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Title: Kinetics of Solid-Solid Phase Transition in Iron

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Solid-Solid Phase Transition Measurements in Iron

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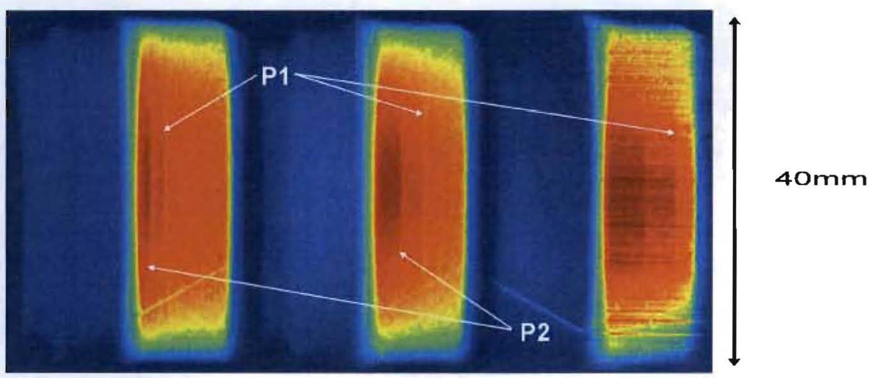
Previously, dynamic experiments on iron have observed a non-zero transition time and width in the solid-solid α-ε phase transition.[1,2] Using Proton Radiography at the Los Alamos Neutron Science Center, we have performed plate impact experiments on iron to further study the α-ε phase transition which occurs at 13GPa. A 40mm bore powder gun was coupled to a proton radiography beam line and imaging system and synchronized to the impact of the projectile on the target sample with the proton beam pattern. A typical experimental configuration for the iron study, as shown below in 3 color-enhanced radiographs, is a 40mm diameter aluminum sabot impacting a 40mm diameter of polycrystalline ARMCO iron. The iron is backed by a sapphire optical window for velocimetry measurements. The aluminum flyer on the left of the iron is barely visible for visual display purposes.



Direct density jumps were measured[3] which corresponded to calculations to within 1% using a Wondy multi-phase equation of state model. In addition, shock velocities were measured using an edge fitting technique and followed that edge movement from radiograph to radiograph, where radiographs are separated in time by 500 ns. Preliminary measurements give a shock velocity (P1 wave) of 5.251 km/s. The projectile velocity was 0.725 km/s which translate to a peak stress of 17.5 GPa.

Assuming the P1 wave is instantaneous, we are able to calibrate the chromatic, motion, object and camera blur by measuring the width of the P1 wave. This approximation works in this case since each of the two density jumps are small compared to the density of the object. Subtracting the measured width of the P1 wave in quadrature from the width of the P2 wave gives a preliminary measurement of the transition length of 265 μm. Therefore, a preliminary measured phase transition relaxation time τ = transition length/u_s = 265 μm/5.251 km/s = 50 ns.

Both Boettger[1] & Jensen[2] conclude that the transition rate and likely the transition mechanisms depend on the impact stress and the sample thickness. Since Proton Radiography can measure directly the transition length as well as the shock velocity, a transition time can be directly calculated. We propose to perform a series of experiments to measure the phase transition relaxation time, τ, as a function of drive, sample size and crystal orientation.

