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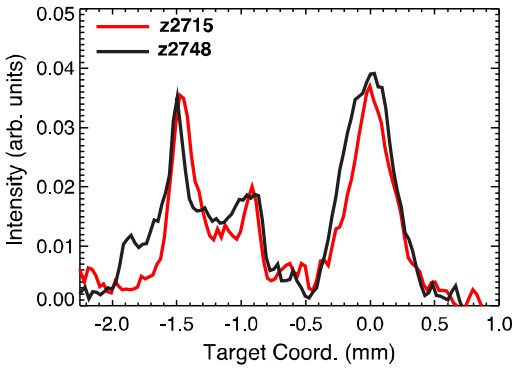

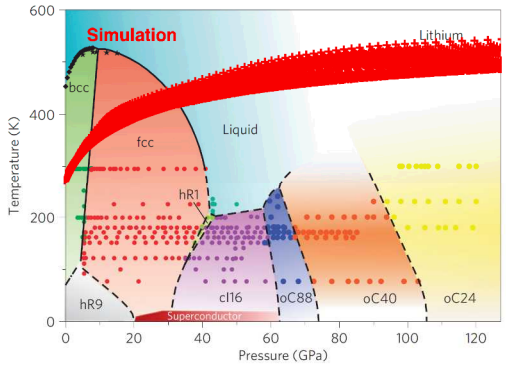

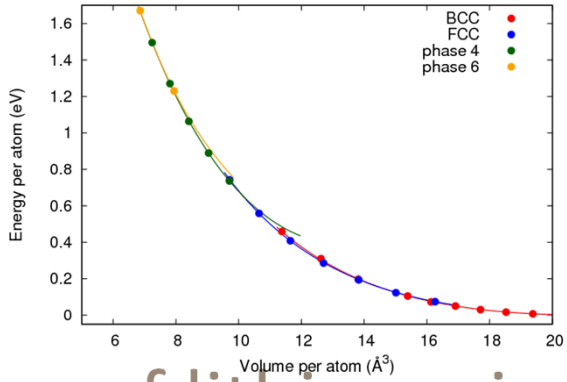

Determining the phase diagram of lithium via ab initio calculation and ramp compression

Luke Shulenburger, Chris Seagle, Tom Haill and Eric Harding

U.S. DEPARTMENT OF ENERGY
National Nuclear Security Administration

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Dynamic compression offers a unique capability for determining the phase diagram of complex materials

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Diamond Anvil Cells

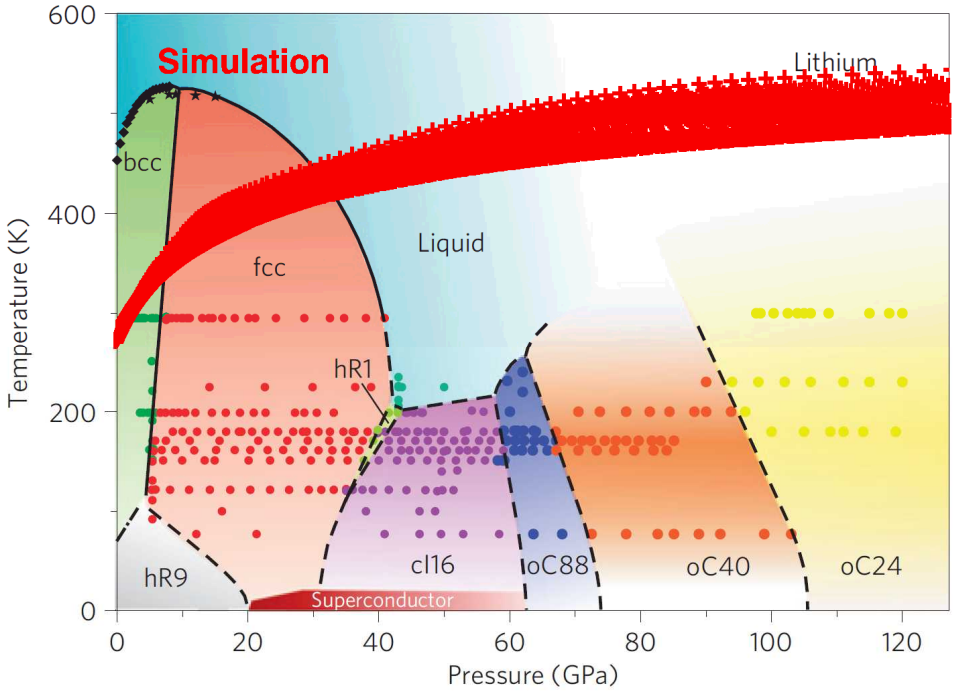
- Stable pressures
- Small sample sizes (~µm)
- Fair to good diagnostic access
- Pressures range 0-200+ GPa
- Temperatures up to several thousand Kelvin (laser heating)
- Chemical reactions with anvils are possible

Dynamic compression

- Transient experiments for 10's to 100's of ns
- Relatively large sample sizes (~mm)
- Challenging diagnostic access
- Pressures depend on the driver, 0-500+ GPa
- Temperatures depend on experiment
- Targeting a thermodynamic state may be challenging

