynamic vs static XRD: gun vs. diamond anvil cell
4. Kinetics of formation of β-Zirconium



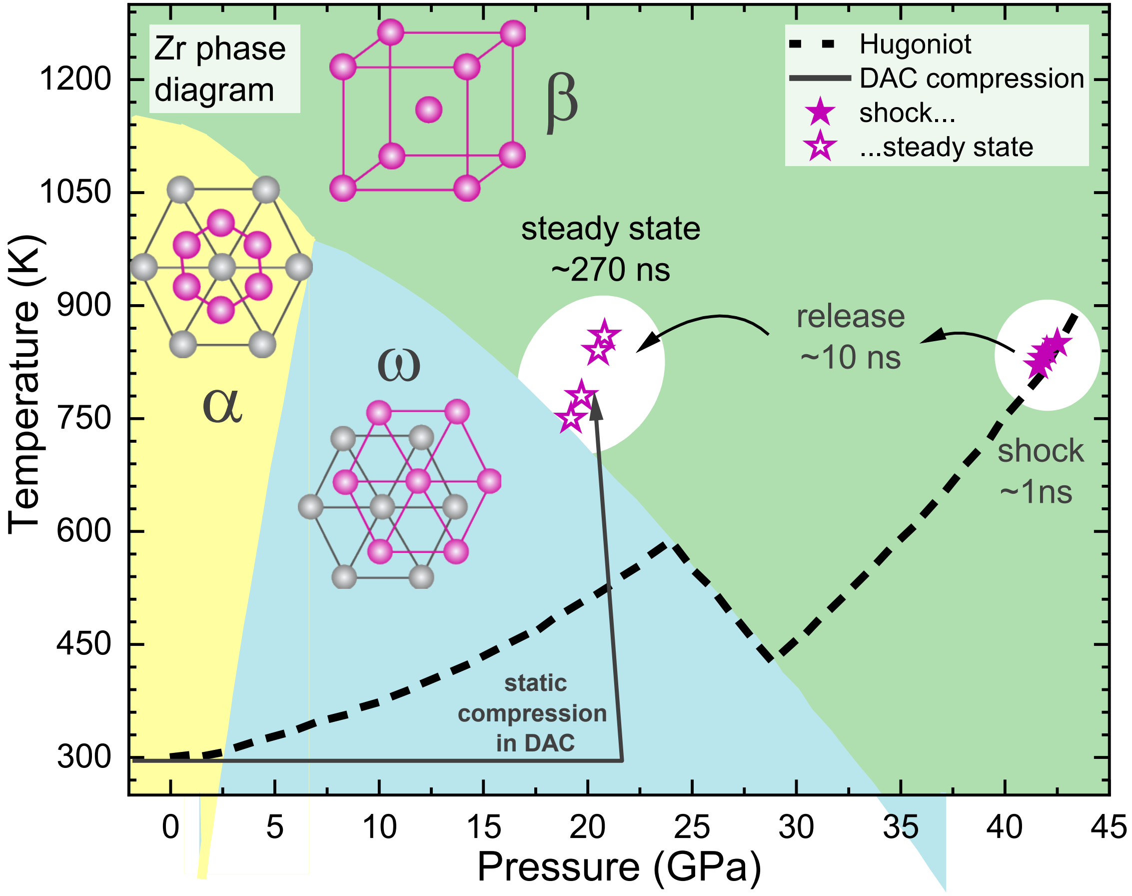


Shock-driven phase transition at atomic and nanosecond scales

- 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



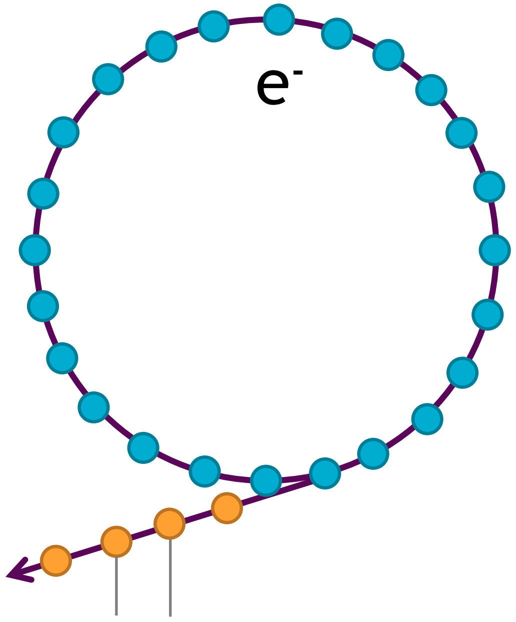
phase diagram after: C. W. Greeff, Modelling and Simulation in Materials Science and Engineering 13, 1015 (2005).

