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Shock Induced Phase Transitions in a High Entropy Rare Earth Sesquioxide, $(La_{0.2}Y_{0.2}Ce_{0.2}Pr_{0.2}Sm_{0.2})_2O_3$

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2023 APS Shock Compression of Condensed Materials
Q05: Mechanisms of Solid-Solid Phase Transformation

Chicago, IL, June 21, 2023, 0935-0955

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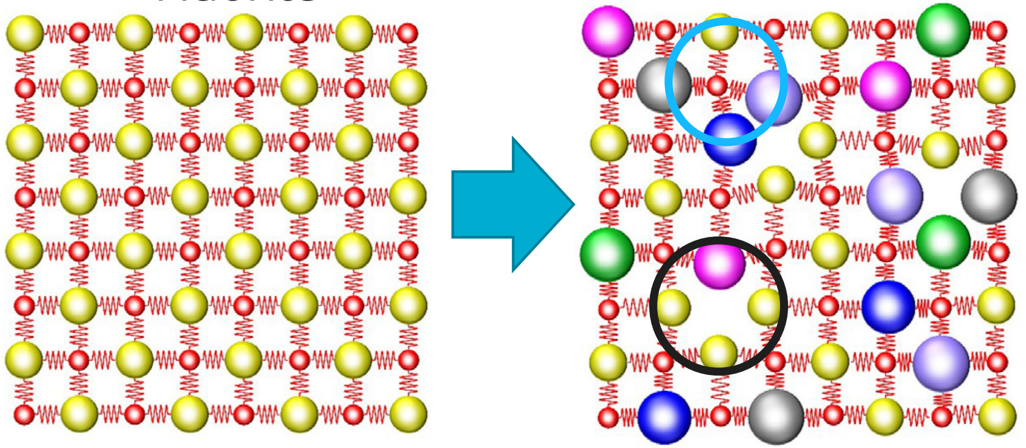
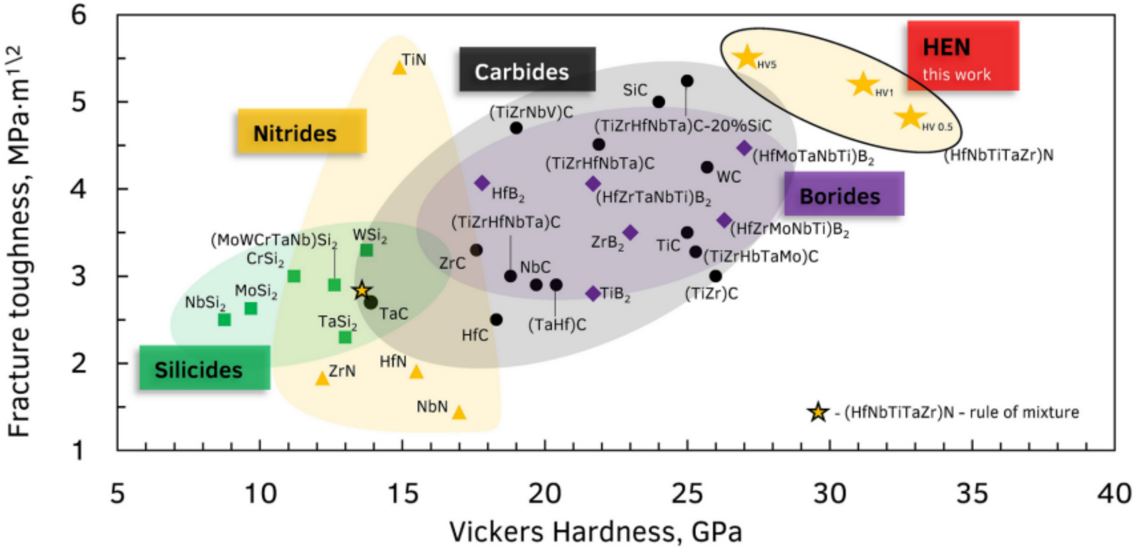
Why are high entropy oxides (HEOs) of interest?

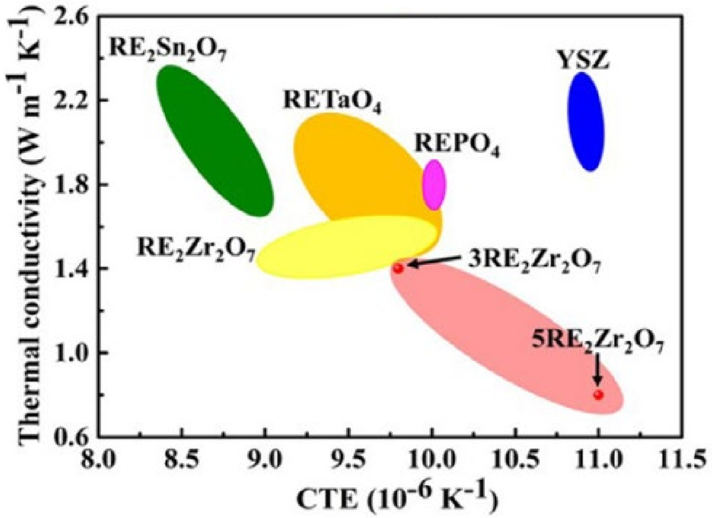
- ≥ 5 cation oxide = high entropy → short range lattice disorder
- May demonstrate entopic stabilization[1] or stable solid solution
  - Metastable phases due to increased configurational entropy
- Property improvement greater than expected from a rule of mixtures approach
  - Improved fracture toughness and hardness[2]
  - Thermal expansion and conductivity[3,4]
  - Thermal barrier and ceramic armor applications