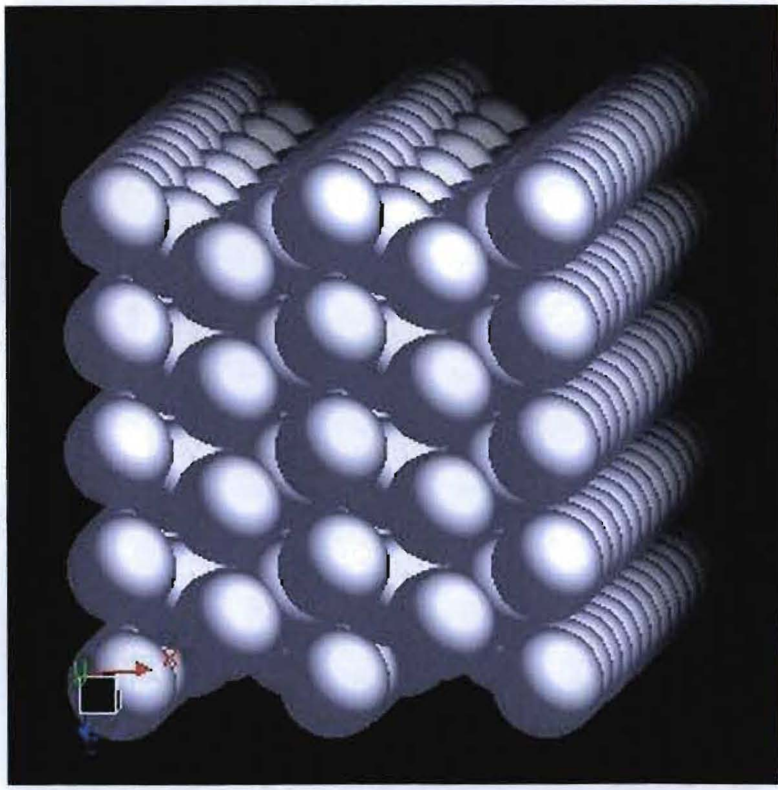
1. J.C. Boettger and D. Wallace, "Metastability and dynamics of the shock-induced phase transition in iron", Phys. Rev. B **55**, 2840 (1997).

2. B.J. Jensen, G.T. Gray III and R.S. Hixson, "Direct measurements for the α-ε transition stress and kinetics for shocked iron", Journ. Appl. Physics **105**, 103502 (2009).

3. P.A. Rigg, C. L. Schwartz, et al., "Proton radiography and accurate density measurements: A window into shock wave processes", Phys. Rev. B **77**, 220101 (2001).

Kinetics of Solid-Solid Phase Transition in Iron ~~for PRIOR~~

Cynthia L. Schwartz and pRad Team
Los Alamos National Laboratory



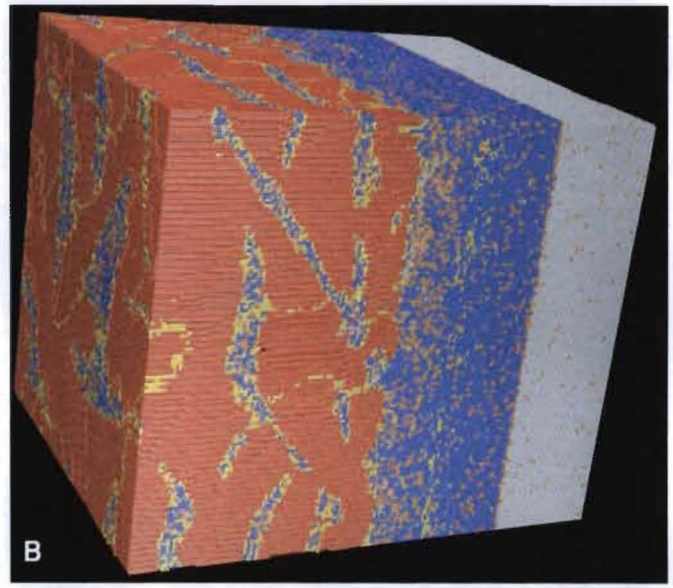
Transition Stress, Mechanisms, Kinetics and Hugoniot response depend on crystal orientation

Polycrystalline Material

- Distribution of grain orientations
- Grain boundaries serve as heterogeneous nucleation sites
- Decreased transformation threshold
- Fast mechanism