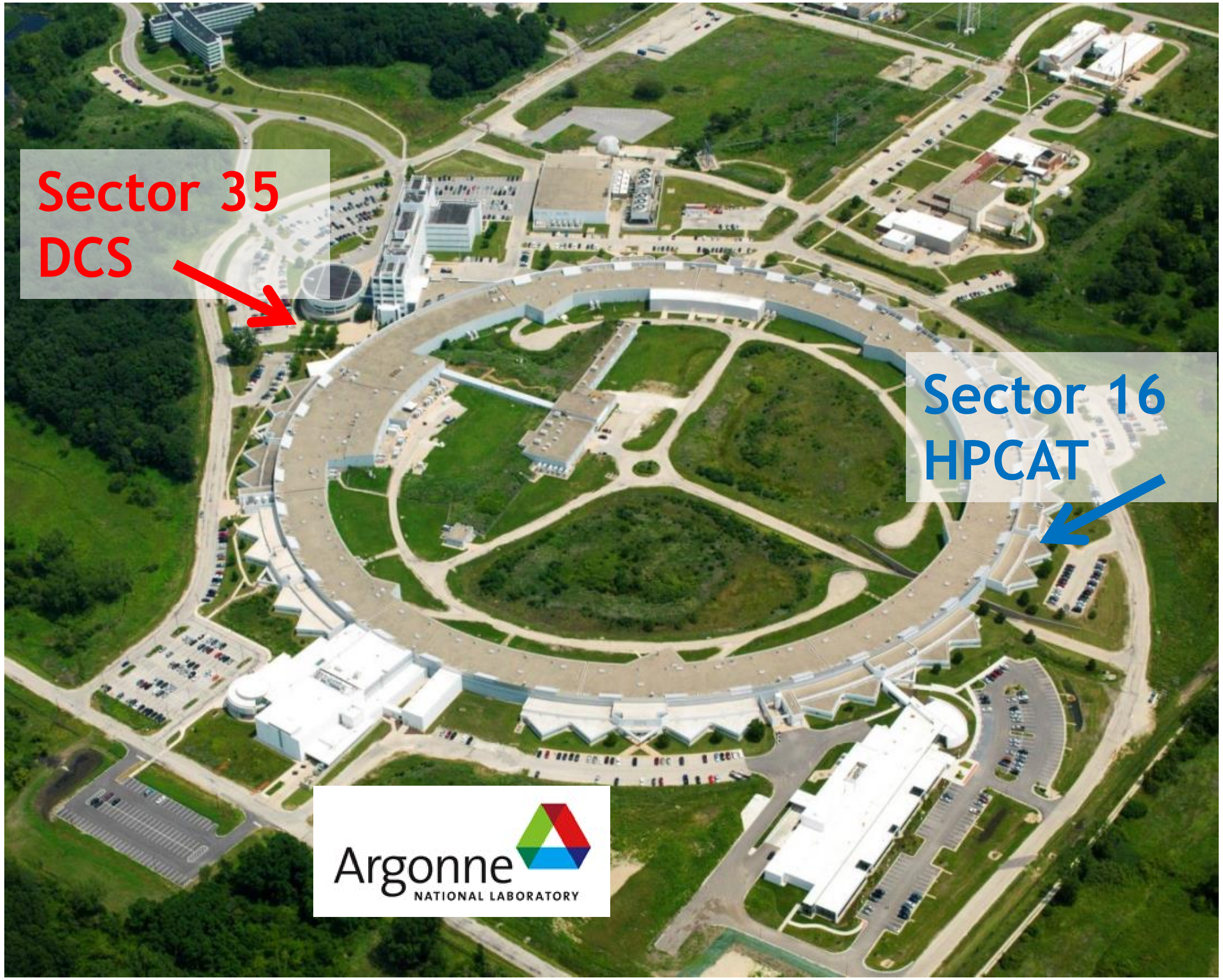
[1] P. W. Bridgman, PNAAS 81, 165 (1952).
[2] H. Xia, S. J. Duclos, A. L. Ruoff, and Y. K. Vohra, PRL 64, 204 (1990).

Advanced Photon Source, ANL

1. Zirconium structures and phase diagram
2. shock and static compression at APS – ANL
3. dynamic vs static XRD
4. kinetics of formation of β-Zirconium

