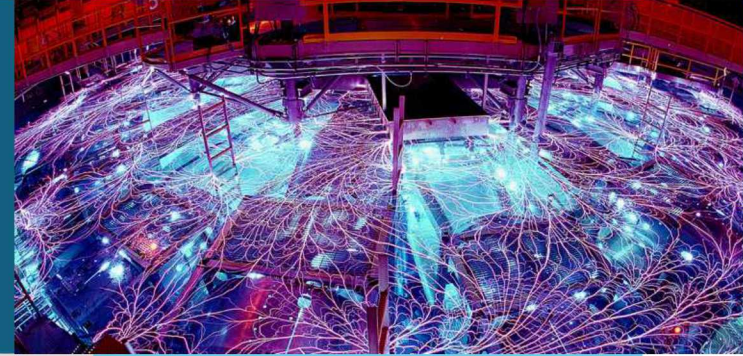


Iron Equation of State Measurements on the Z-Machine



University of Texas: Sean Grant, Todd Ditmire, Jung-Fu Lin, Aaron Bernstein

Sandia National Laboratories: Tommy Ao, Kyle Cochrane, Jean-Paul Davis,
Daniel Dolan, Andrew Porwitzky, Christopher Seagle,
John Benage, Dawn Flicker

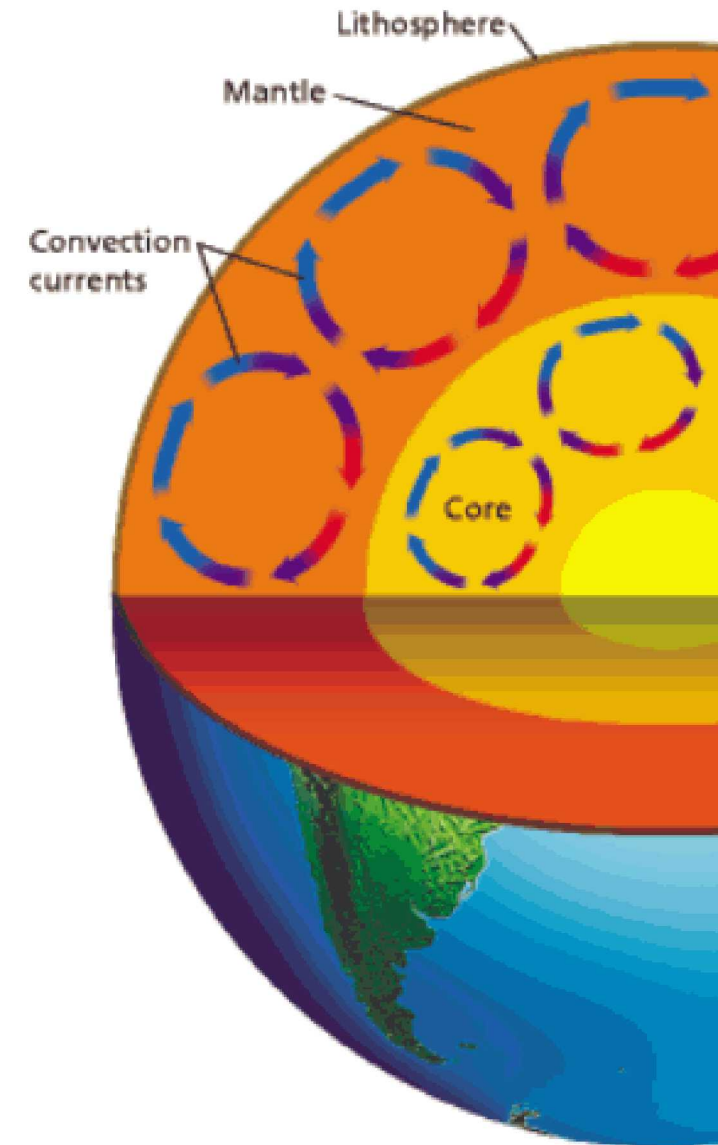
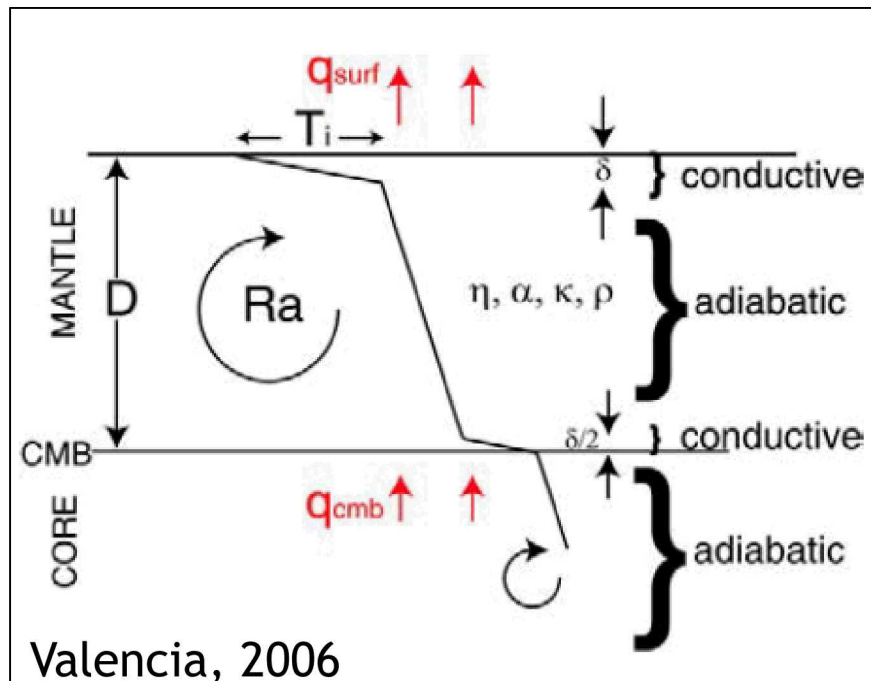


Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration. SAND2019-9398C

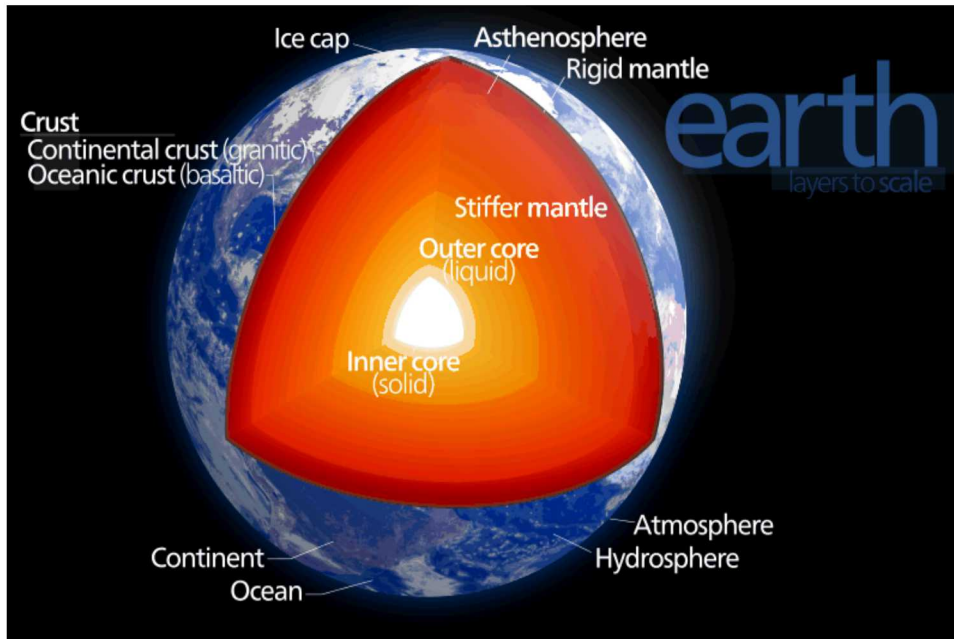
Iron is an important material for planetary sciences and many other high energy density applications

Important Current Research:

- Measuring the P - ρ equation of state (EOS) of liquid iron at previously unexplored off-Hugoniot isentropes
- Isentropic compression is an extremely useful way to study planetary equations of state