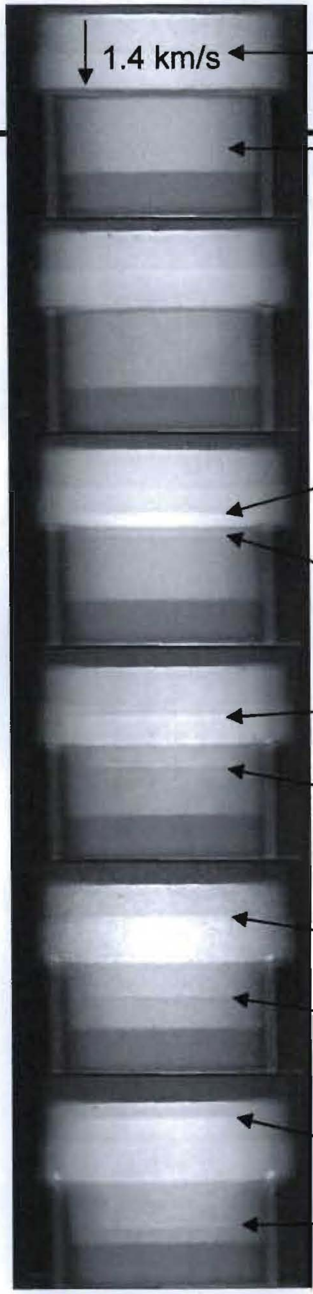
Single Crystal Material

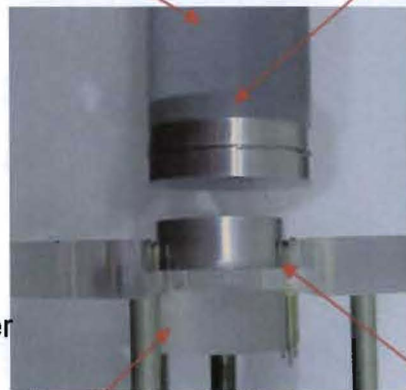
- Mulitmillion atom MD simulations for single crystal iron
- Homgeneous nucleation
- Slower mechanism
- Increased transformation threshold

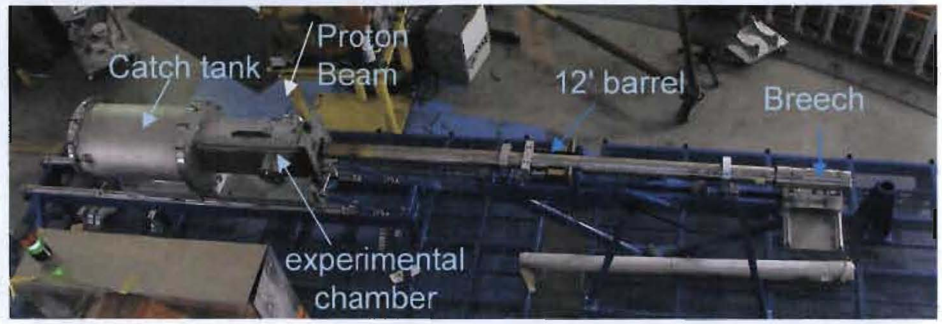


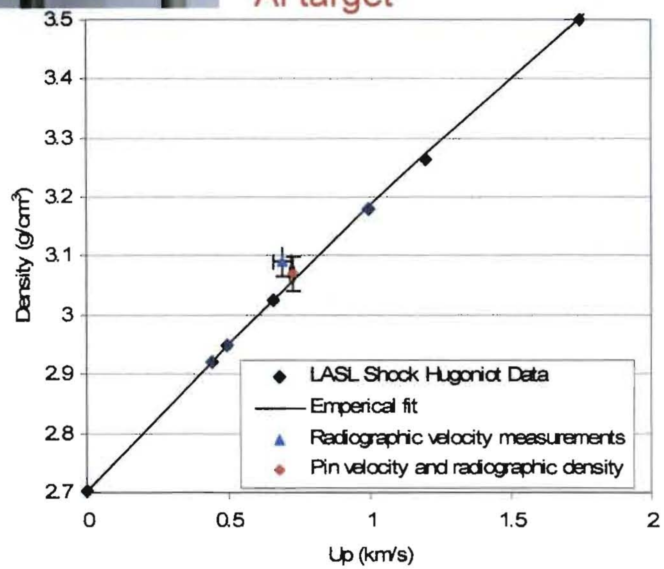
K. Kadau, T. C. Germann, P. S. Lomdahl, and B. L. Holian, *Science* **296**, 1681 2002.