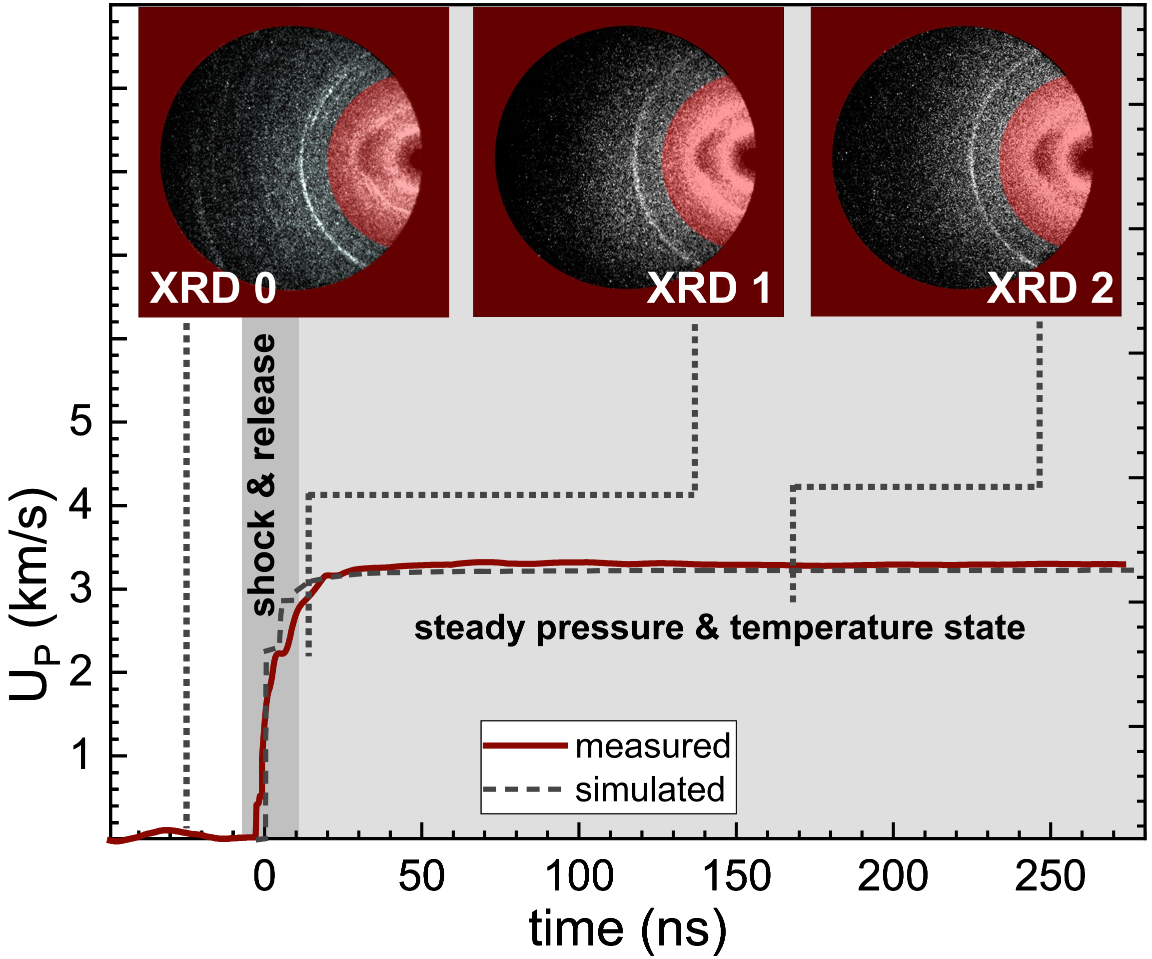
- 3[rd] generation synchrotron source
- 1,104m = 3,622 ft.
- X-rays ON 24h/day