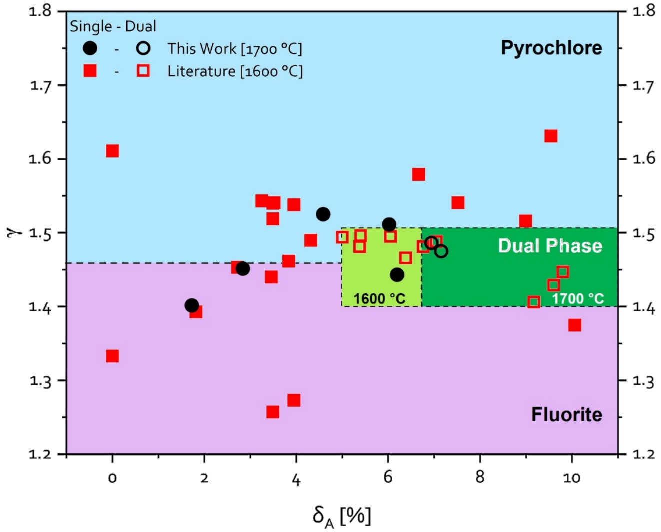
Fluorite

HEO Fluorite



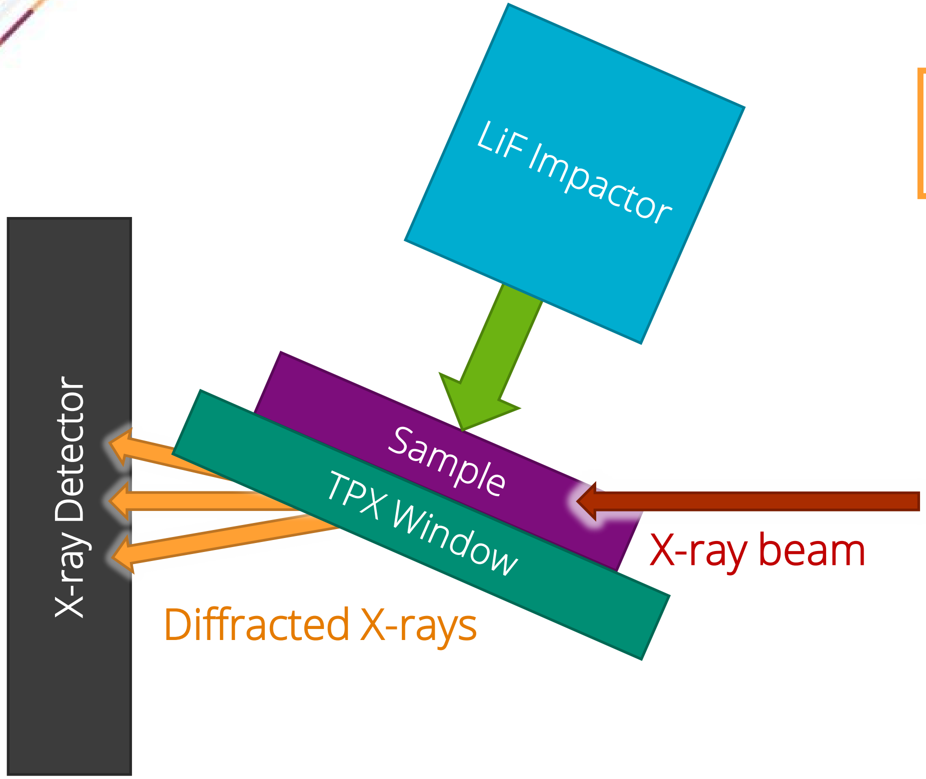






[1]C.M. Rost, Nature Comm. 6 (2015)
[2]D. Moskovskikh, Scientific Reports 10 (2020)
[3]K. Ren, Scripta Materialia 178 (2020)
[4]Lowry, JACerS (2023) *accepted*

Dynamic Compression with *In Situ* X-ray Diffraction (XRD)



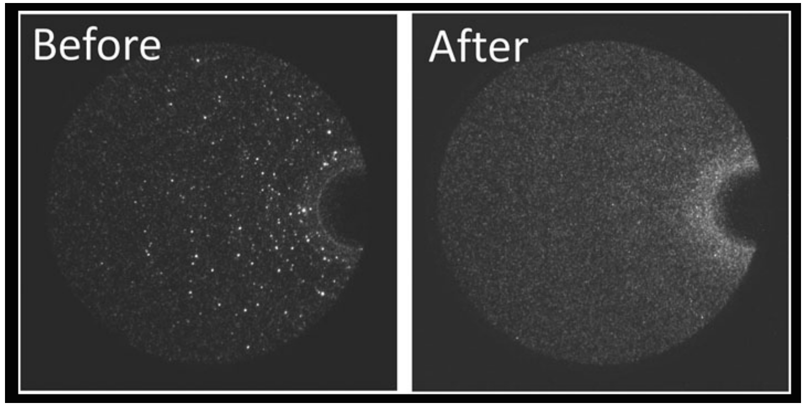
Investigate the effect of dynamic compression on the phase stability and transformations in a compositionally complex oxide