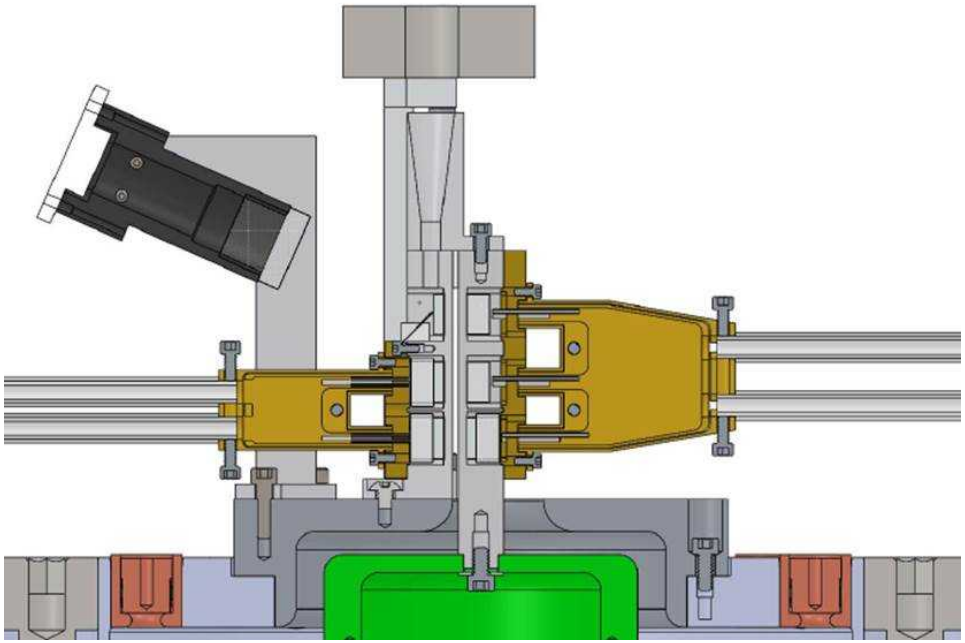
Lithium is an ideal material for developing ramp compression capabilities

- Many solid phases
- Required pressure range is not too great
- Temperatures are comparatively low
- Diamond Anvil Cell experiments are limited by reactivity
- Uncertainty in solid-solid phase boundaries from both theory and experiment
- Must understand affects from strength and kinetics
- Melt boundary above ~60 GPa is unknown



Phase diagram from Guillaume et. al., Nature Physics 2011

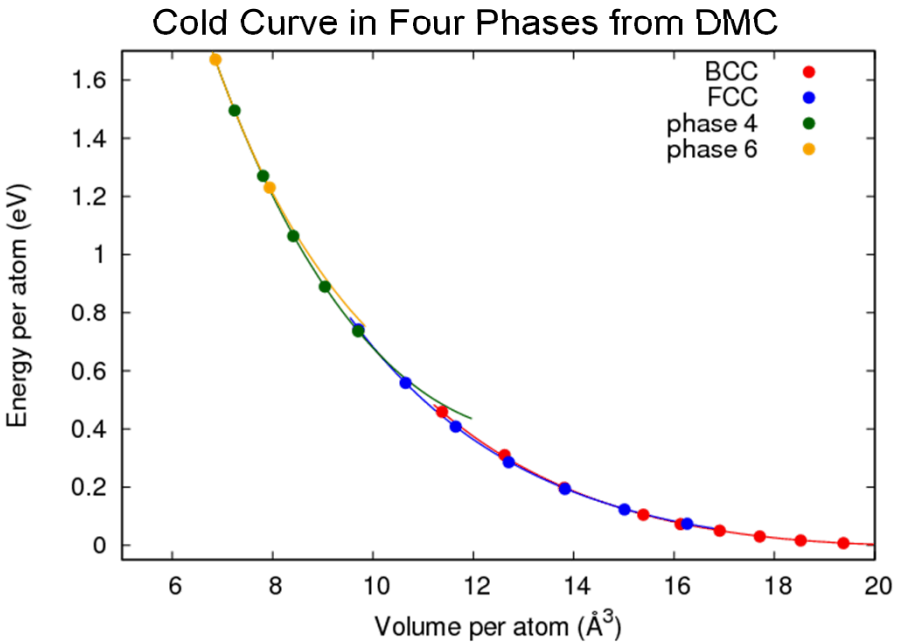
Experimental design



- Stripline load configuration
- Samples on both sides of anode-cathode gap
- Aluminum drive surface
- LiF windows
- Primary diagnostic is VISAR
- Top sample configured for X-ray Thomson Scattering (XRTS)
- Load current designed to avoid shocking samples