- 6 days/week





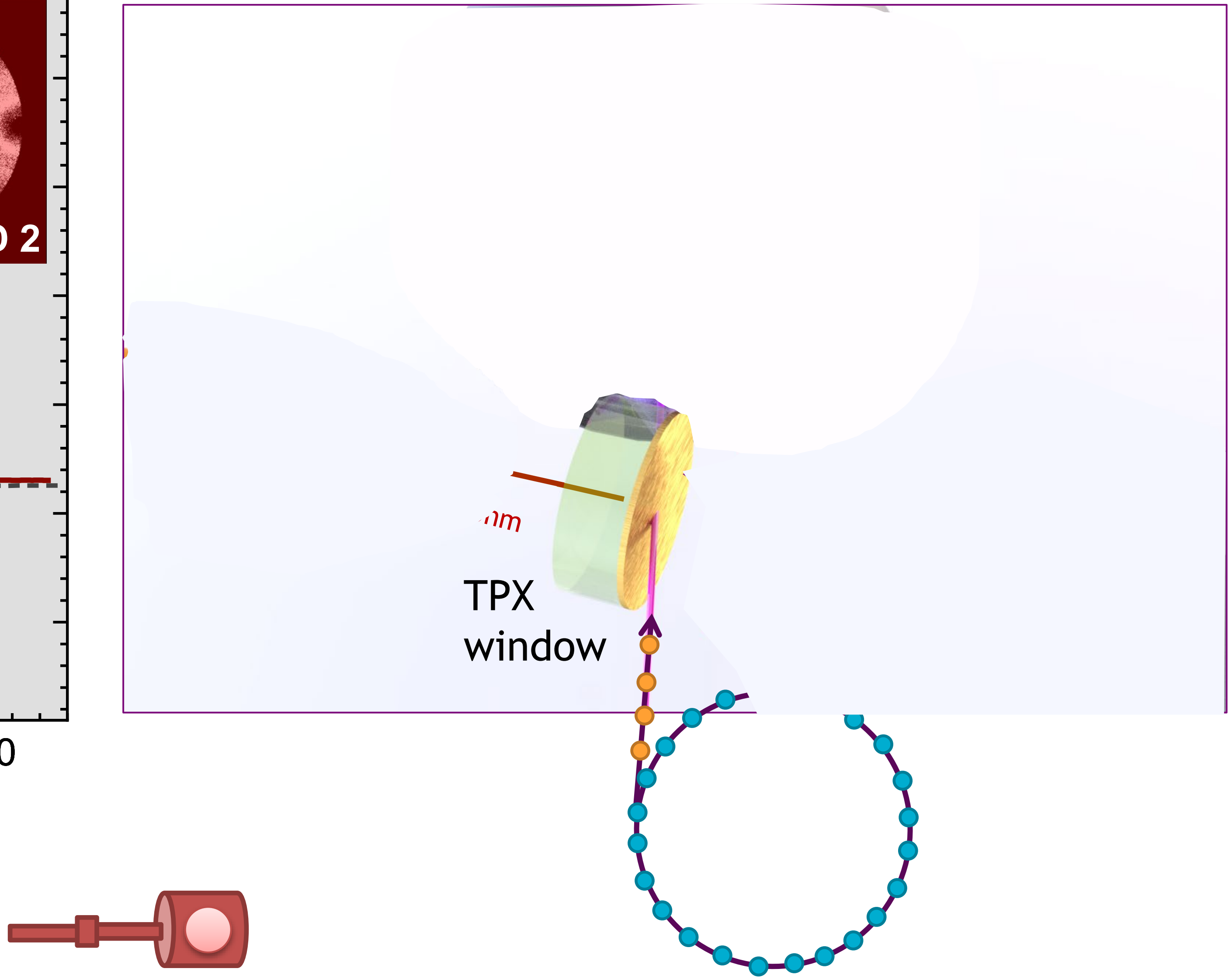
Advanced Photon Source Image Bank (aps.anl.gov)