Demonstration Powder Gun Experiment









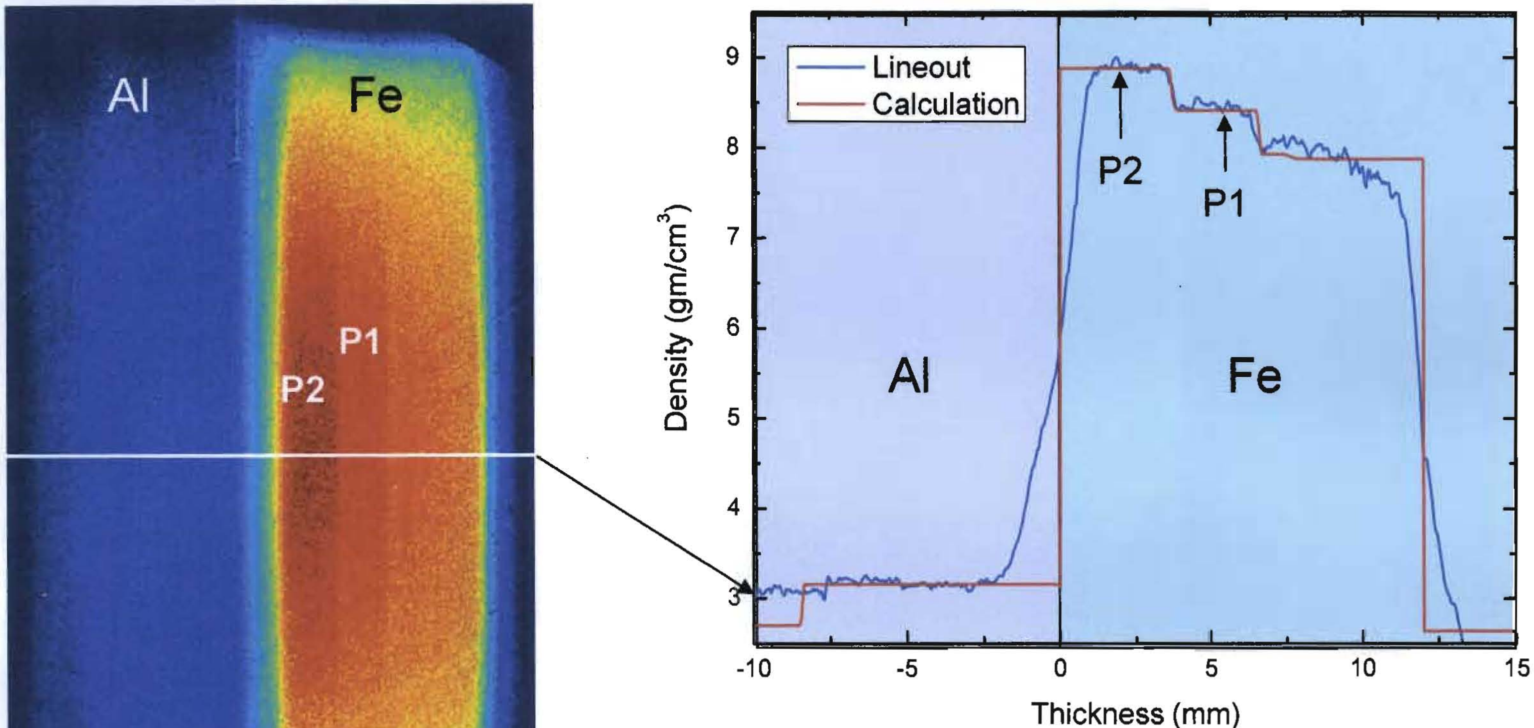
Two methods of measuring a point on shock Hugoniot per dynamic event:

- Radiographic measurement of density behind shock front.
- Simultaneous measurement of particle and shock velocity

Invited Talk : Paulo Rigg, *Shock Compression of Condensed Matter*, 2007

Rigg, Schwartz, et al., *Phys. Rev. B*, Jun 08, vol. 77, iss. 22 220101

Powder Gun-Driven
Measured and Calculated Densities - Iron



Schwartz, Rigg, et. al, IP Conference Proceedings (12 Dec. 2007) vol.955, no.1, p.1135-8