The conductivity of iron is important for understanding the evolution of planetary cores

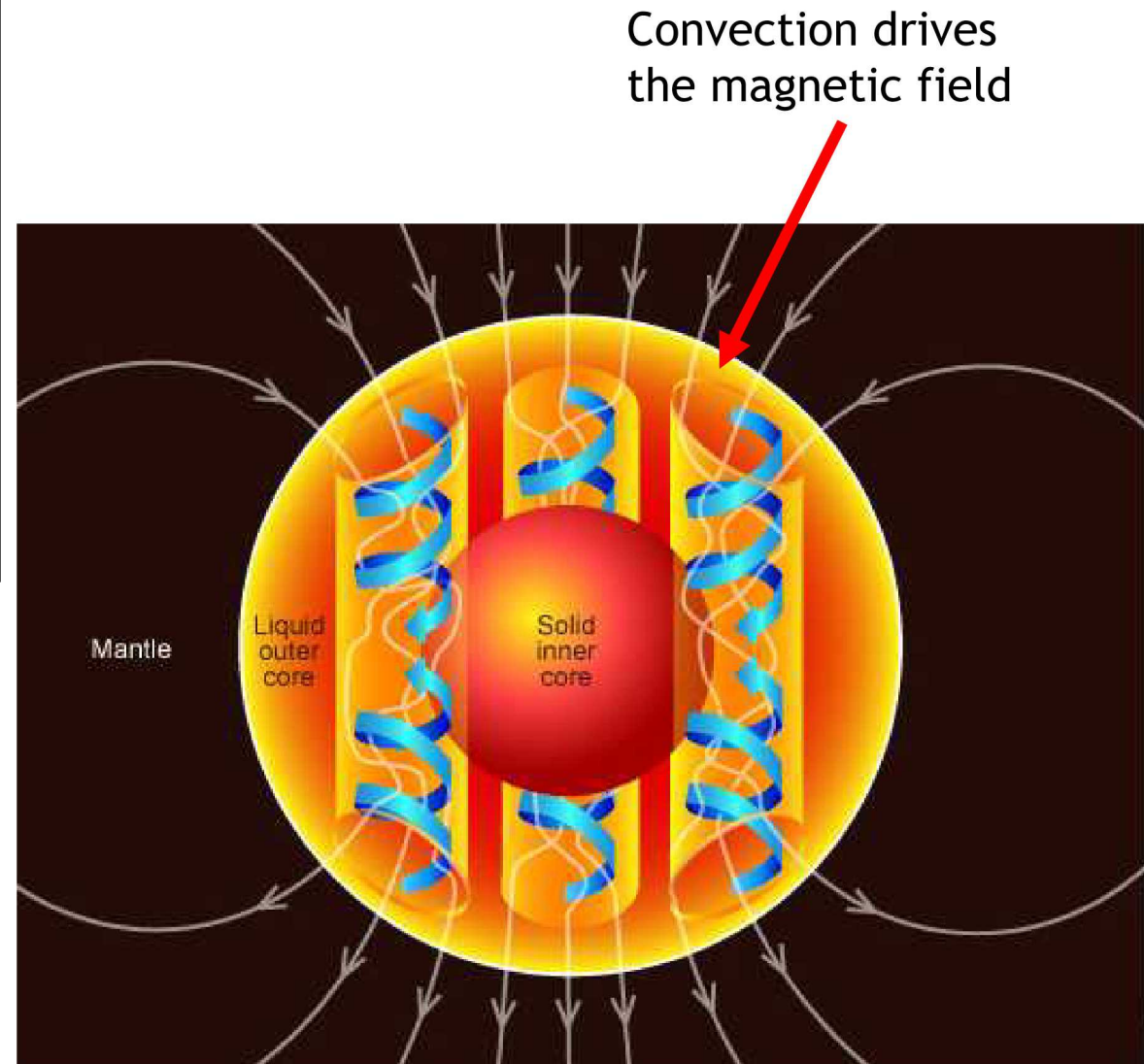


Unresolved Question:

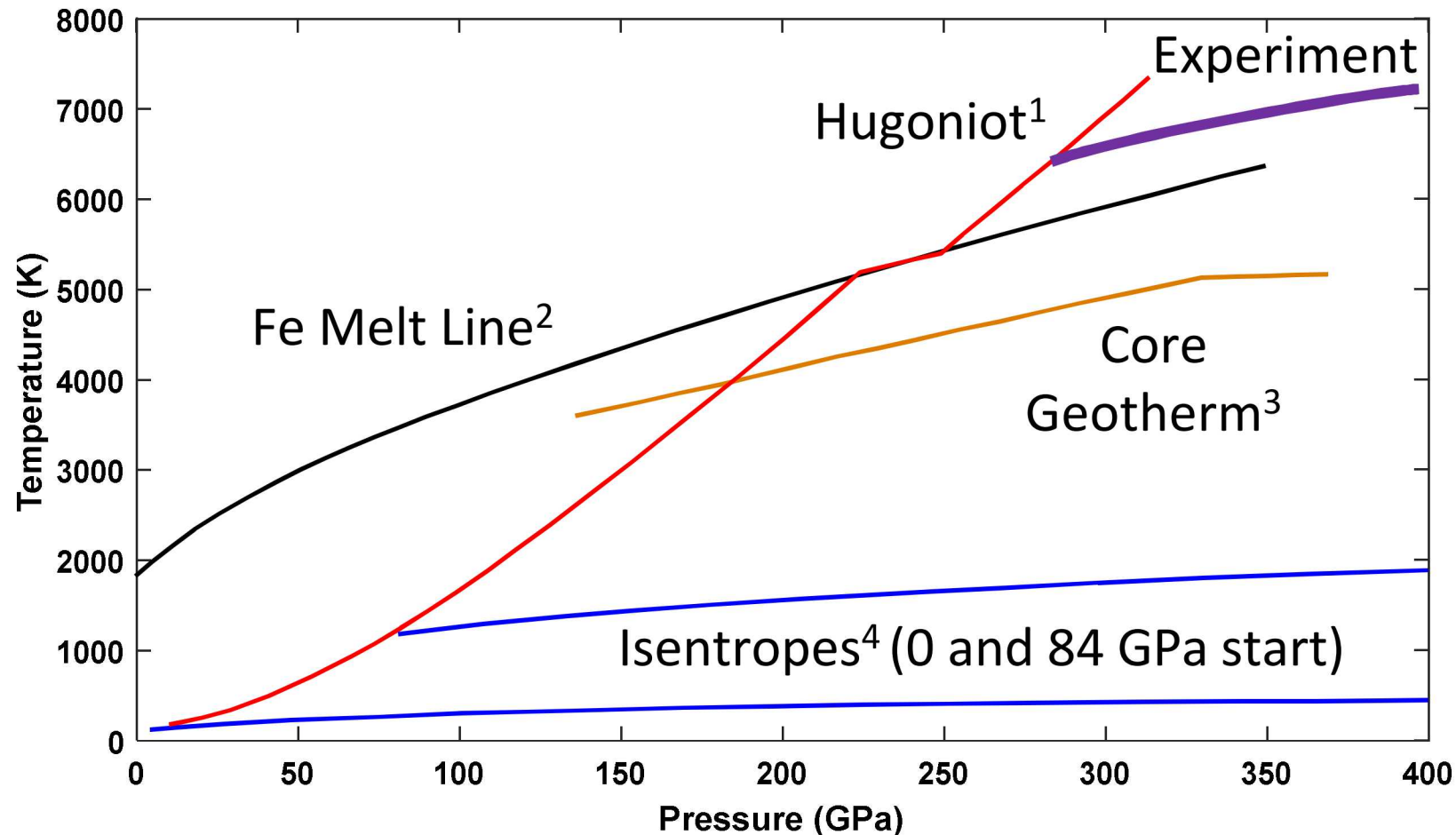
- Current estimates of the conductivity of the Earth's core could produce an inner core ranging from 4 billion to 1 billion years old

Important Current Research:

- Measuring conductivity of liquid iron at planetary core conditions



We designed an experimental path close to the conditions of the Earth's core



¹J. M. Brown and R. G. McQueen, J. Geophys. Res. 91, 7485, doi:10.1029/ JB091iB07p07485 (1986).