Dynamic XRD setup: a shock experiment with an extended steady-state

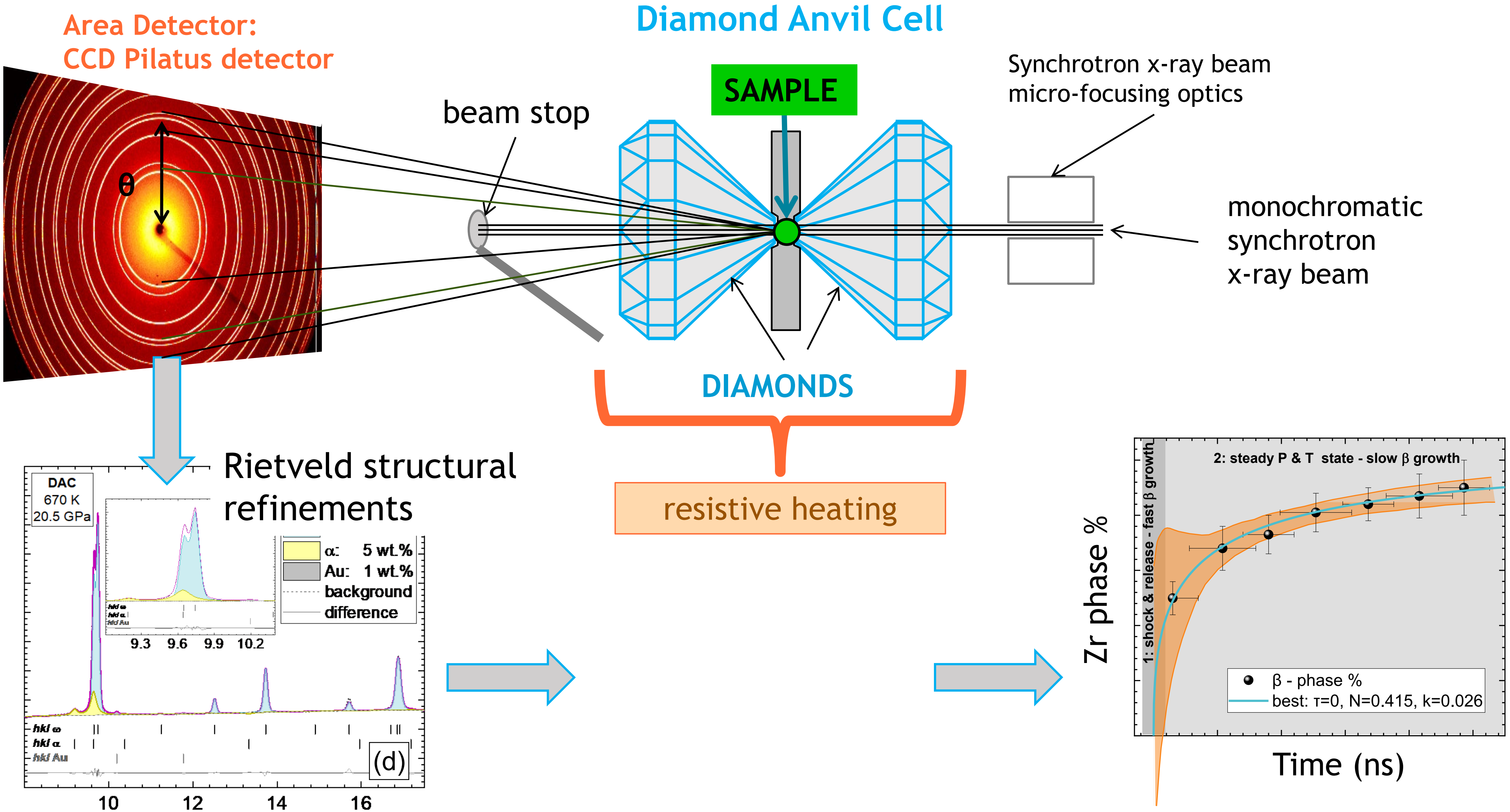


PDV velocimetry

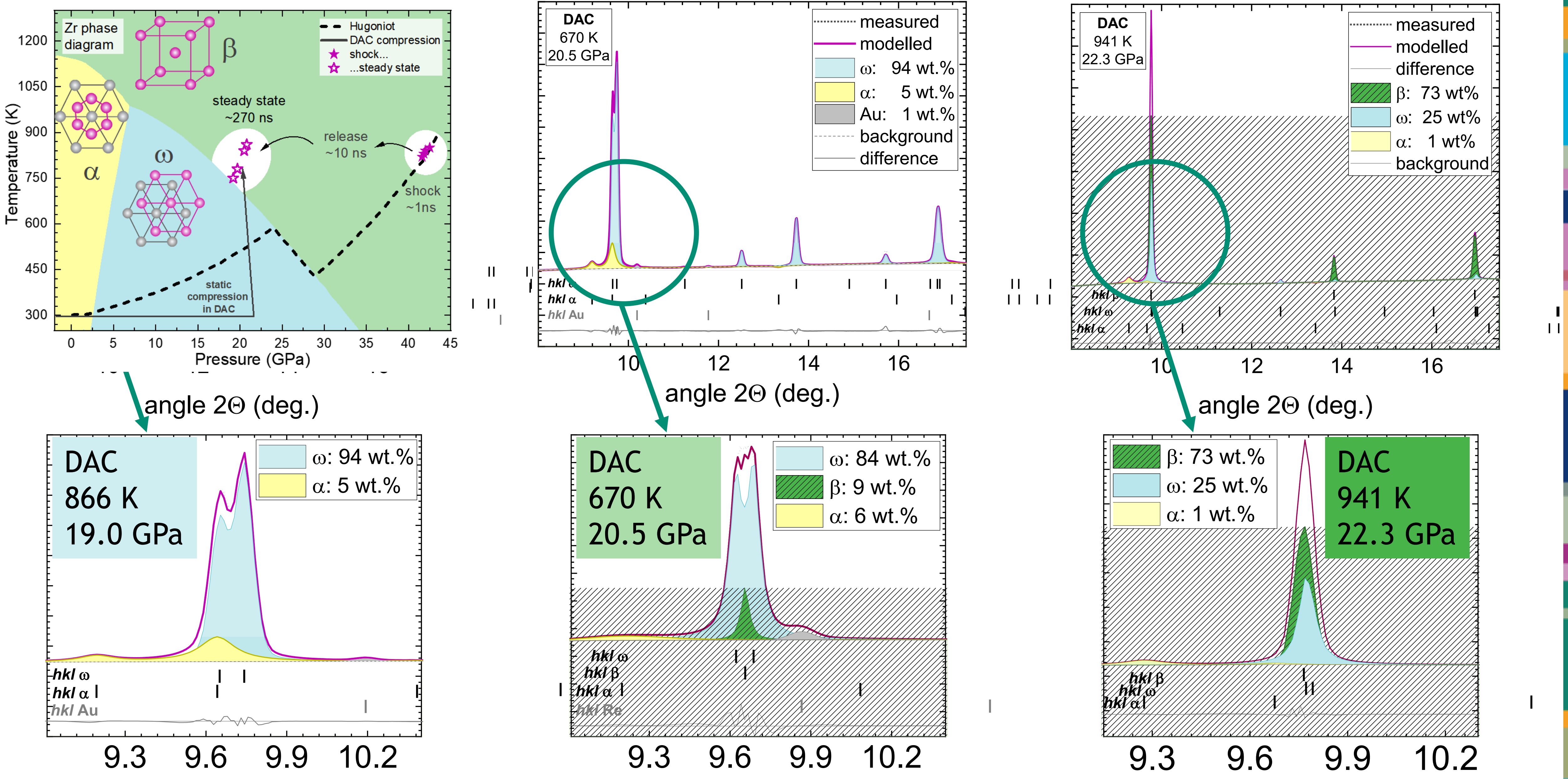
Dynamic XRD setup at DCS, APS, ANL



DAC compression diagram