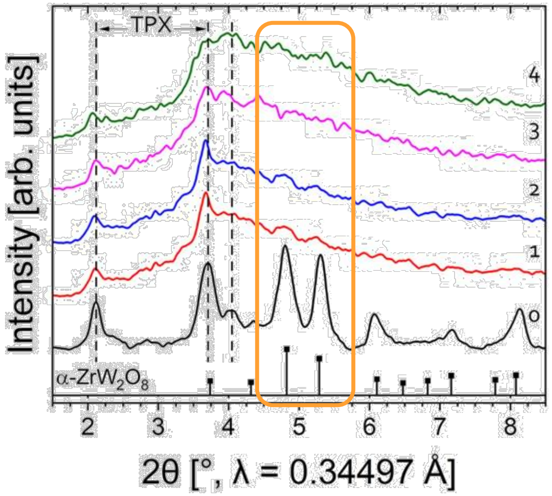
- Dynamic Compression Sector at Argonne National Laboratory – Advanced Photon Source
- Understand behavior of compression-driven phase transformations, their pathways, and kinetics

Pressure induced amorphization in $(La_{0.2}Y_{0.2}Ce_{0.2}Pr_{0.2}Sm_{0.2})_2O_3$ during hydrostatic loading[5]

- Four diffraction patterns acquired at ~153 ns intervals
- 2 Stage powder gun for impact velocities up to 6.8 km/s

Pressure Induced Amorphization of ZrW_2O_8 at 3 GPa[6]