²S. Anzellini, A. Dewaele, M. Mezouar, P. Loubeyre, & G. Morard, (2013). Science, 340(6131), 464-466.

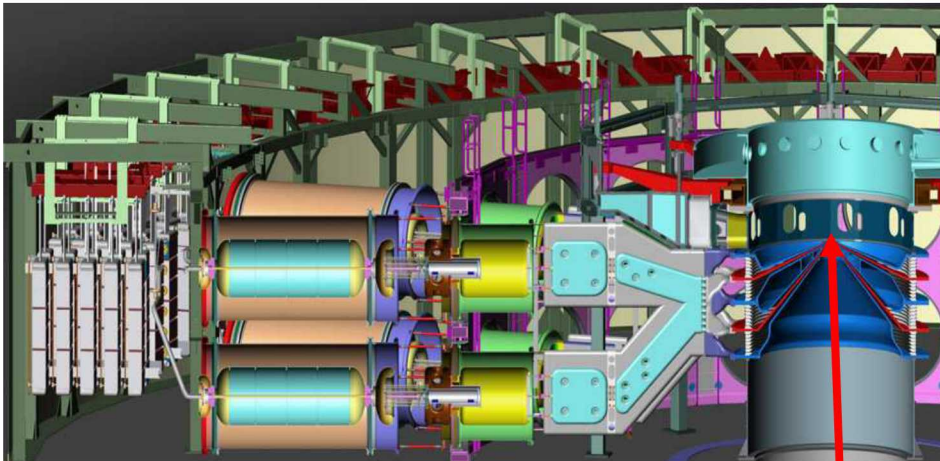
³F. D. Stacey, *Physics of the Earth*, 4th ed. (Cambridge University Press, Cambridge, 2008).

⁴J. Wang, R. F. Smith, J. H. Eggert, D. G. Braun, T. R. Boehly, J. Reed Patterson, P. M. Celliers, R. Jeanloz, G. W. Collins, and T. S. Duffy. Journal of Applied Physics, 114(2), p.023513. doi:10.1063/1.4813091 (2013).

The strip-line target configuration is a common method of driving planar samples to high pressure and density states on Z

Load hardware details

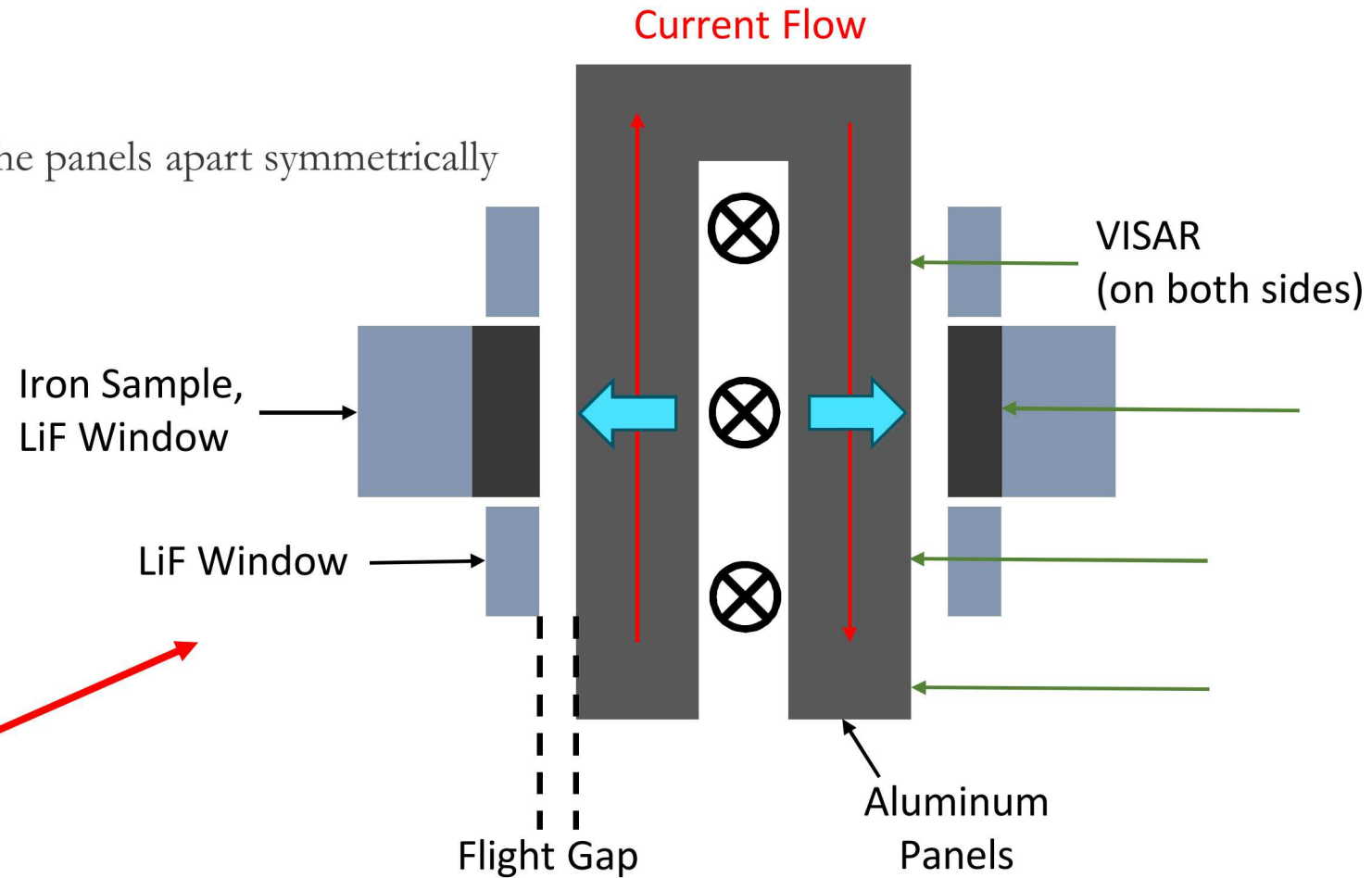
- Top Sample Pair Shown
- Parallel counter-propagating current drives the panels apart symmetrically
- Flight gap leads to initial shock



Marx Banks

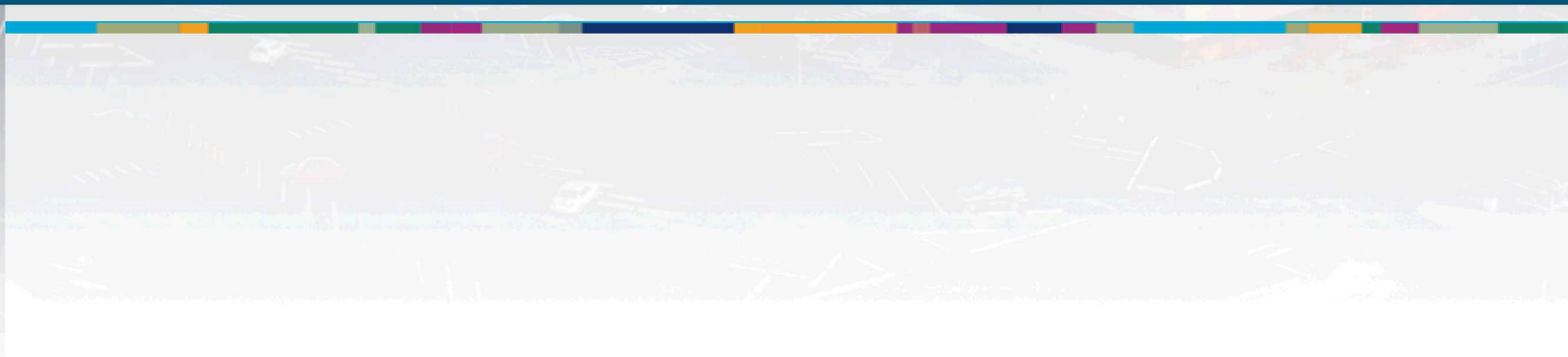
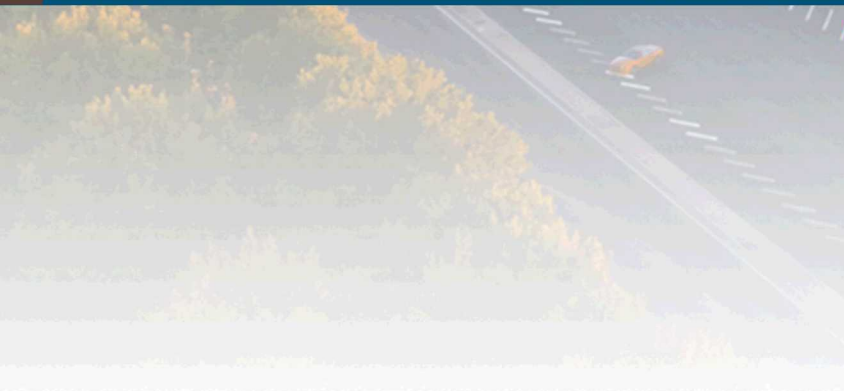
Triggering
and Pulse
Shaping