Static Compression XRD in DAC at high T



Shock compression: dynamic XRD at nanosecond scale

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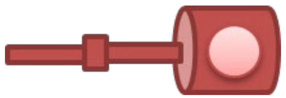
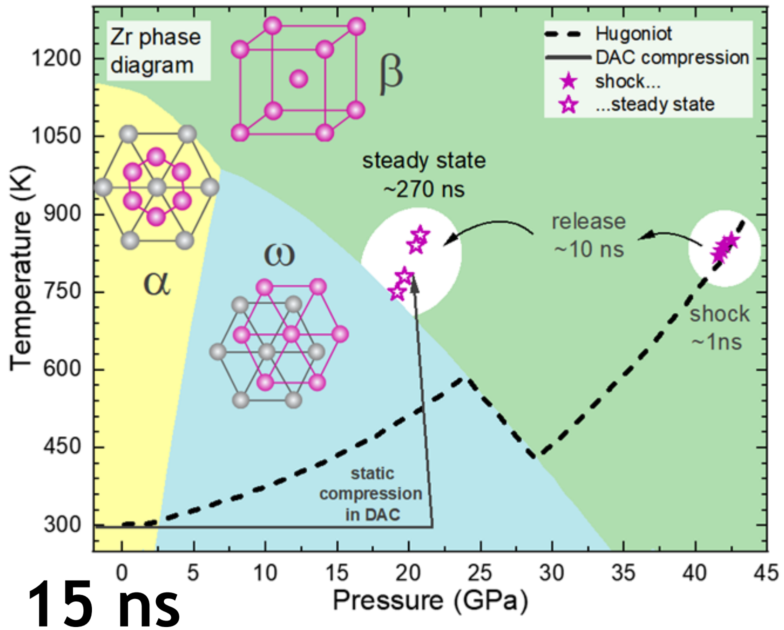
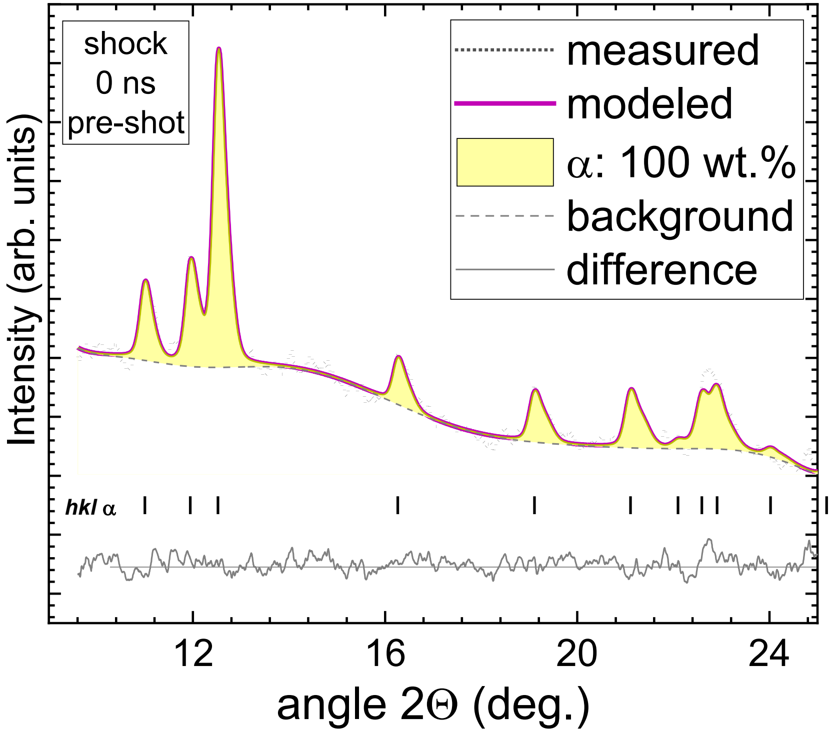