Ab initio calculations provide starting point for pulse shaping

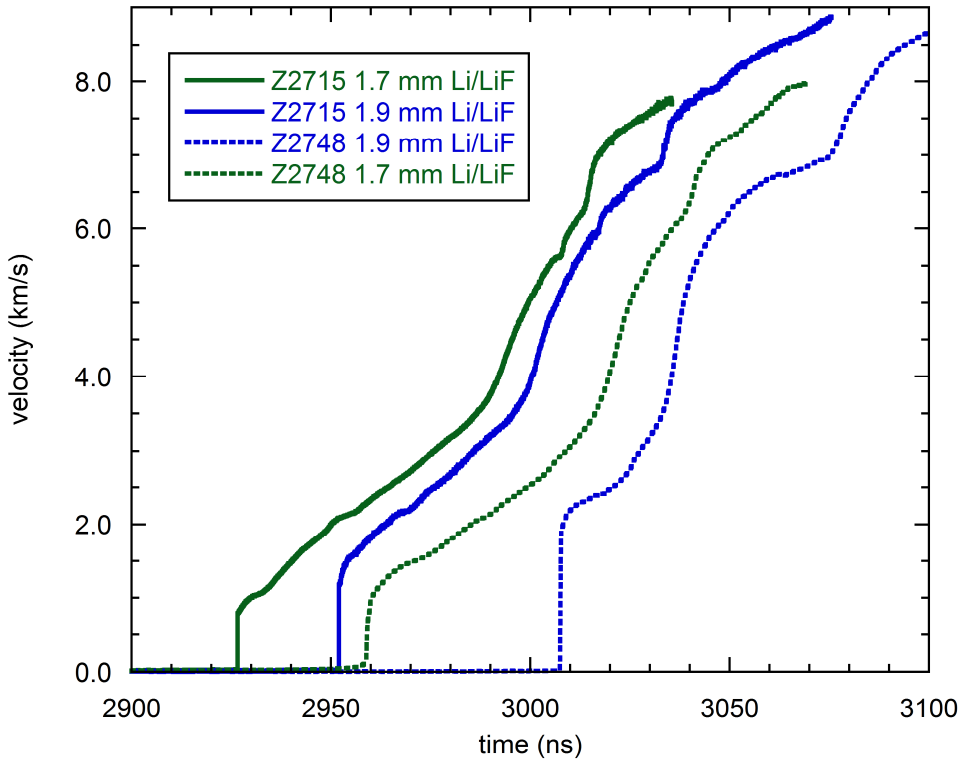
- Diffusion Monte Carlo calculations provide cold curve in four different low pressure phases
- Ion thermal piece of EOS inferred from quasiharmonic calculations of phonons
- Liquid EOS from QMD calculations along isotherms



- BCC-> FCC Transition 8.6 GPa
- FCC->cI16 Transition 30.2 GPa
- cI16 ->oC40 Transition 66.5 GPa

Experiments suggest several phase transitions

- Two experiments performed with similar results
- VISAR measures Li / LiF interface velocity
- Traces show several interesting features



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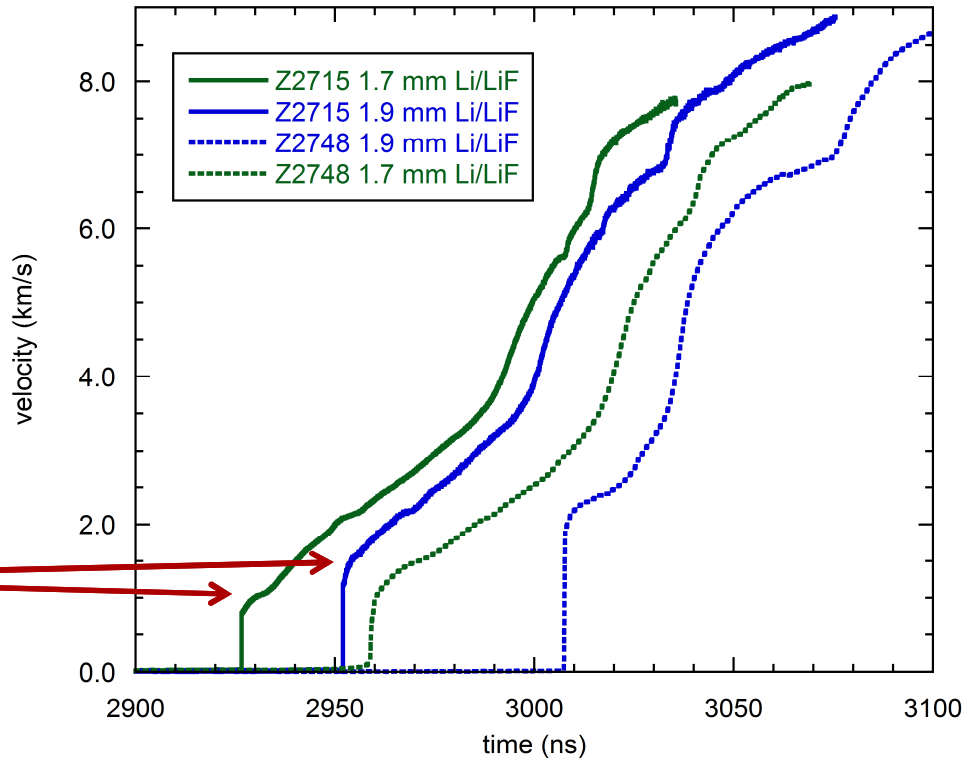
- Initial shock