Center
Section:
Load
Hardware

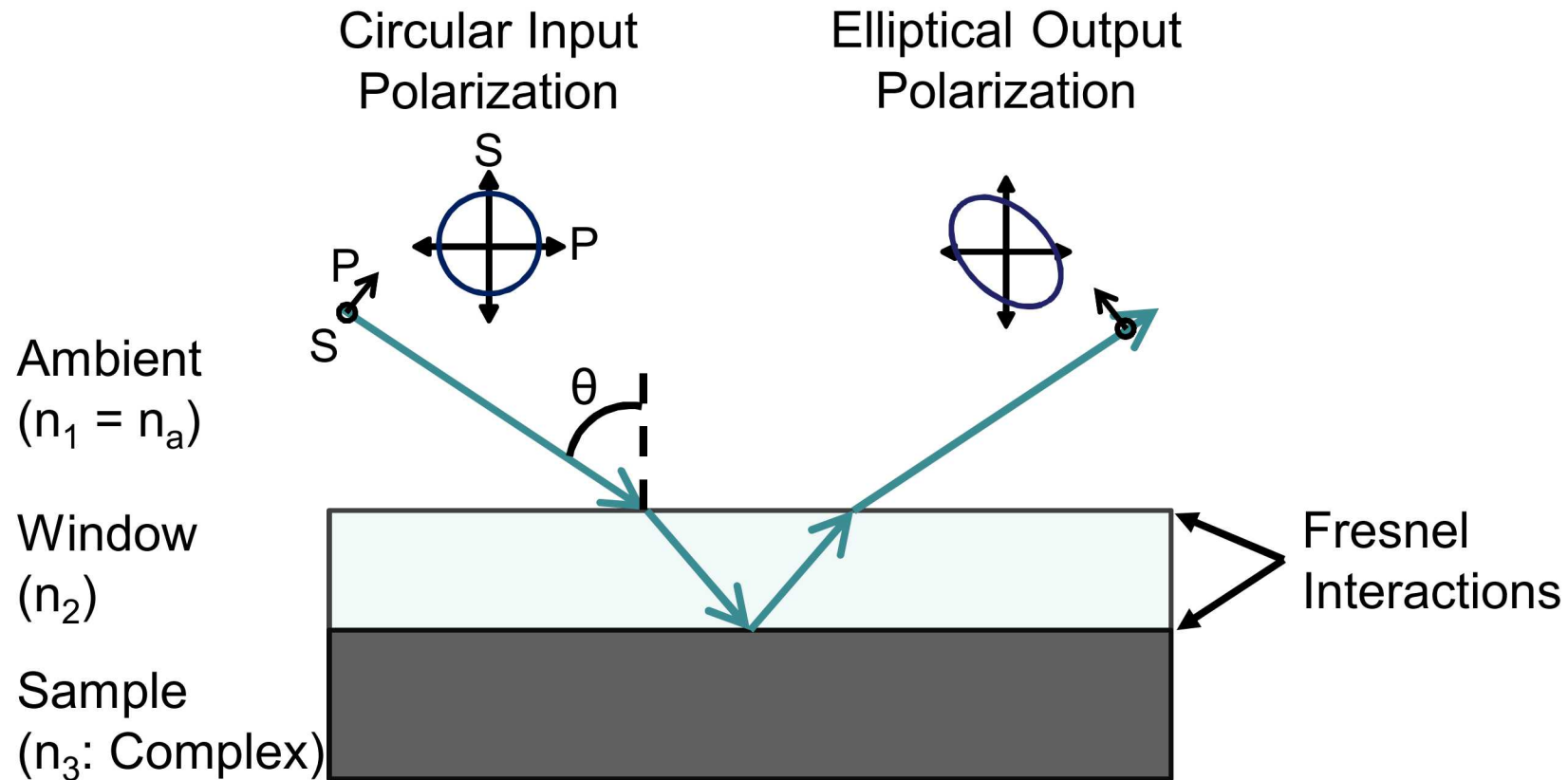




Conductivity Measurements with Ellipsometry



Ellipsometry uses a polarized laser to probe material dielectric properties at the laser wavelength



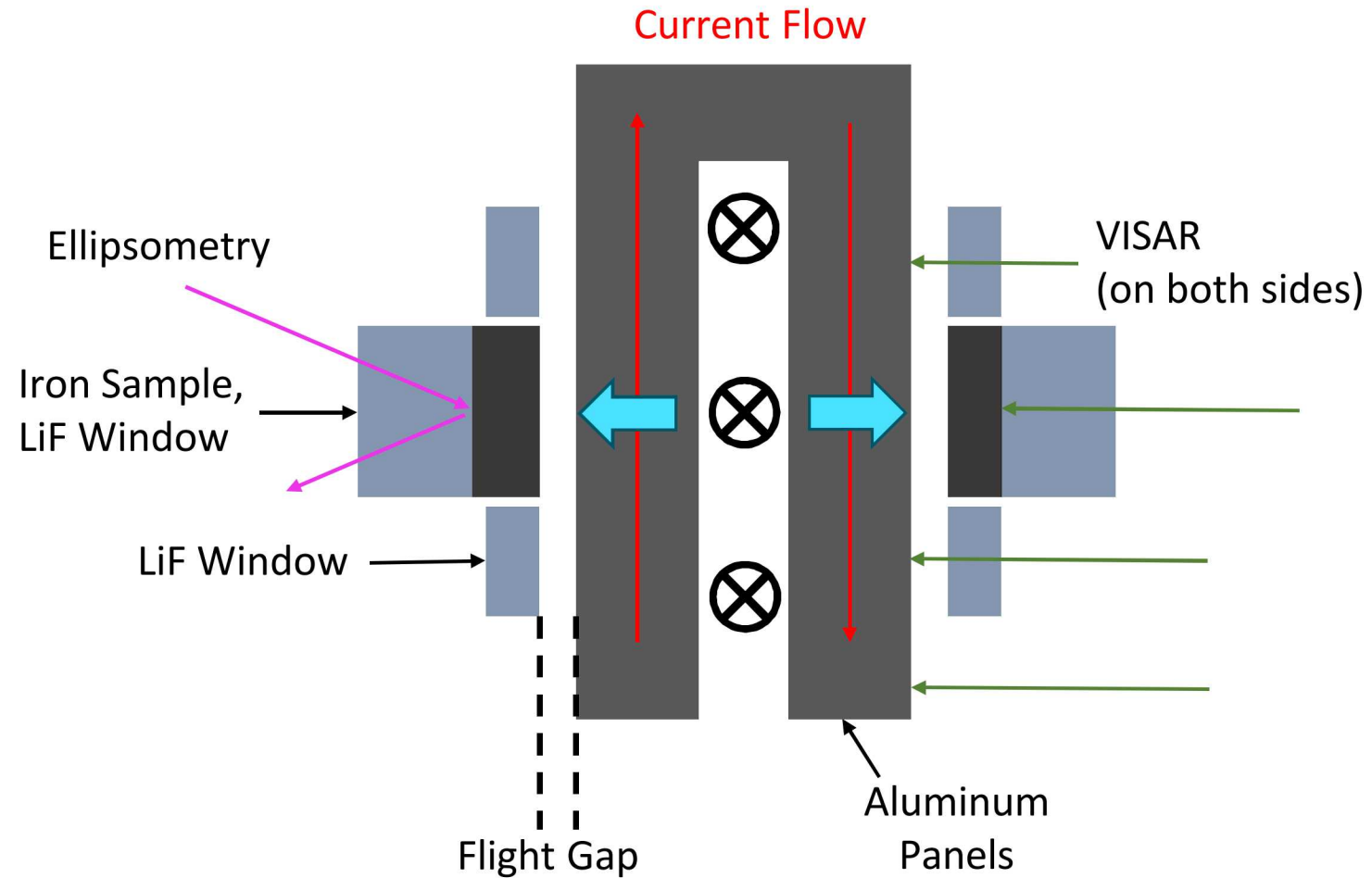
Along with the standard VISAR diagnostics, we have been fielding ellipsometry on one to two samples