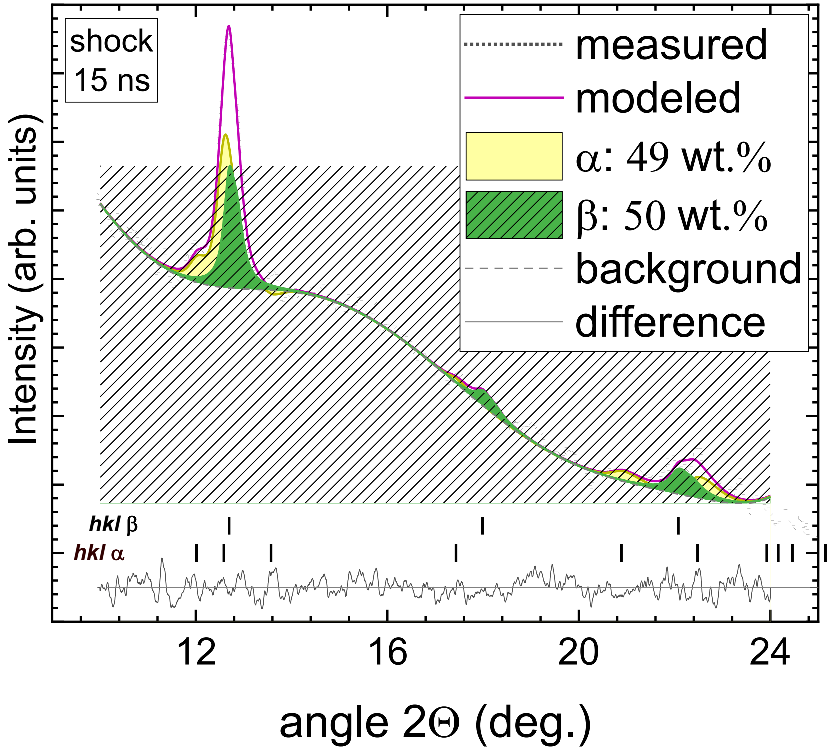


times are with respect to impact

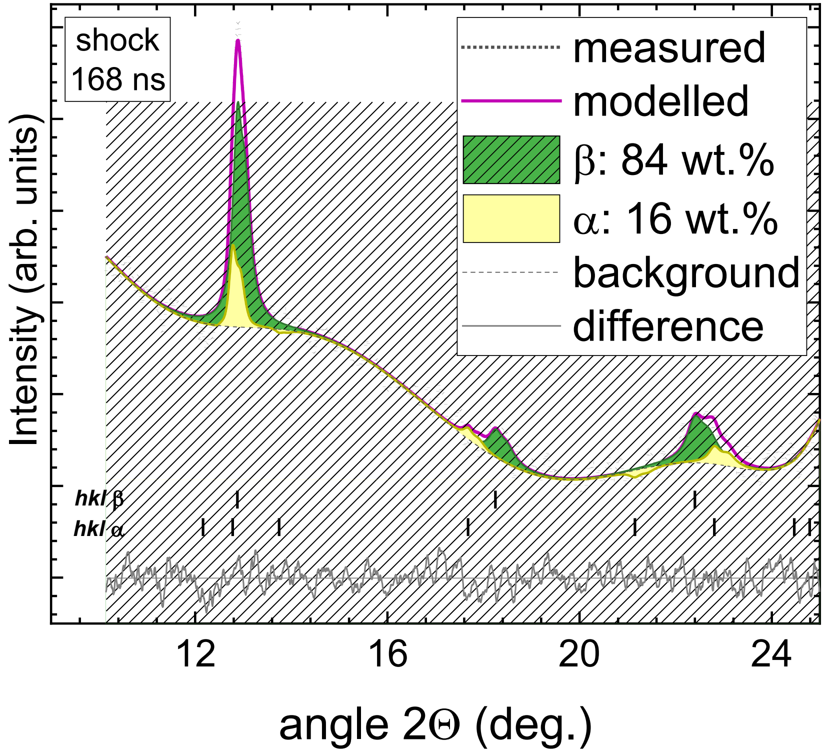
0 ns



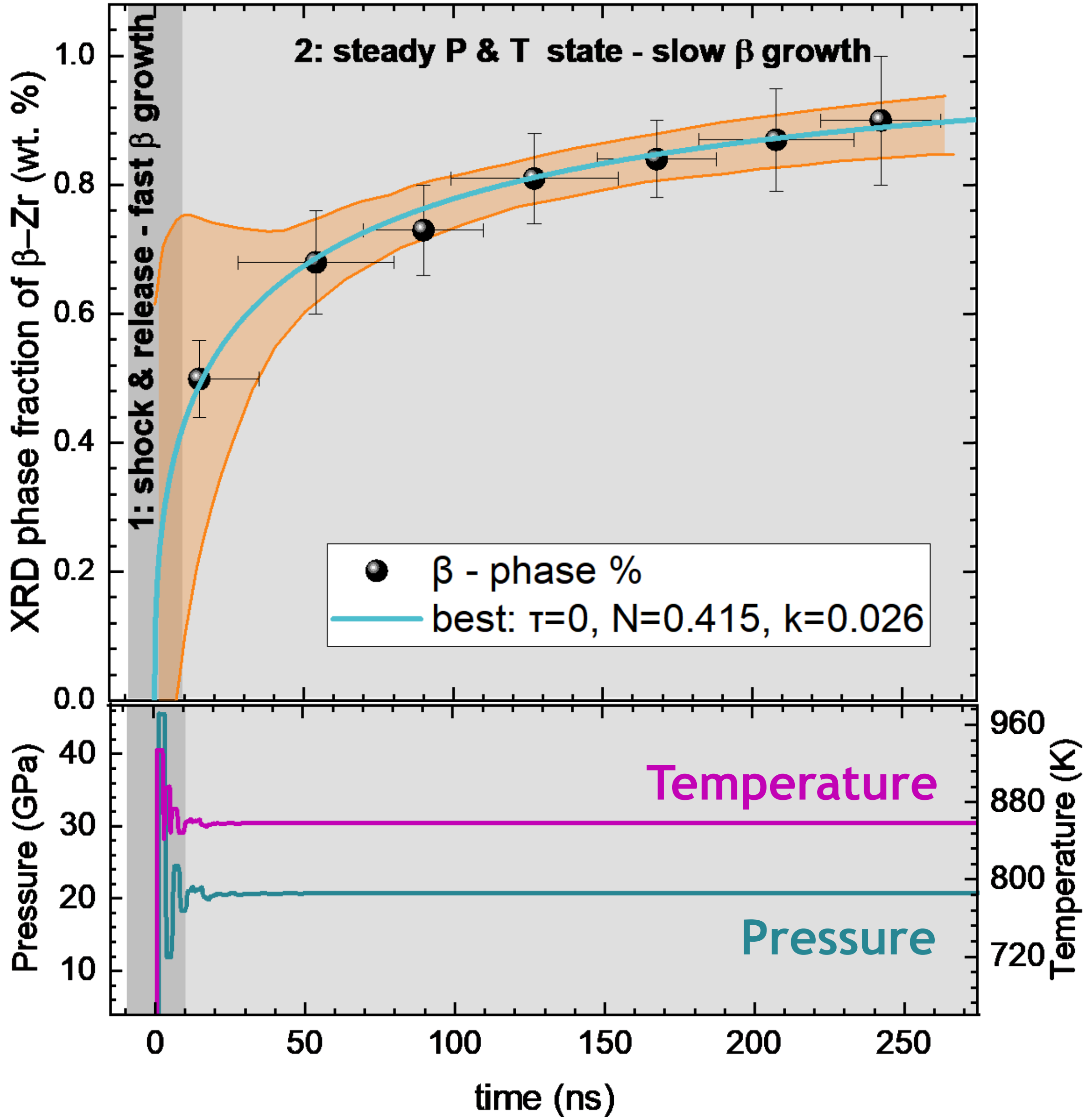
15 ns



168 ns



Kinetics of β-Zr under shock



- short incubation time τ~0 ns and ~250 ns needed to complete the transition are consistent with a first-order martensitic kinetics pathway
- atomic displacement during transition requires tens of ns to complete the process
- N < 1: heterogeneous nucleation and simultaneous diffusion-controlled crystallization
- our N = 0.415: heterogeneous distribution of nucleation sites and a distribution of grain sizes, where transformation begins on the surface of grains

KJMA Model of kinetics

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

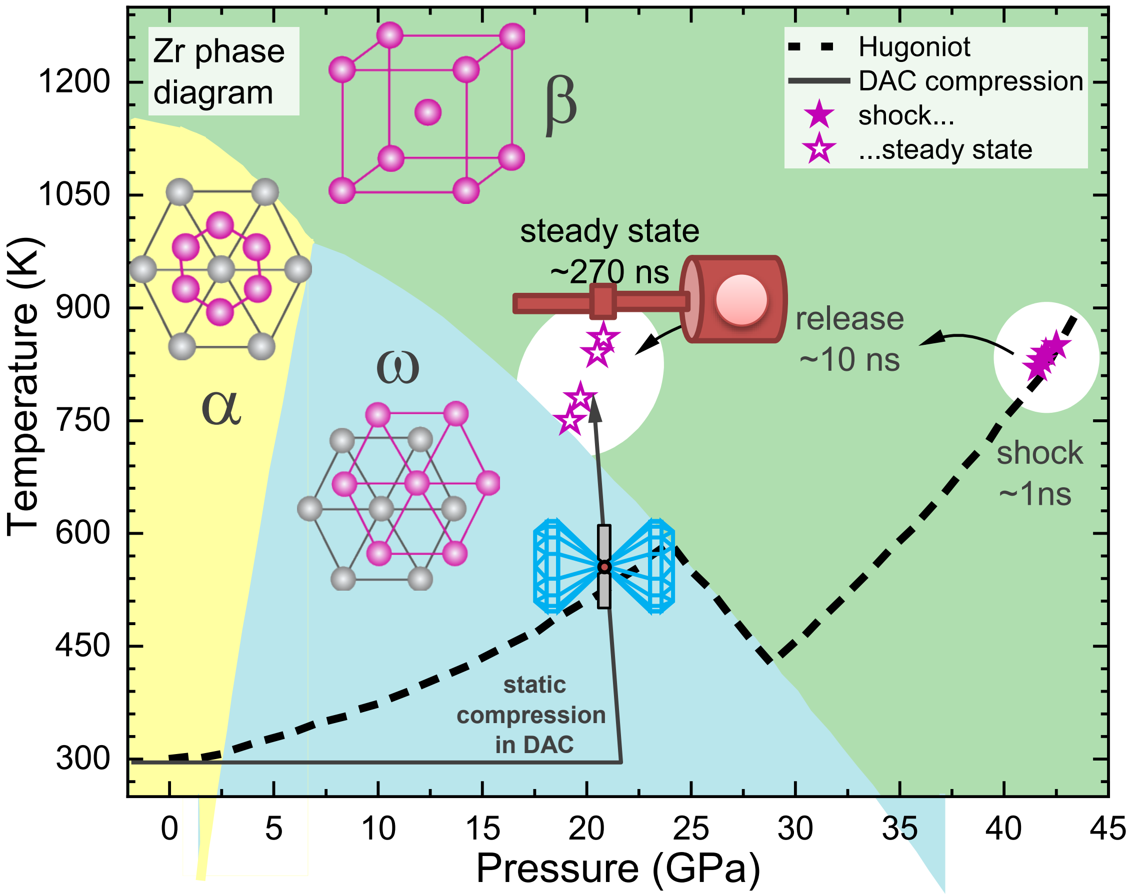
incubation time (τ)

crystallization rate (k)

Avrami parameter (N)

Summary - takeaway

- **dynamic compression of Zr**: first-order, martensitic phase transition to β, skipping the ω phase
- **static compression of Zr:** path to the same thermodynamic end-state, but the α + ω + β phase sequence is a direct reflection of the thermodynamic pathway
- the shocked end state β -Zr is not aware of the existence of any intermediate ω-Zr state nor does it need to pass through ω-Zr before transitioning to the β -Zr phase.
- 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



Acknowledgements!

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- 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.
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- **Carrie Blada** and **Dr. Marius Schollmeier** of SNL created the fabulous! rendering of the DXRD setup.