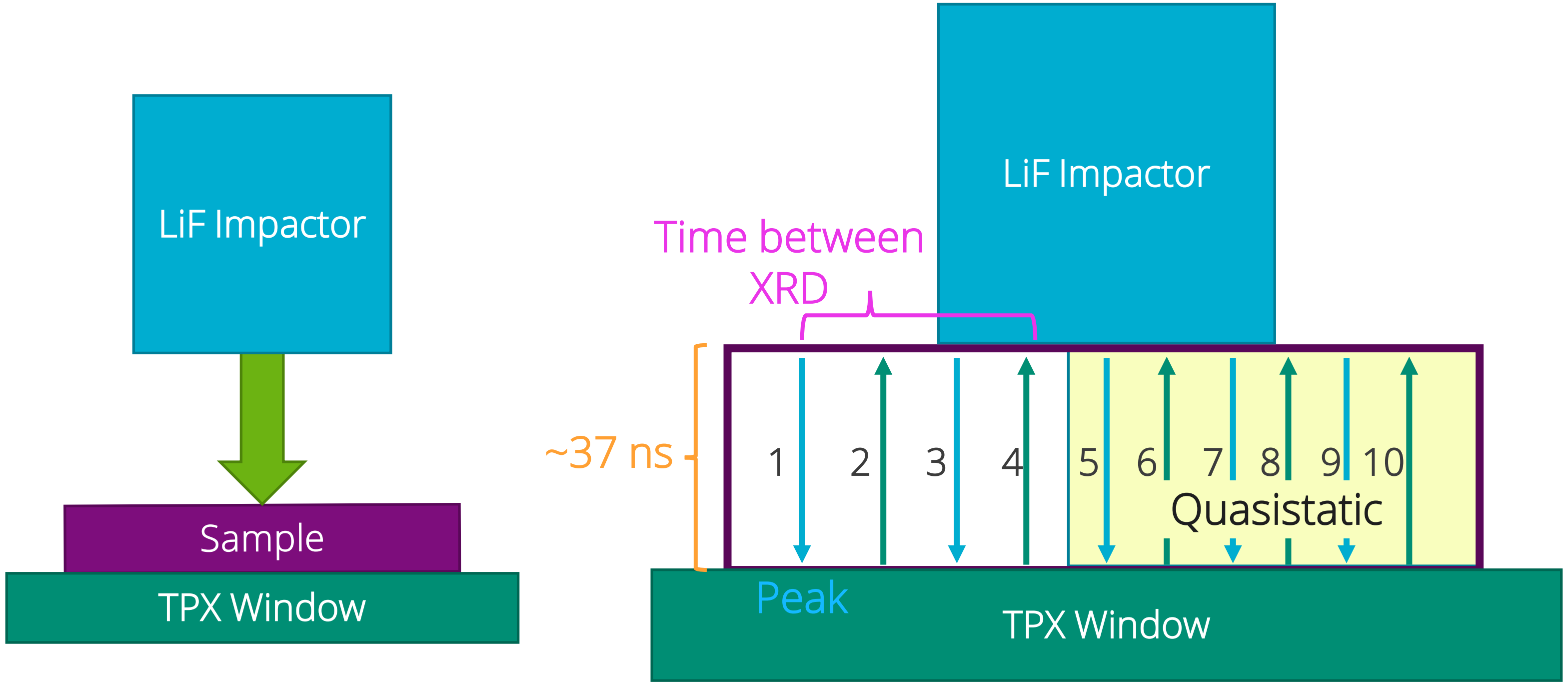


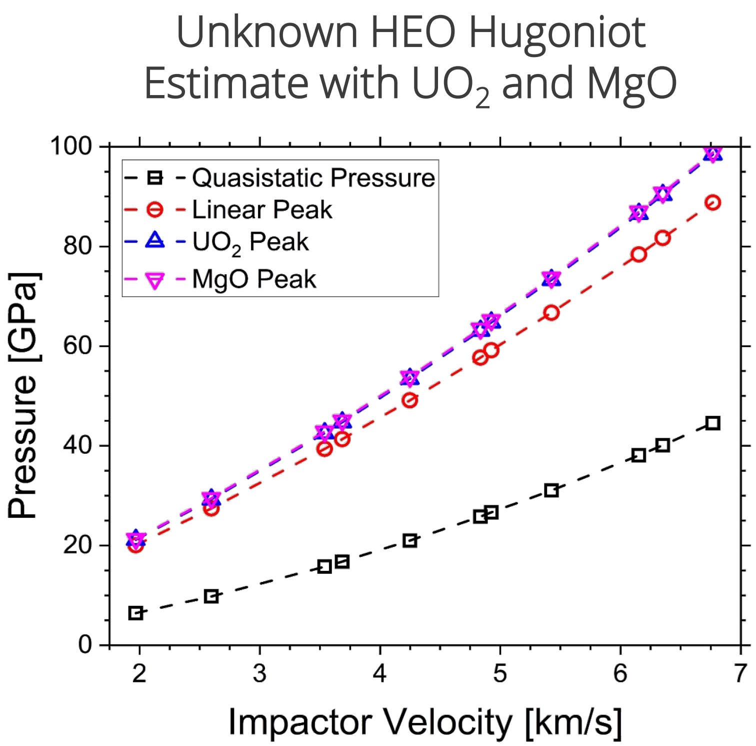


Impact on processing → Thermal Spray[7]

[5]B. Cheng, Comm. Chem. 2 (2019)
[6]S.R. Bishop, D.R.Lowry, AIP Advances (2023)
[7]S. Suresh, Acta Materialia (2020)