Experiments suggest several phase transitions

- Two experiments performed with similar results
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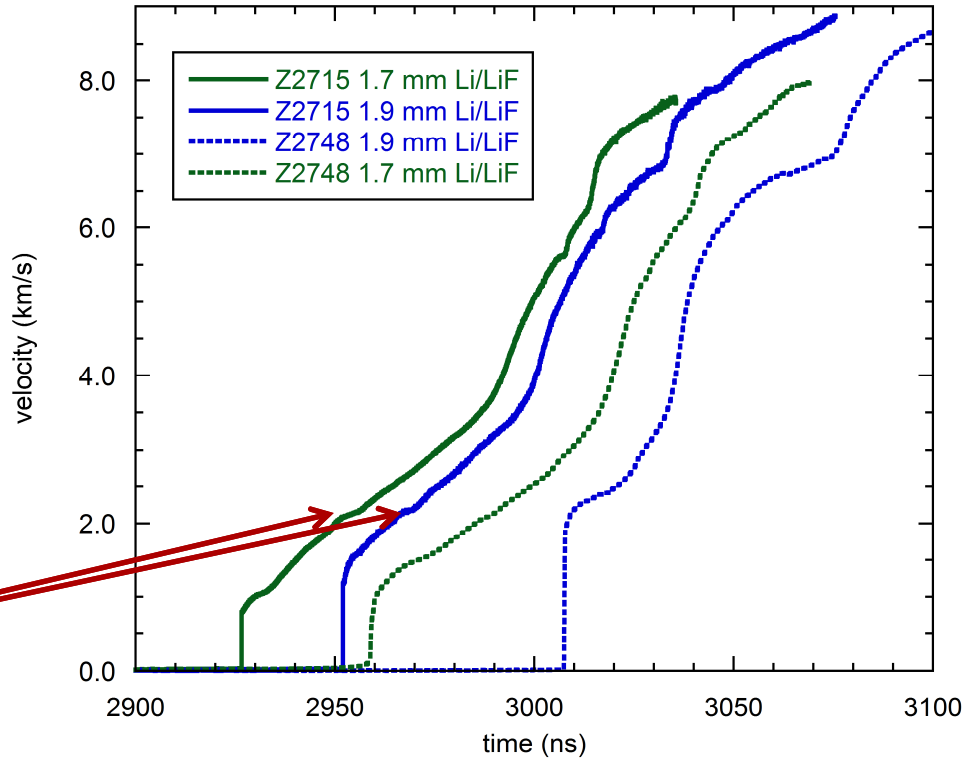
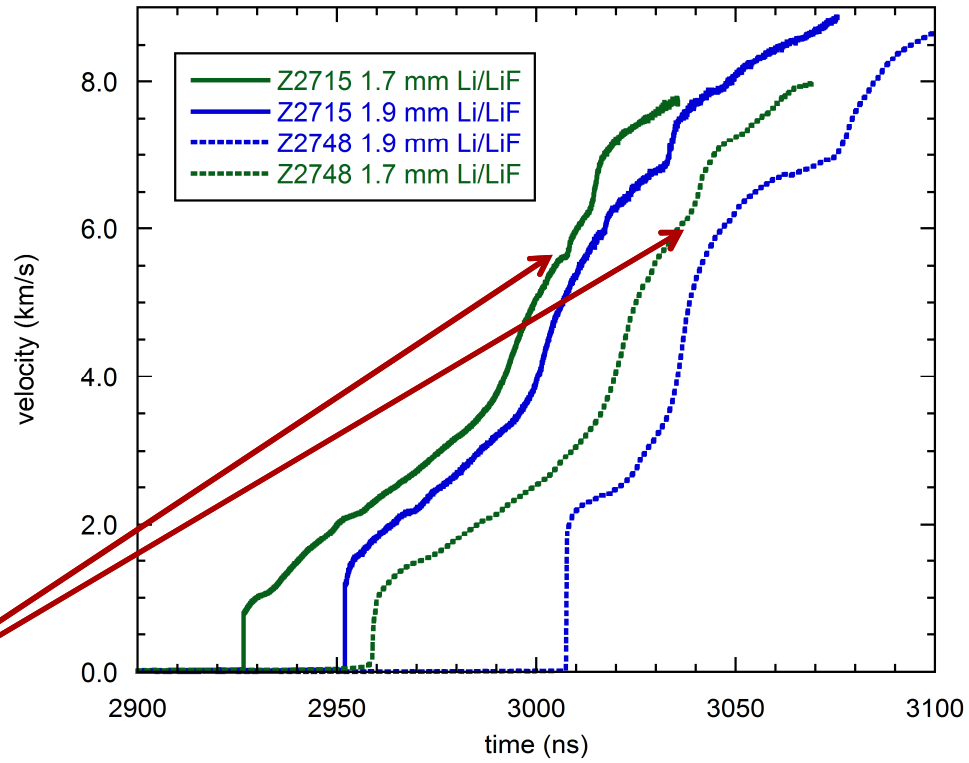
- Initial shock
- First softening