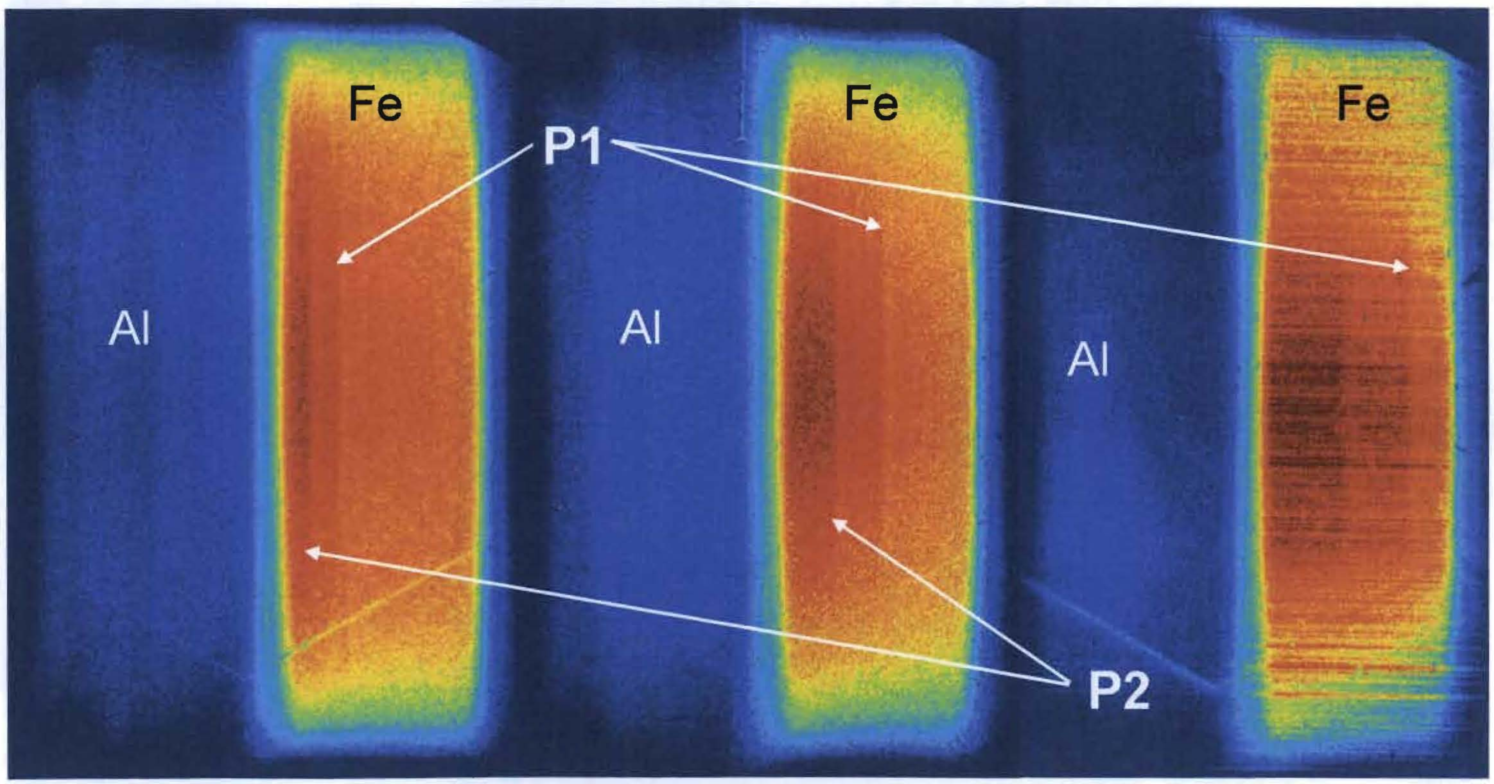
Fe Densities

State	Measured	Calculated*	Agreement
P1	8.346	8.342	<0.1%
P2	8.854	8.846	0.1%

*calculated values from 1-D Multi-Phase EOS for Fe model

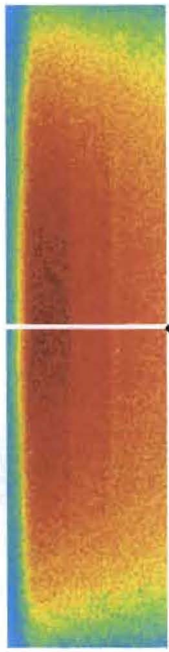
Two-wave structure observed in Iron

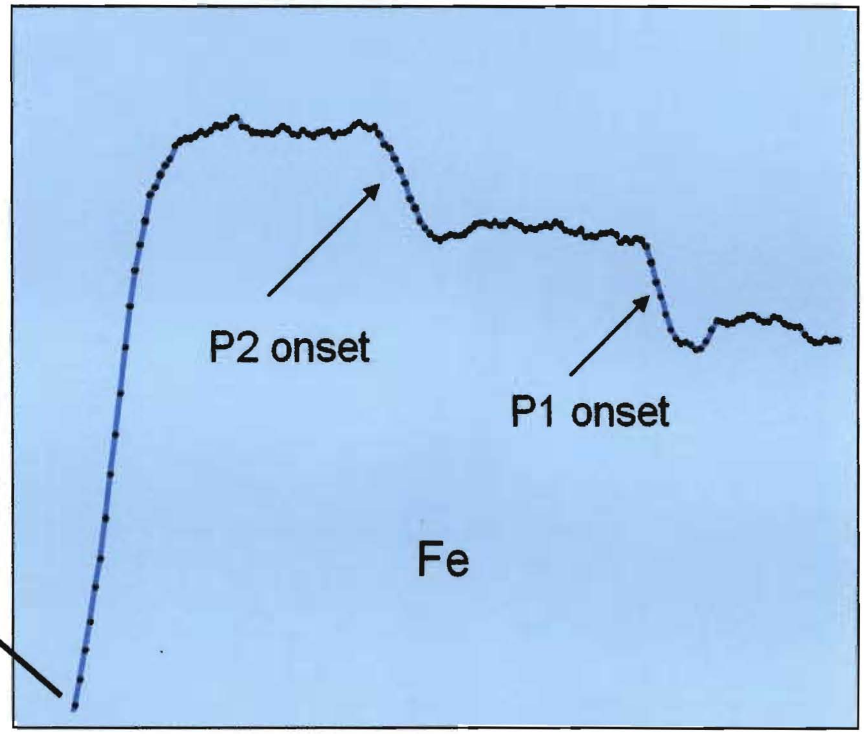
- Aluminum impacting Iron backed by Sapphire @ 1.45 km/s -> 175 kbar in Fe
- 3X pRad Magnifier used to enhance contrast and sharpness
- 3 camera times captured separated by 500ns



Resolution Calibration

The nearly instantaneous P1 wave can be used to calibrate the resolution of the radiographic system.