Determining pressure from impactor velocity

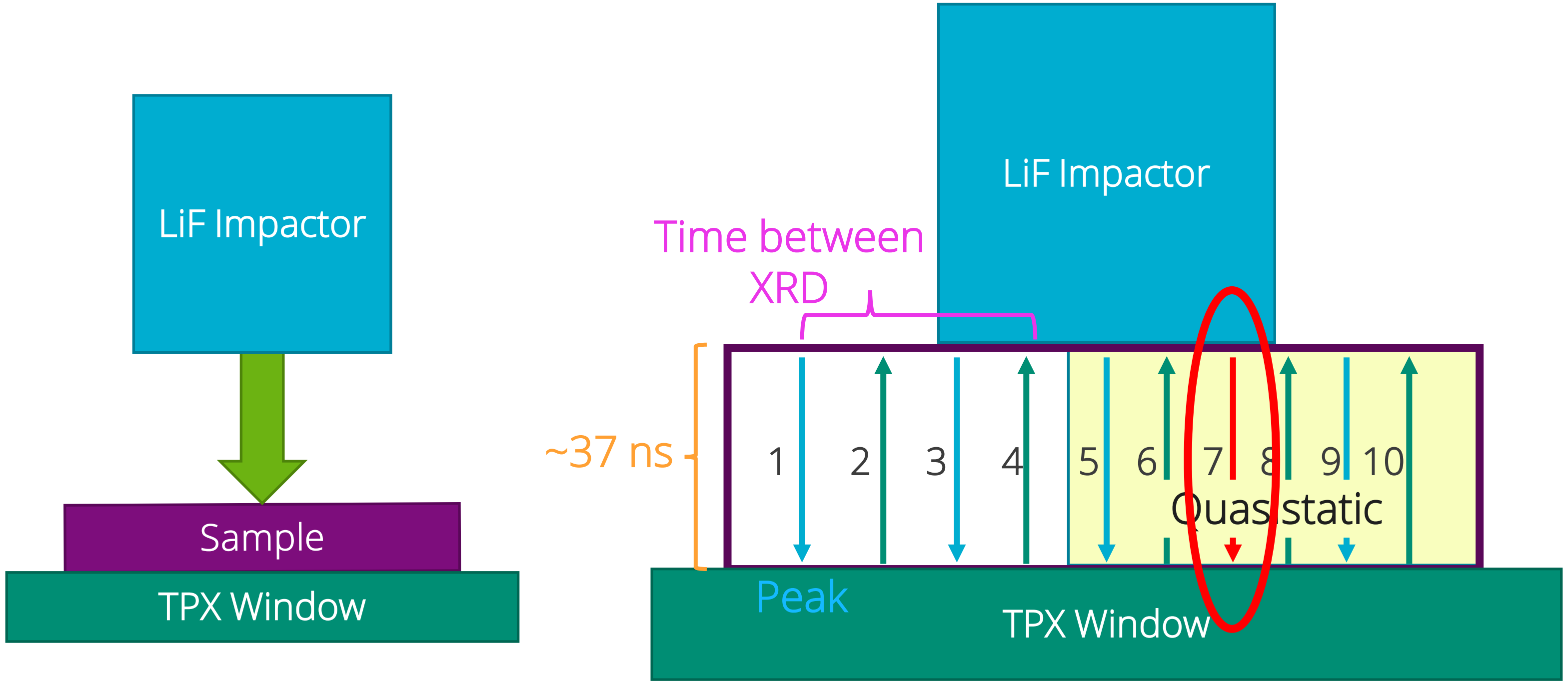




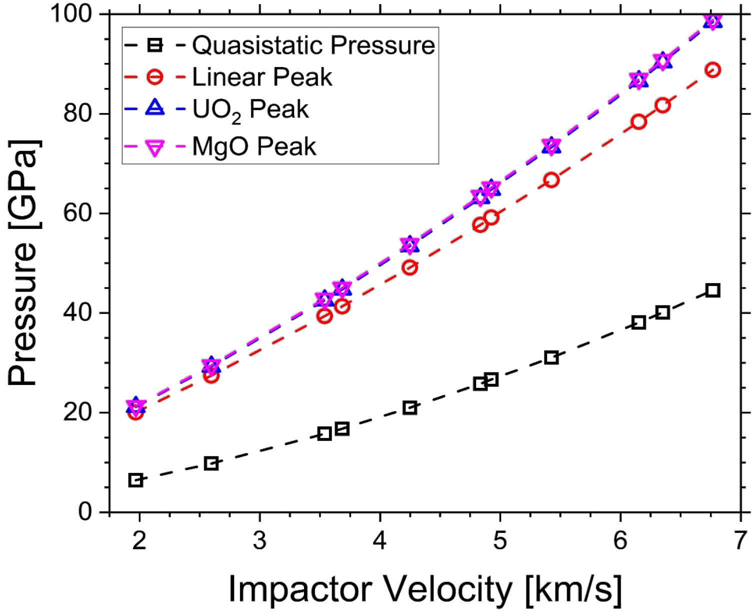
- Impact velocities from 1.9 → 6.8 km/s
- Peak pressure estimates from UO_2 and MgO Hugoniot[6]

[6]S.P. Marsh, LASL Shock Hugoniot Data (1980)

Determining pressure from impactor velocity



Unknown HEO Hugoniot Estimate with UO_2 and MgO



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$(La_{0.2}Y_{0.2}Ce_{0.2}Pr_{0.2}Sm_{0.2})_2O_3$ was prepared by the solid state method