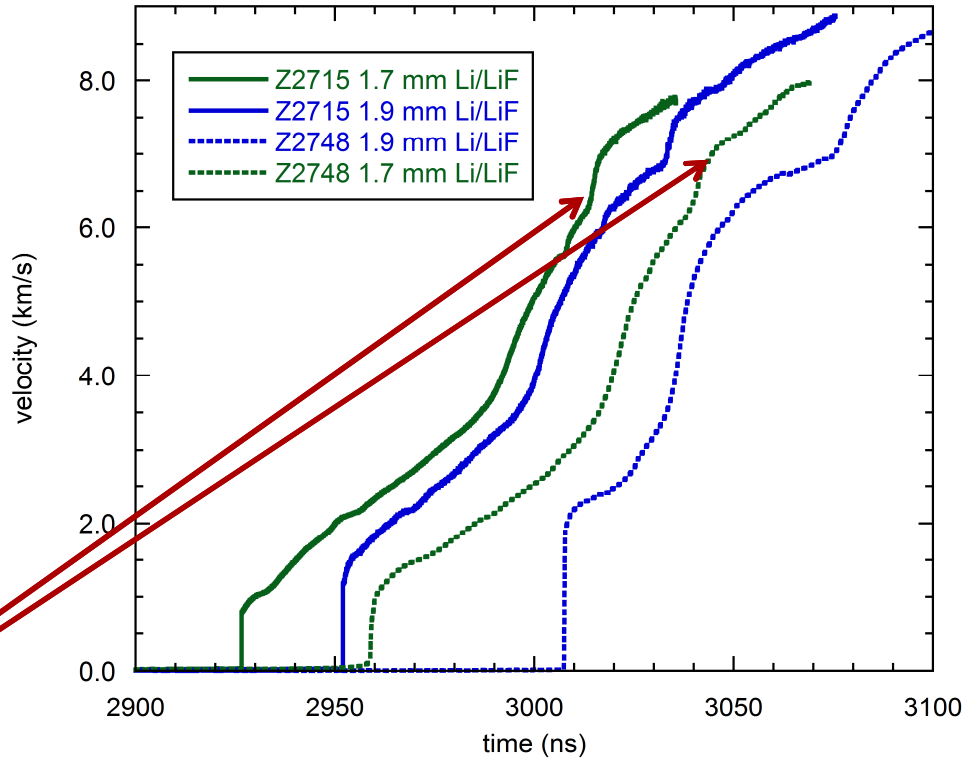
Experiments suggest several phase transitions

- Two experiments performed with similar results
- VISAR measures Li / LiF interface velocity
- Traces show several interesting features
- Initial shock
- First softening
- Late time softening