Implementation of New Diagnostic

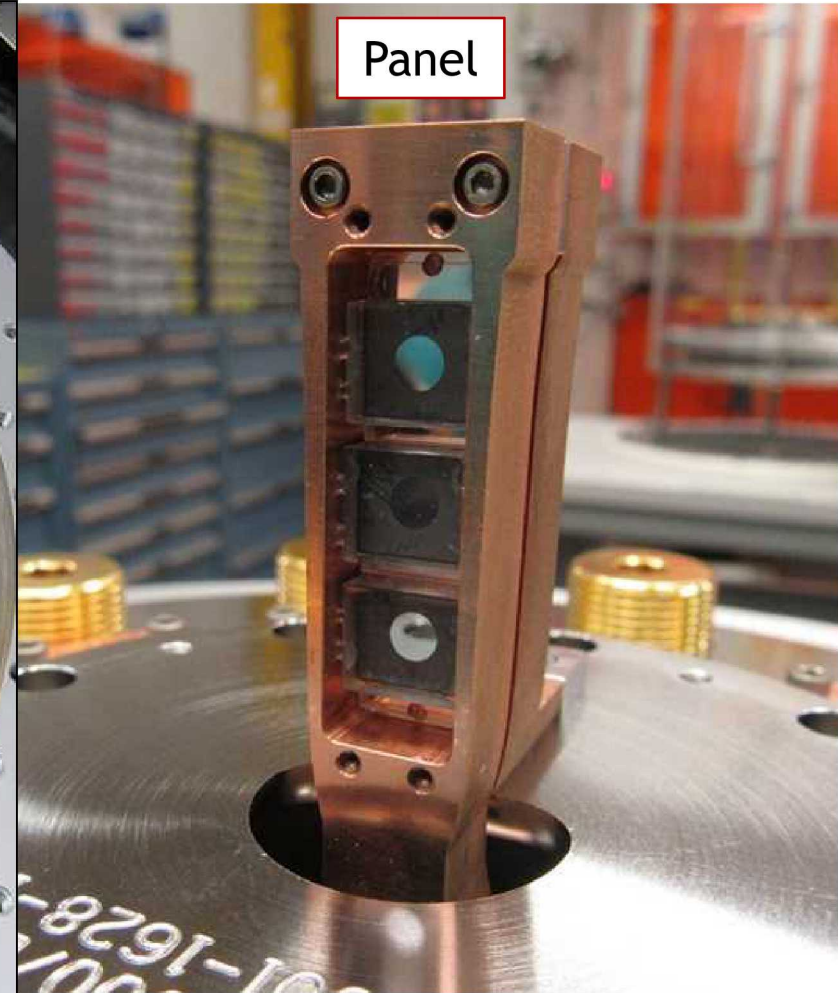
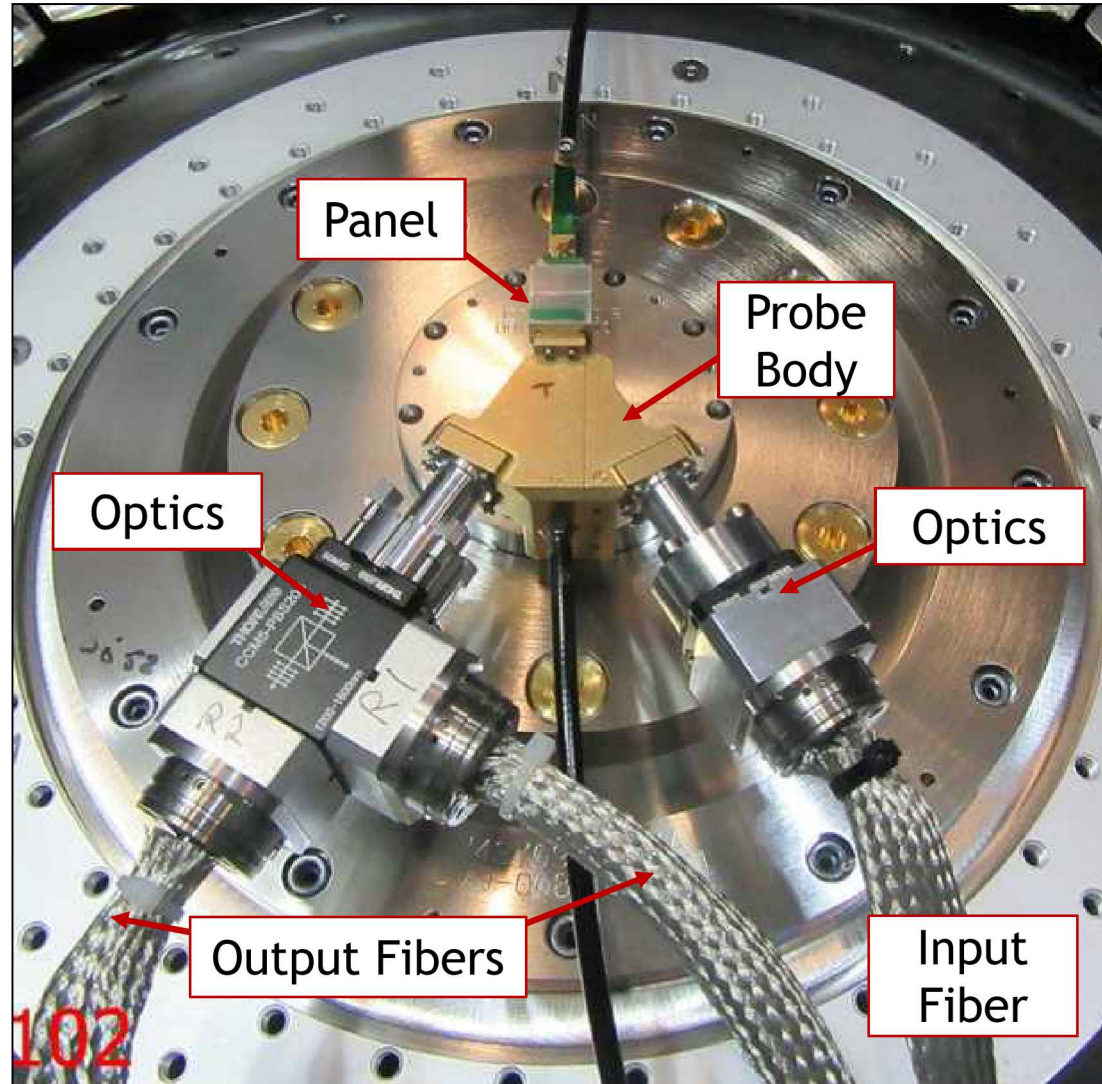
- Hardware/Procedural Changes
- No negative impact on other diagnostics or experiment

Advantages of this Experiment

- Overdriving detrimental window effects
- Minimal tilt compared to gas guns
- AC conductivity closely matches DC conductivity at these wavelengths