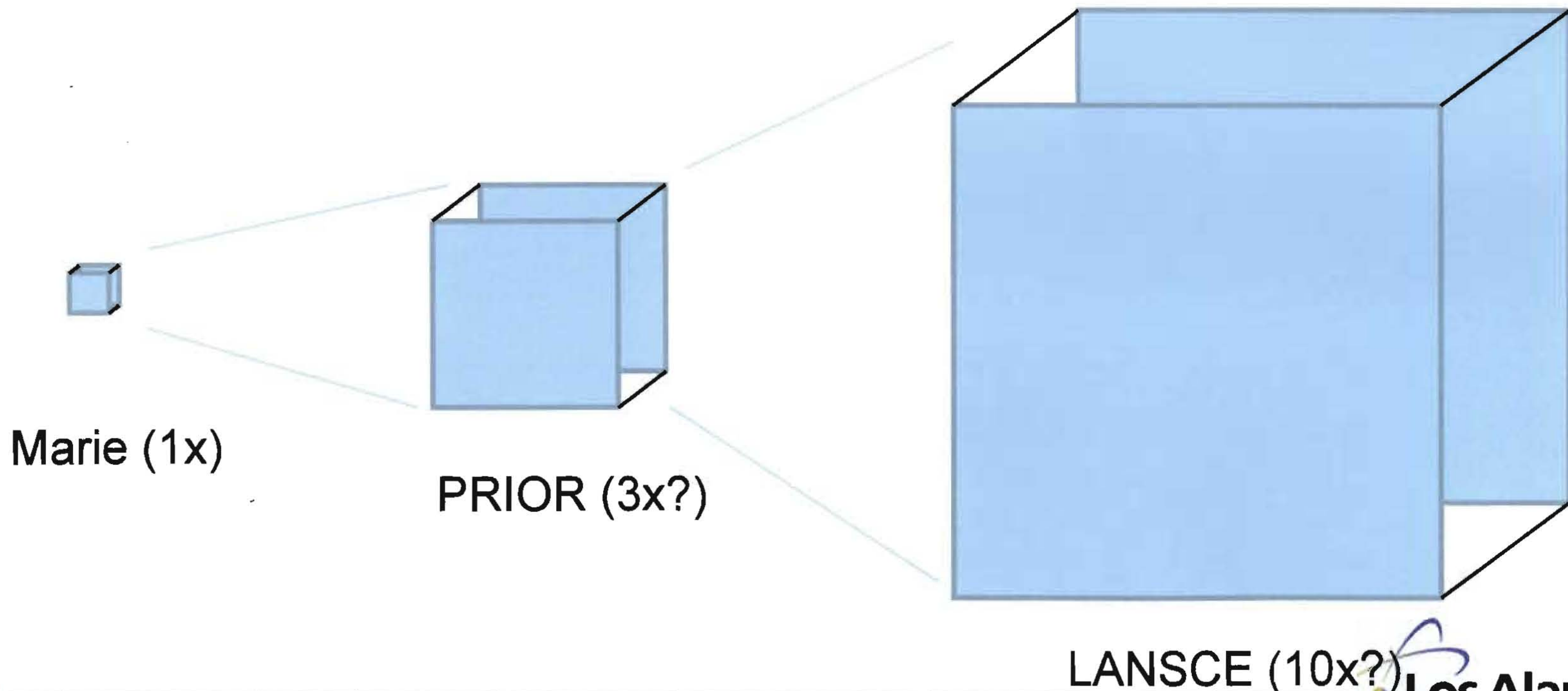




P2 slope:	66 g/cm^2/cm
P1 slope:	98 g/cm^2/cm
Residual P2 onset slope:	72 g/cm^2/cm

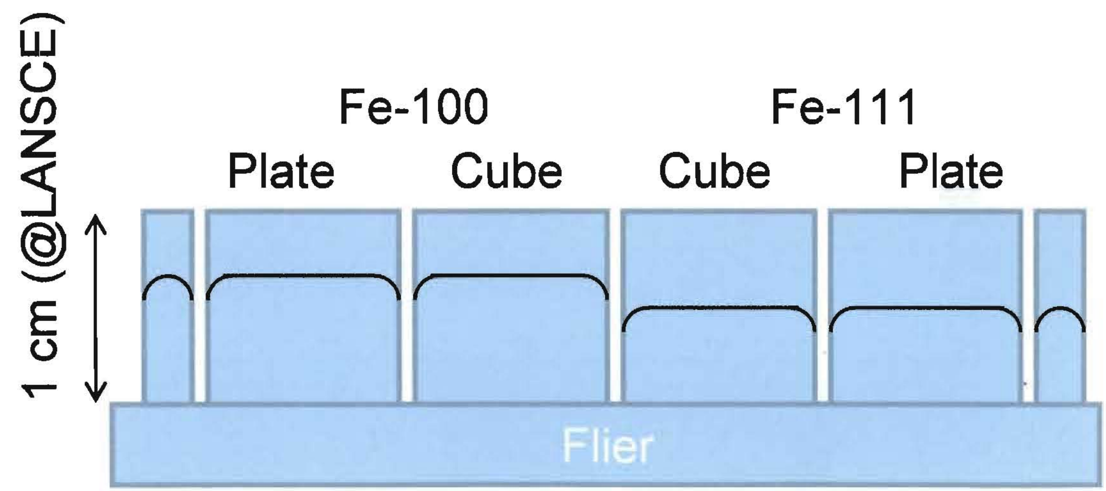
Scaled MaRIE-type experiments

- How important are edge effects on the Marie physics?
- pRad @ Line C or PRIOR cannot reach Marie scales
- But they can access large scale replicas of Marie experiments
- Edge effects are expected to scale with experiment size



Proposal: single shot, multiple experiments To be done at LANSCE and PRIOR

- Mount multiple objects to be hit by single flier
- Scale experiment to LANSCE and PRIOR FOV and resolution
- Radiograph experiment both directions simultaneously
- Actual experiments TBD; Fe crystals as example



Summary

- Perform experiments on a Fe
  - well studied
  - atomistic MD simulations to compare to
  - Experimental data to compare to
- Perform experiments with multiple single crystal orientations as well as polycrystalline in iron to understand the affect of crystal orientation on Hugoniot response
  - Measure shape and evolution of P2 wave using P1 wave as a resolution calibration
- Begin off-Hugoniot studies
  - Design deep release experiments
  - Measure shape and evolution of release isentrope for iron to calibrate and validate EOS models
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