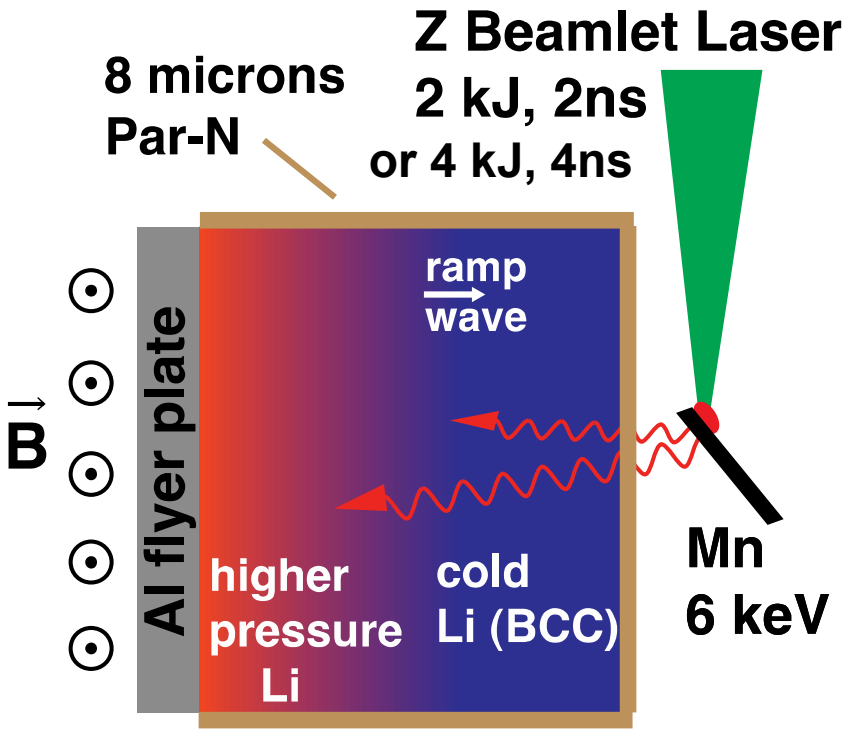


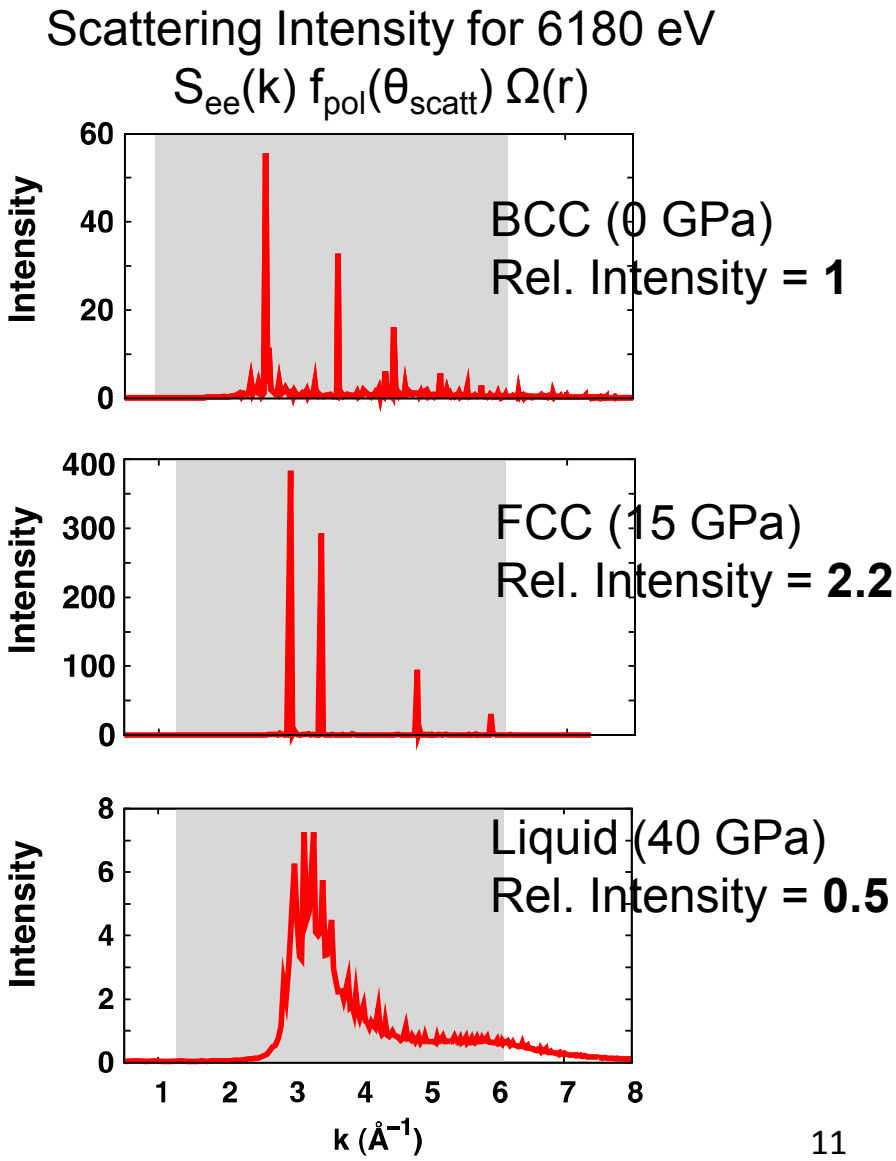
Experiments suggest several phase transitions

- Two experiments performed with similar results
- VISAR measures Li / LiF interface velocity
- Traces show several interesting features
- Initial shock
- First softening
- Late time softening
- Reverberation