- 9 The Z hardware engineers made the fielding of this diagnostic possible



Obtaining specular reflections on dynamic experiments is difficult

Surface roughness and impactor tilt can severely hinder such measurements

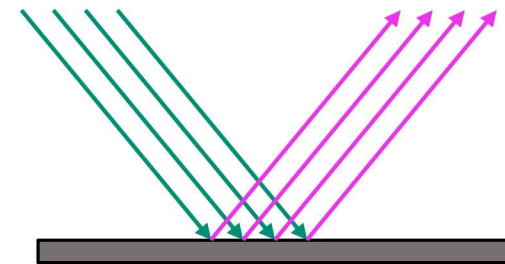
- Surface roughness can be propagated through the shock wave

Ellipsometry depends on AOI

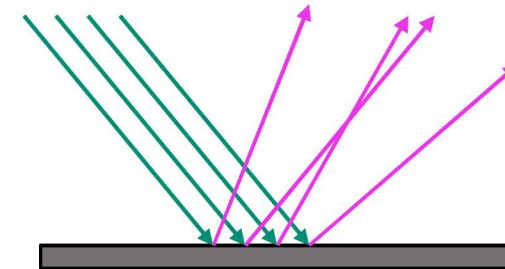
- cannot simply increase the collection

Ensure all surfaces are as smooth as possible

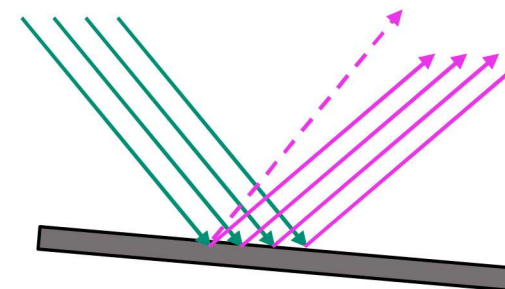
- Diamond turned metals (maybe lapping too)
 - 10-30 nm Ra
- Polished single crystal LiF
 - 20/10 scratch/dig