La_2O_3, Y_2O_3, Sm_2O_3, CeO_2, Pr_6O_{11}

Annealed in Ar

Mill 24hrs in EtOH

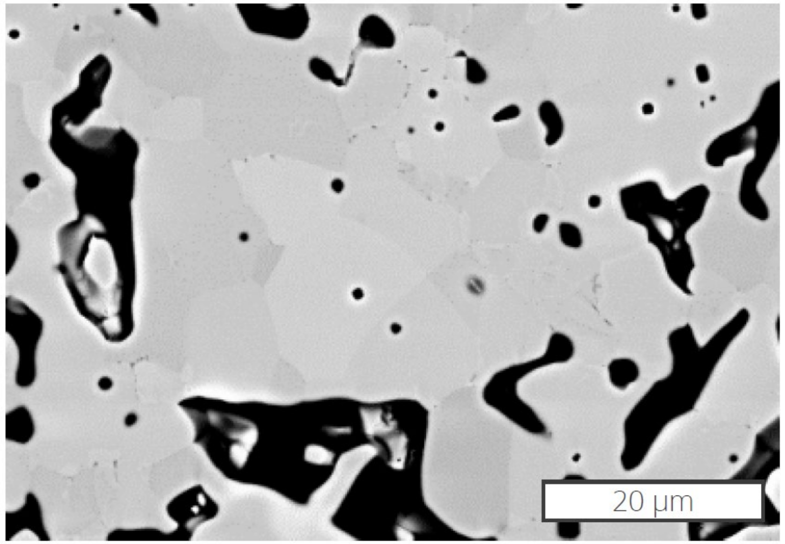
Annealed in Air

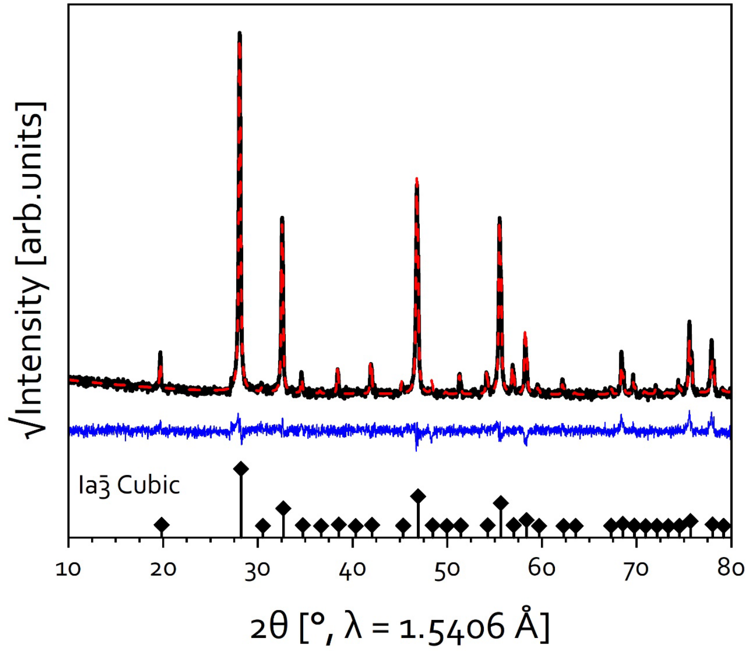
Dry and Pelletize

1600 °C
12 Hr
Quench

Slice to ~160 μm thick and mount to TPX windows for DCS experiments

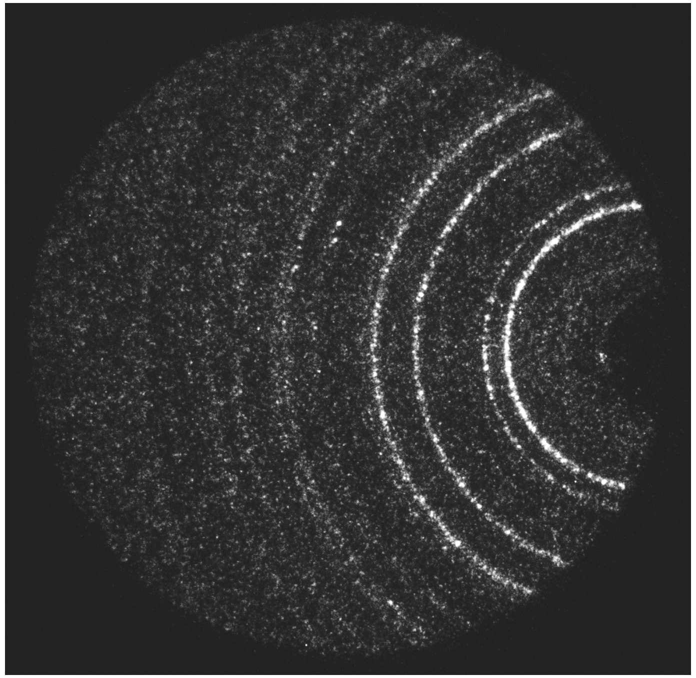
- ~93% dense
- Single phase cubic "Bixbyite" structure ($Ia\bar{3}$)
- ~37 ns for shock wave to transit sample



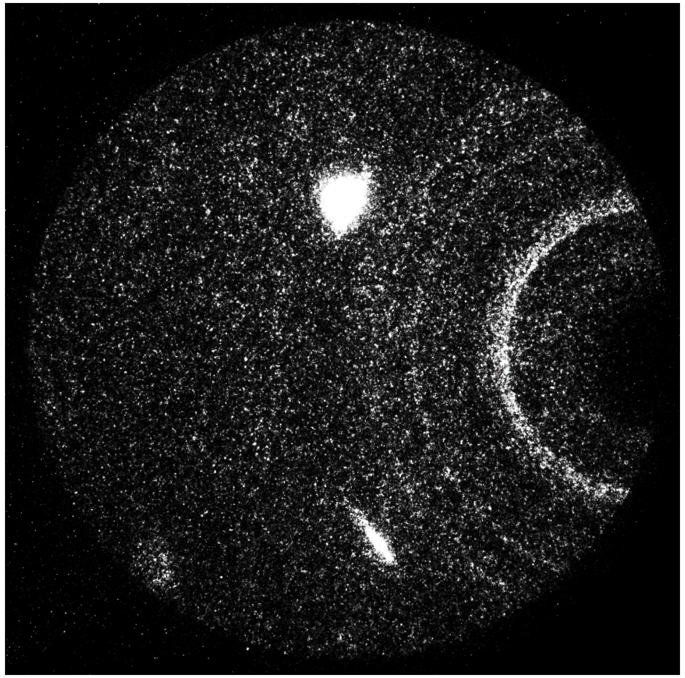


In situ XRD shows that $(La_{0.2}Y_{0.2}Ce_{0.2}Pr_{0.2}Sm_{0.2})_2O_3$ undergoes a FCC to BCC phase transformation in response to mechanical shock!