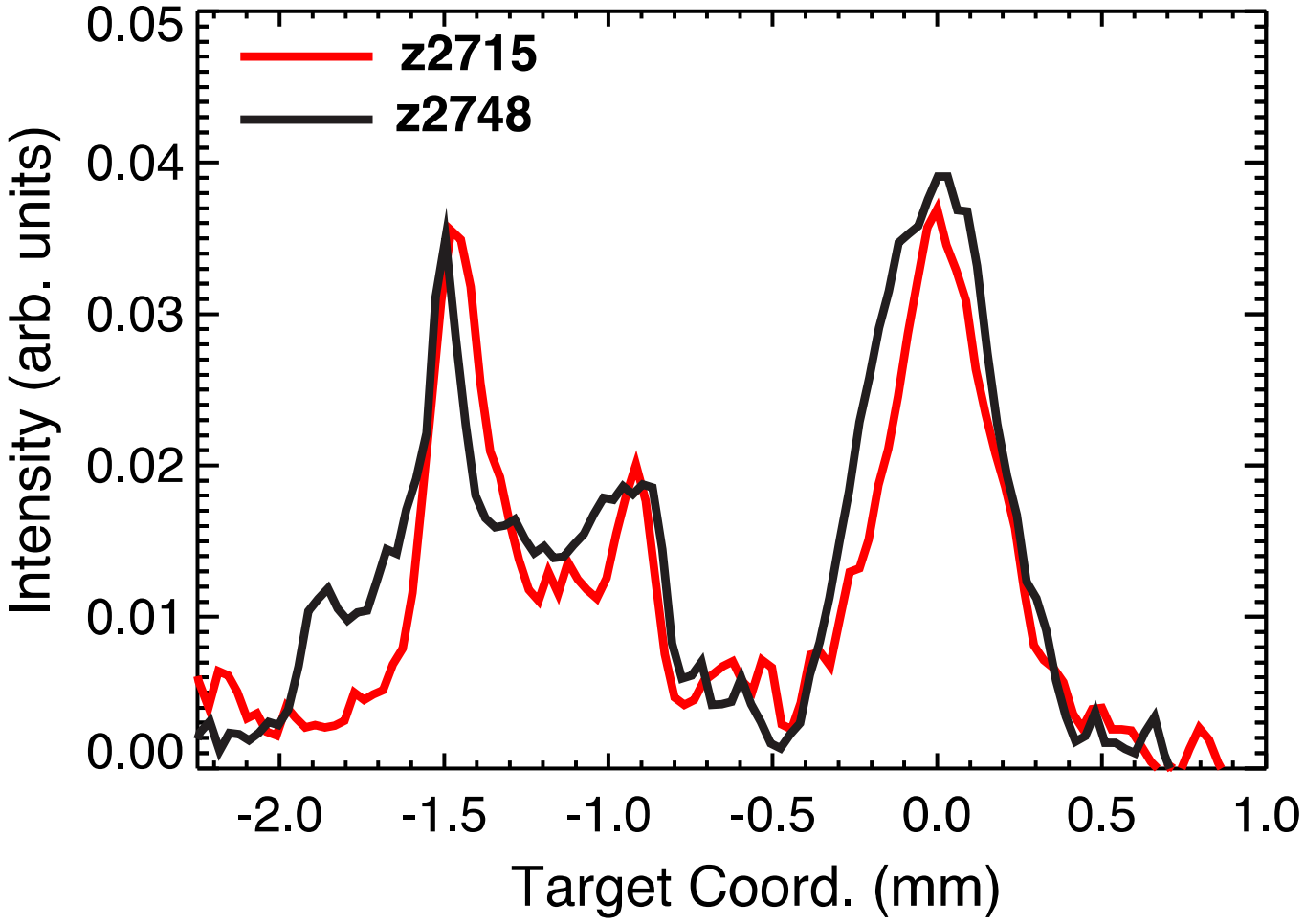


XRTS spectrometer gives spatially dependent probe of material state





The spatially resolved lineouts (width = 70 eV) show similar structure and overall intensity for both shots.



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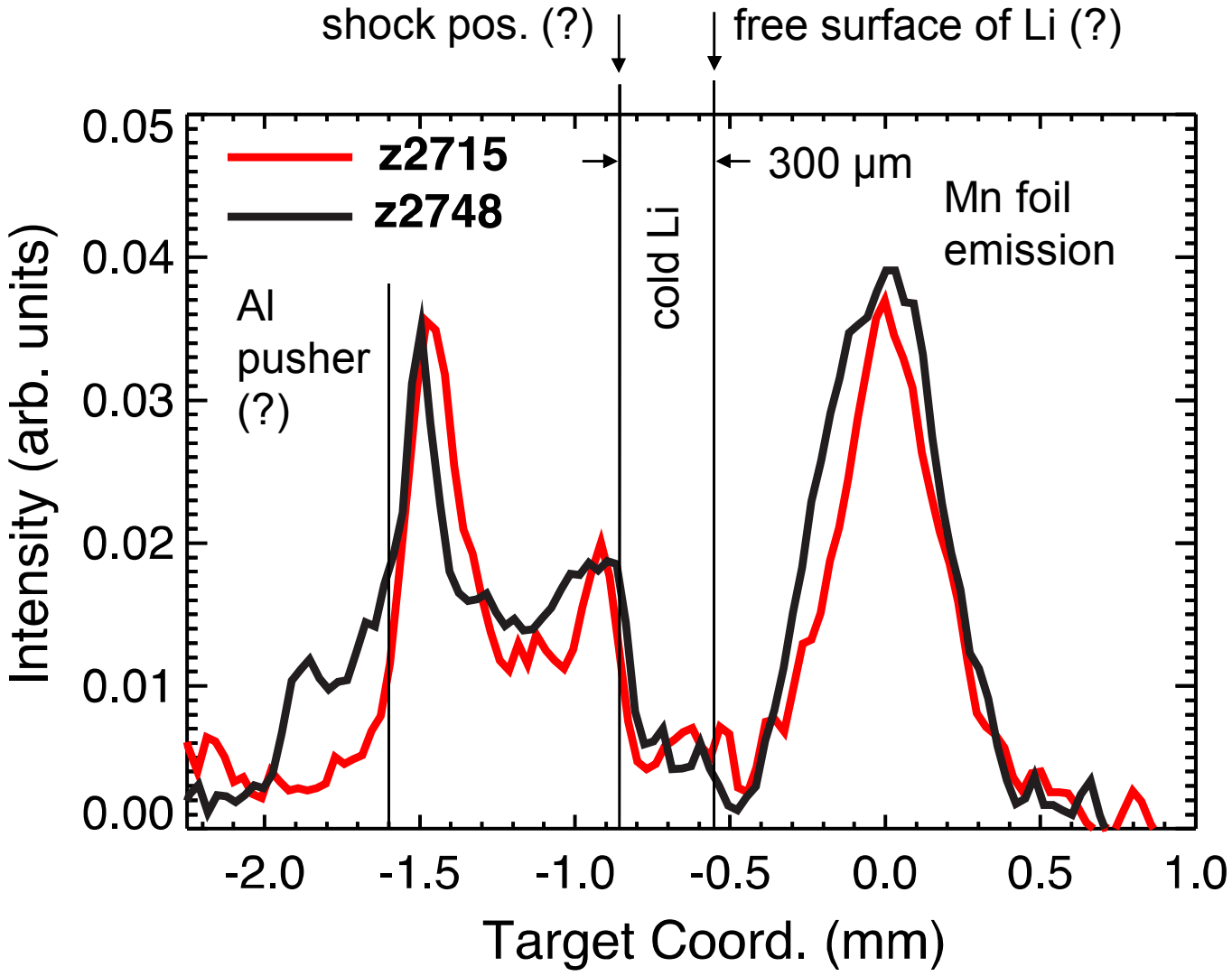