Specular Reflection

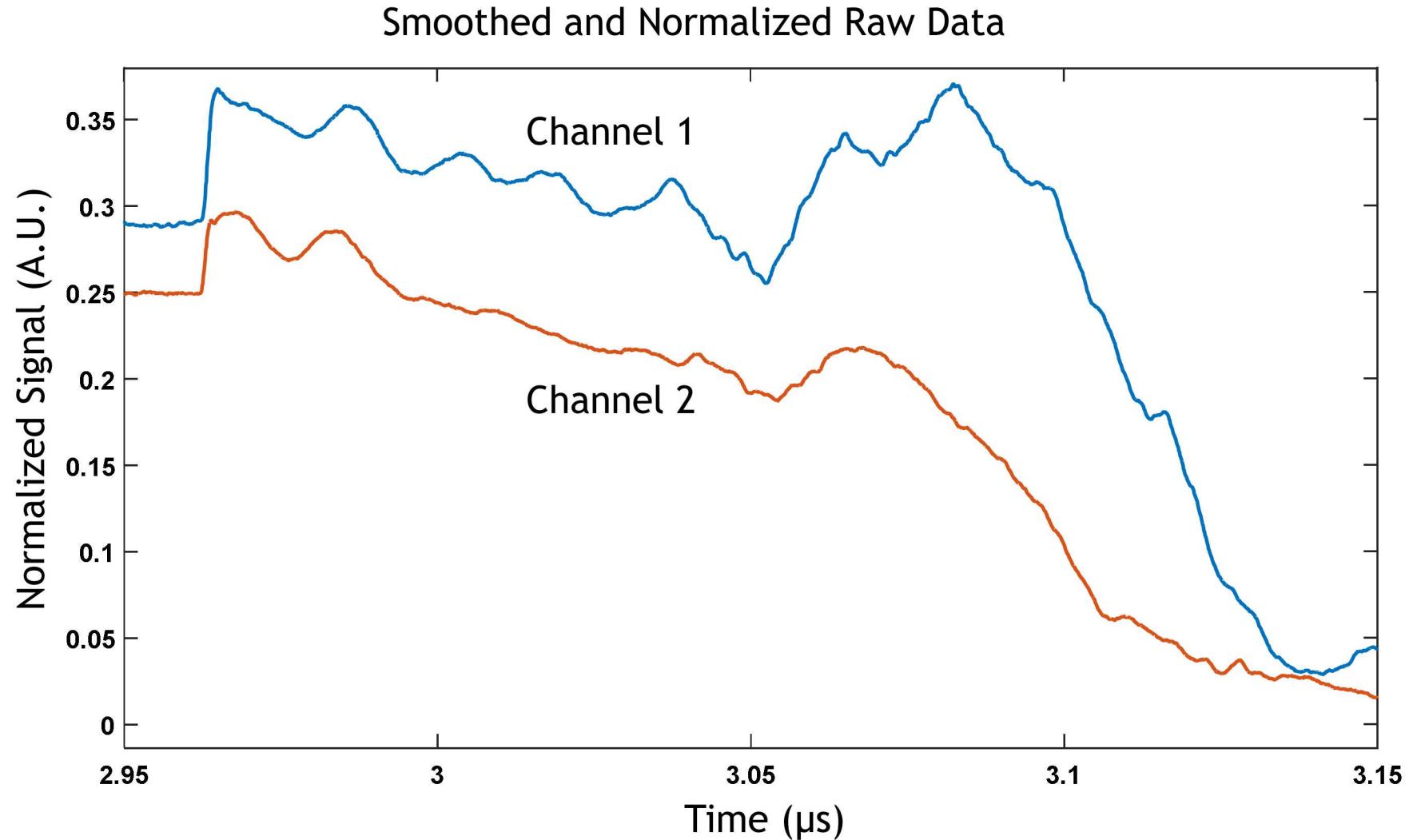


Scattered Reflection

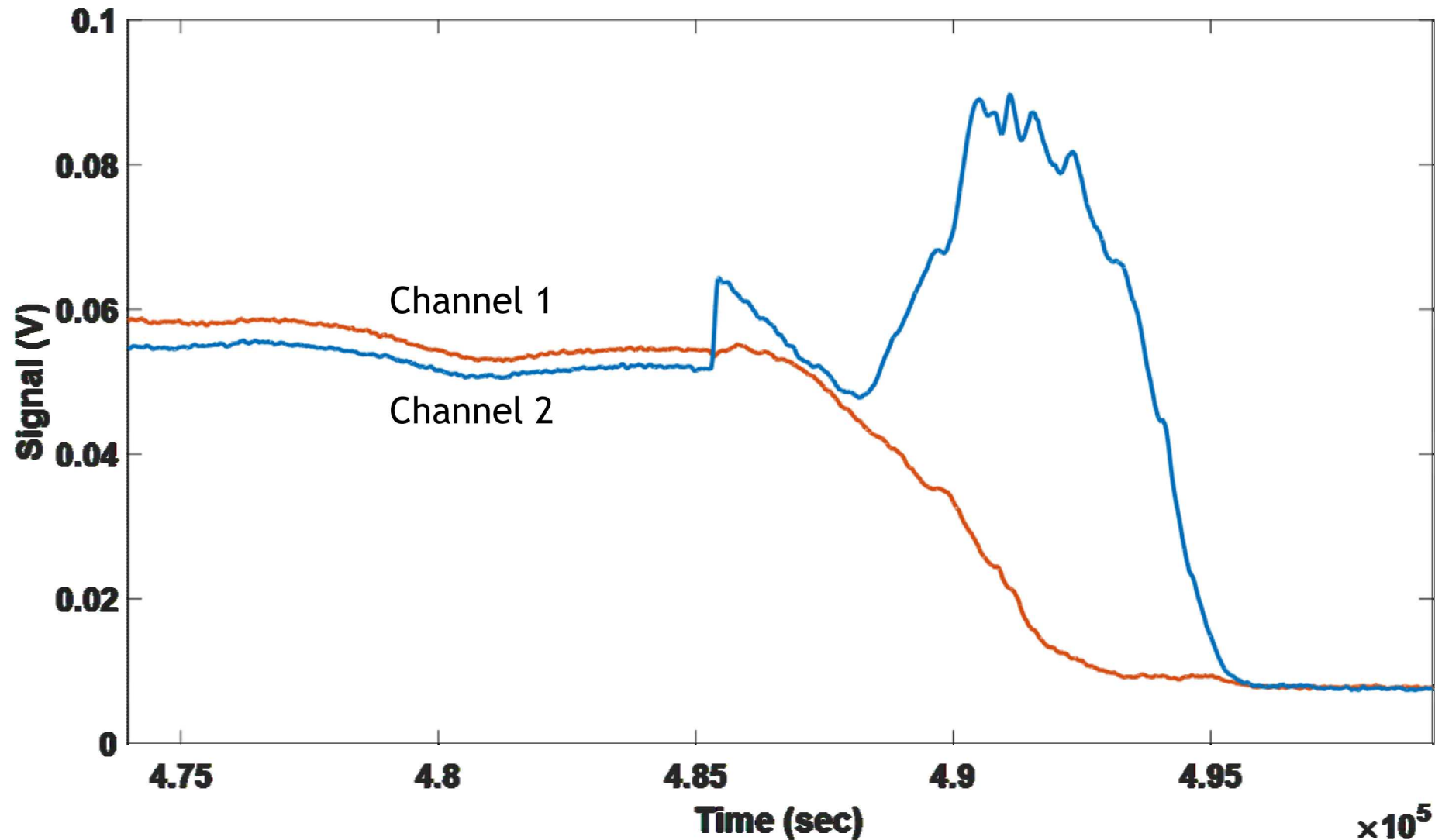


Tilted Reflection

Using a polished LiF 'sample' we obtained our best collection yet

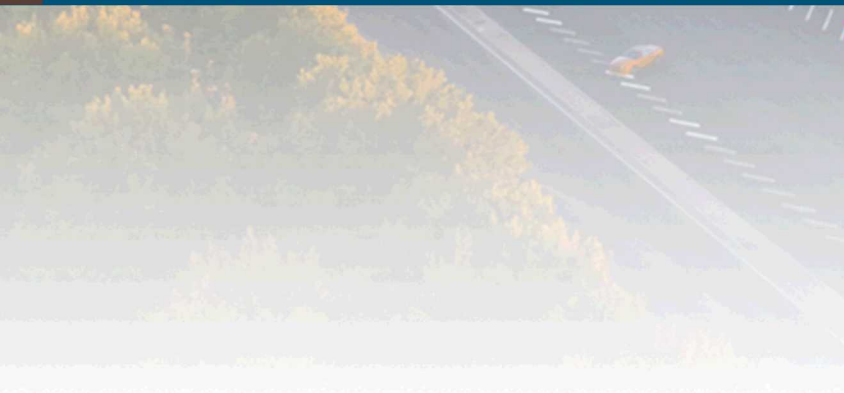


With increased focused on polishing, we were also able to see significant improvement on with an iron sample, though not as much as for the LiF sample arrangement

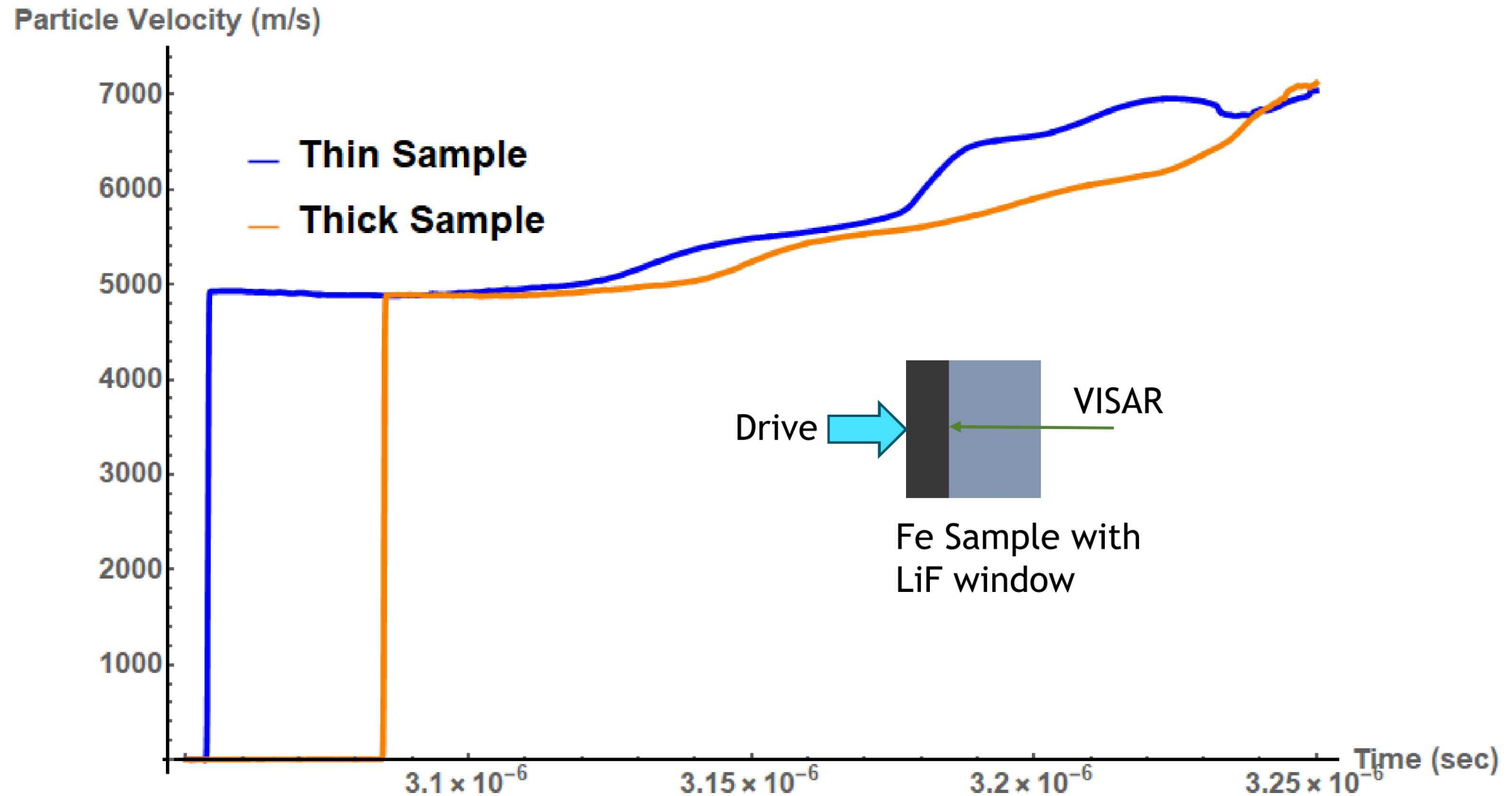




Equation of State



We use measurements of the particle velocity at all of the sample-window interfaces, provided by VISAR



An iterative backward-integration forward Lagrangian analysis is used to build the equation of state