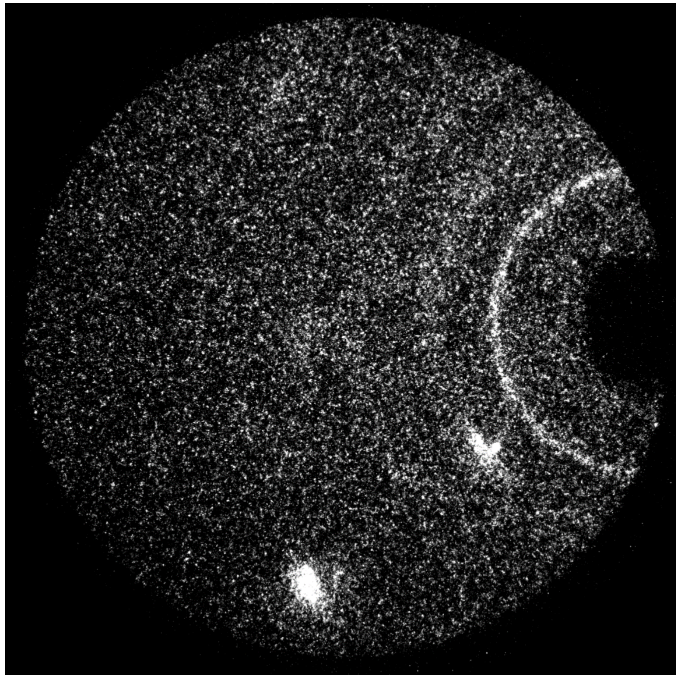
Ambient – FCC



10 GPa – FCC + BCC

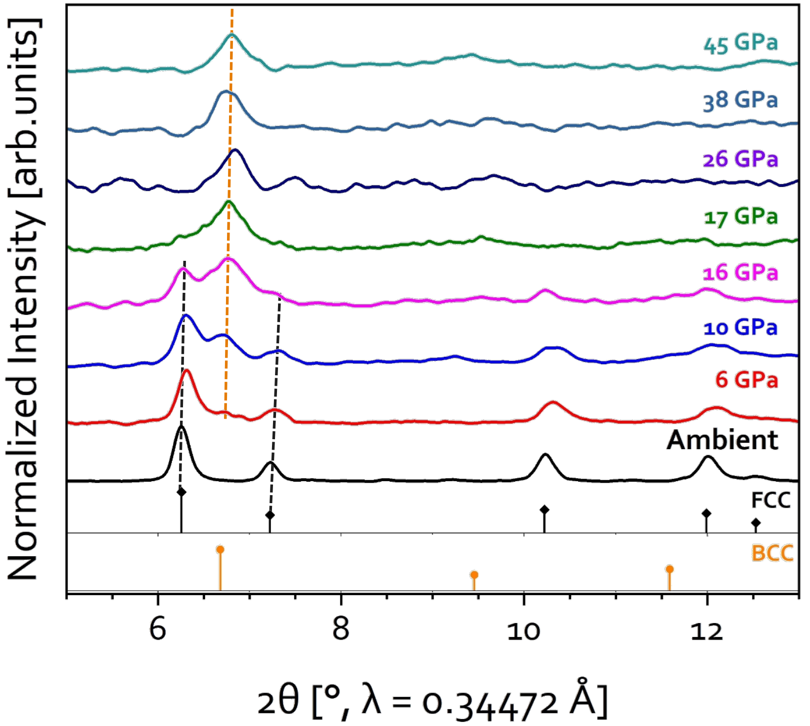


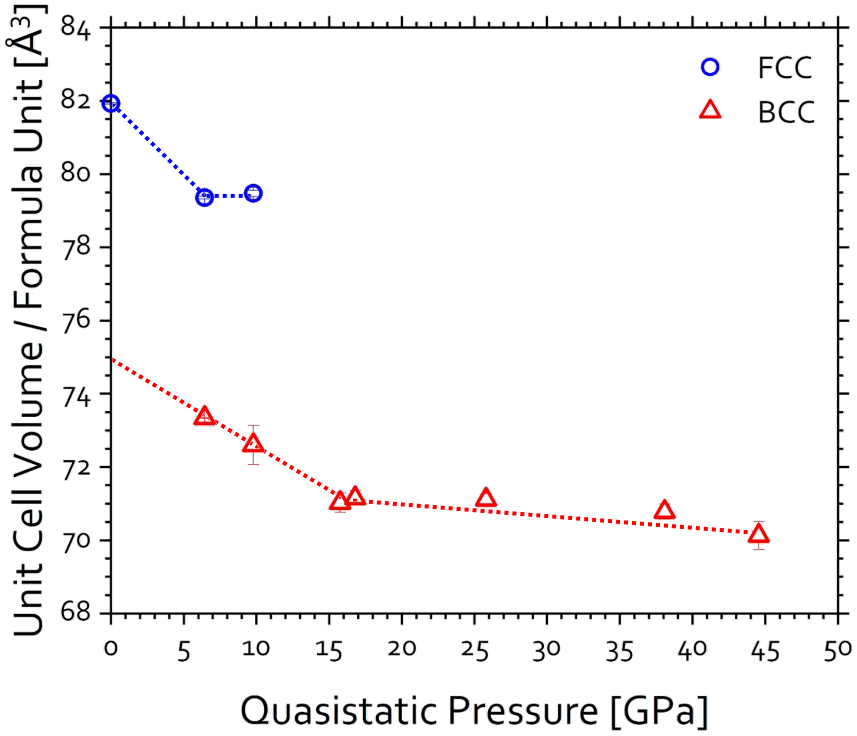
45 GPa – BCC



- Indexed phases include the FCC and BCC structures
- Strong BCC (110) reflection observed at all pressures
- Bright spots → LiF impactor

At low pressure FCC and BCC phases coexist while at higher pressures BCC exhibits reduced compression