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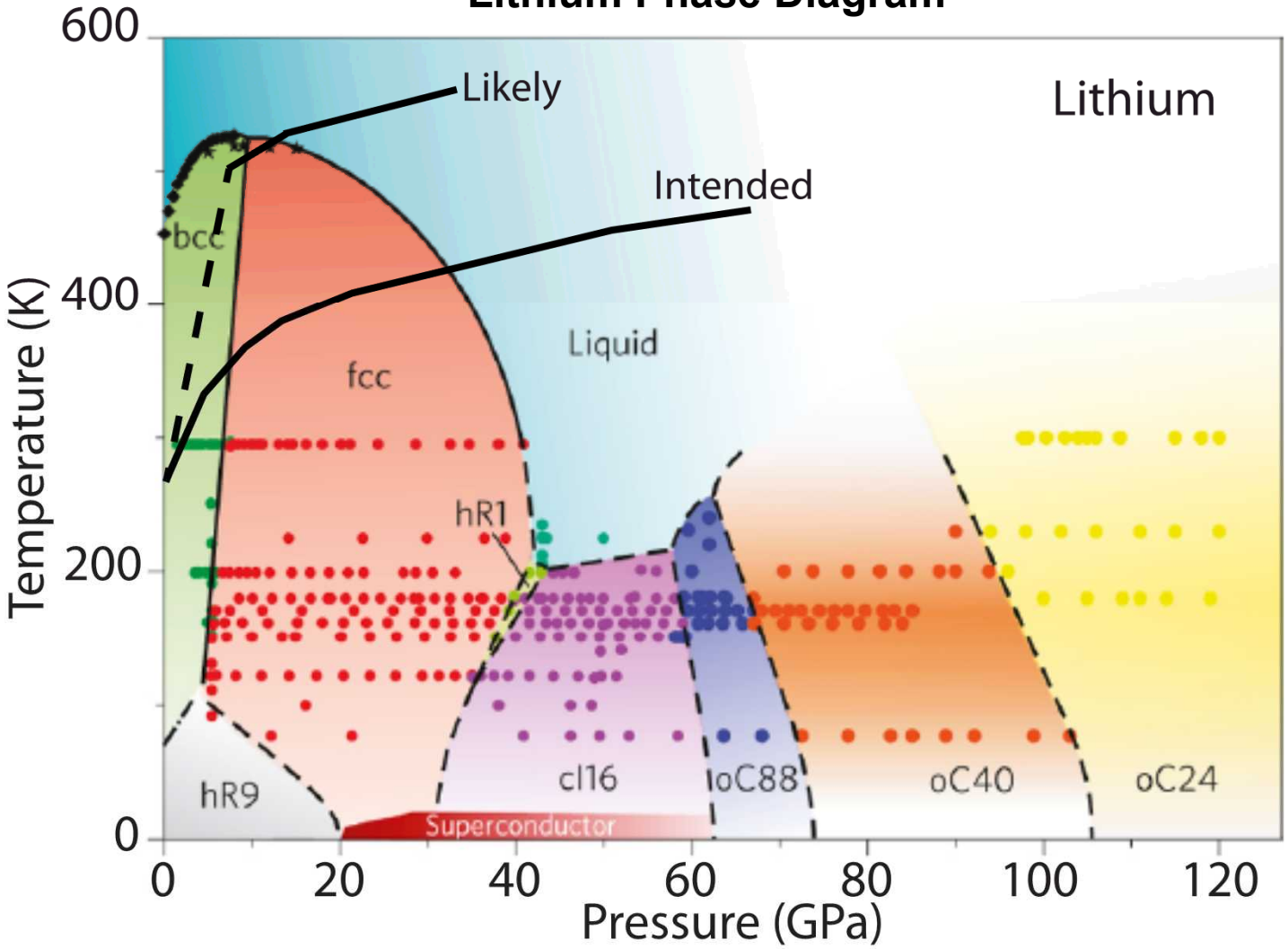
Lithium Phase Diagram*



Phase diagram from Guillaume et. al., Nature Physics 2011

Initial ramp compression experiments on Li show promise for understanding high pressure phase transitions

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- Ab inito calculations provide initial EOS for designing experiment
- VISAR traces show initial shock followed by several potential phase transitions
- Spatially resolved XRTS gives insight into early time behavior during ramp compression
- Future experiments will seek to remove initial shock
- Late time behavior in VISAR suggests unexplained high pressure phase transition
  - Freezing?