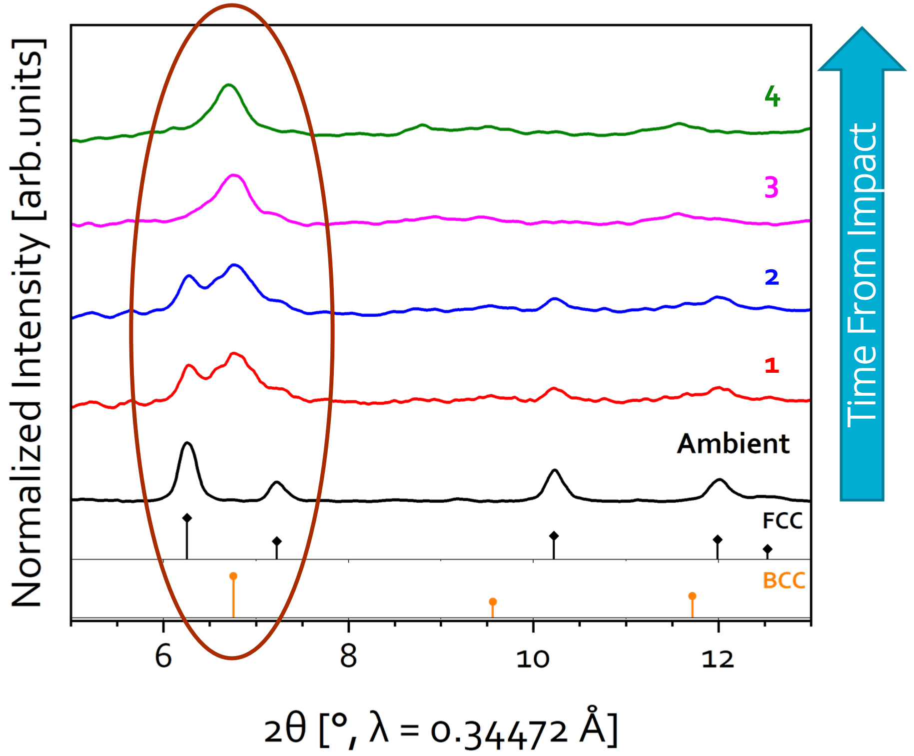


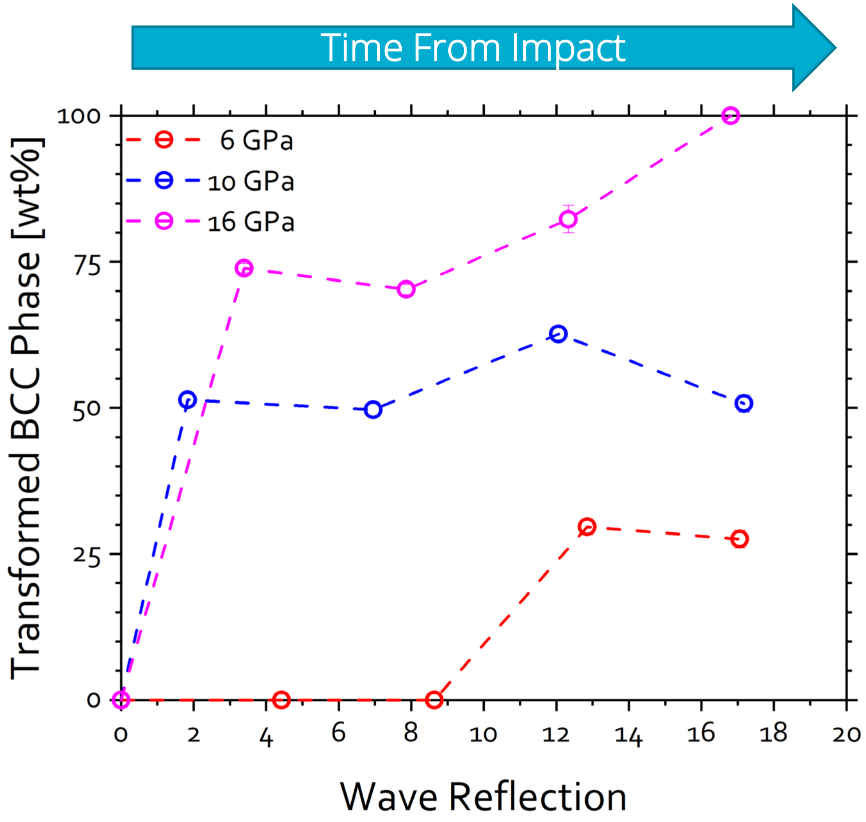
- XRD patterns for each pressure after 7 reflections
- BCC crystalline phase retained up to 45 GPa

- 3 % compression of FCC before full transformation
- Significant BCC compression up to 16 GPa
- Beyond 16 GPa BCC shows reduced compression

Low quasistatic pressure demonstrates delayed FCC → BCC transformation

16 GPa





- Peak pressure in ~37 ns
  → limited atomic diffusion for phase transformations

Summary

- FCC → BCC transformation induced due to mechanical shock
- Under dynamic compression, pressure induced amorphization was not observed
  - Contrary to PIA under hydrostatic compression in literature
- In low pressure (< 17 GPa) quasistatic condition the phase transformation demonstrates kinetic delay
  - Possible pressure induced heating

Next Steps

- PDV analysis for better insight into pressure and timing
  - Correct for timing mismatch
  - Determine pressure for pre-quasistatic frames
- Extract displacement errors (if any) for refined lattice parameters and unit cell volume

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Questions?

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