Backward Integration

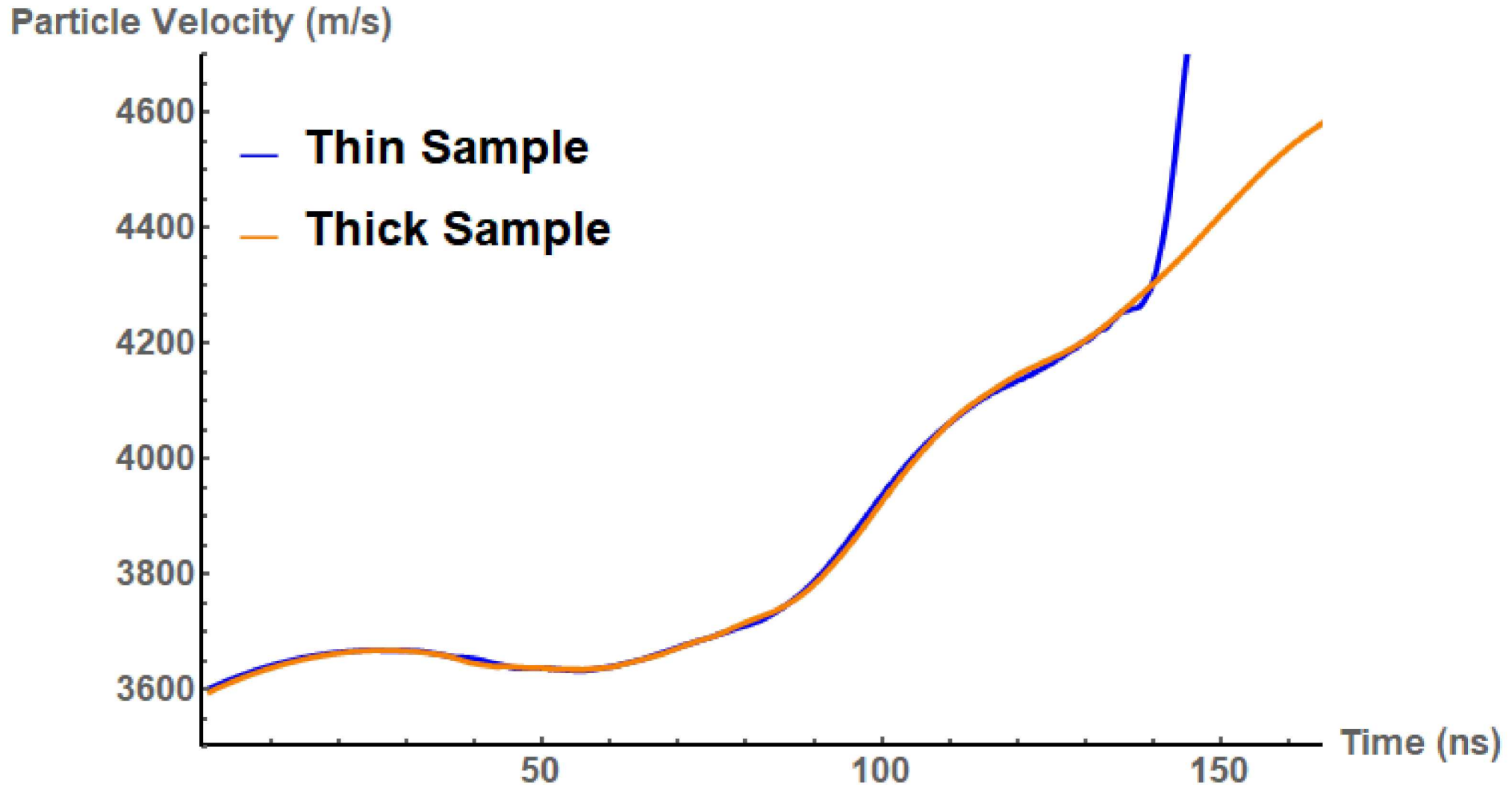
- The Lagrangian hydrodynamic equations along with a guess of the equation of state are backward integrated to obtain the drive profile at the sample-impactor interface:

$$\frac{\delta[P(\rho)]}{\delta x} = -\rho_0 \frac{\delta u}{\delta t}$$
$$\frac{1}{\rho_0} \frac{\delta u}{\delta x} = \frac{\delta \left[\frac{1}{\rho} \right]}{\delta t}$$

Davis, J.-P. "Experimental measurement of the principal isentrope for aluminum 6061-T6 to 240 GPa." *Journal of applied physics* 99.10 (2006): 103512.

Seagle, C. T., and A. J. Porwitzky. "Shock-ramp compression of tin near the melt line." *AIP Conference Proceedings*. Vol. 1979. No. 1. AIP Publishing, 2018.

The drive conditions for the two samples should be equal until the release wave from the thin sample reaches this interface



An iterative backward-integration forward Lagrangian analysis is used to build the equation of state

Backward Integration

- The Lagrangian hydrodynamic equations along with a guess of the equation of state are backward integrated to obtain the drive profile at the sample-impactor interface:

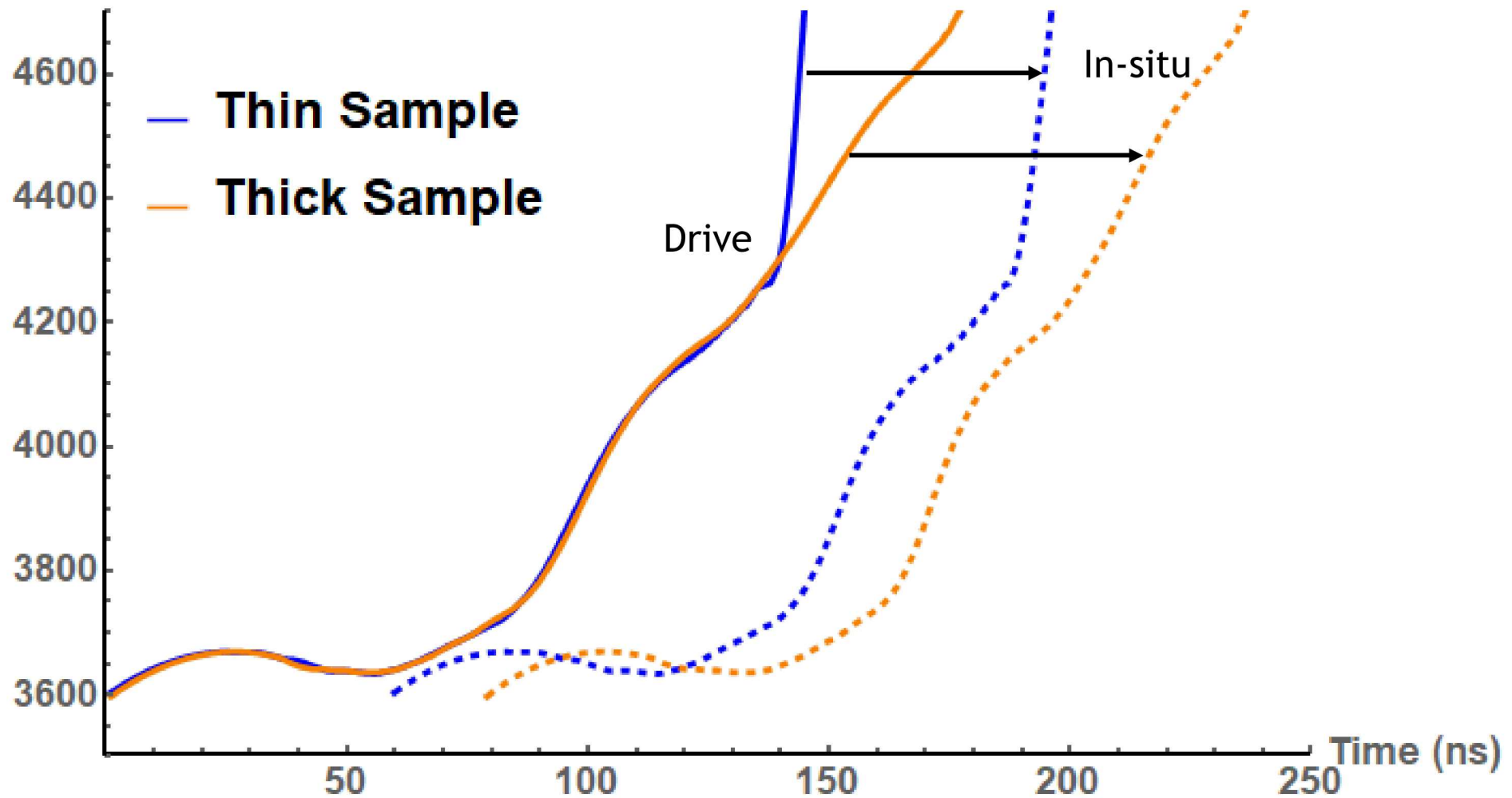
Forward Propagation

- The drive state can then be propagated forward to the sample-window interface to obtain the *in-situ* particle velocity (the particle velocity that would have been present at that location had there not been a release interface)

$$\frac{\delta[P(\rho)]}{\delta x} = -\rho_0 \frac{\delta u}{\delta t}$$
$$\frac{1}{\rho_0} \frac{\delta u}{\delta x} = \frac{\delta \left[\frac{1}{\rho} \right]}{\delta t}$$

The drive condition is propagated forward to the sample-window interface location

Particle Velocity (m/s)



An iterative backward-integration forward Lagrangian analysis is used to build the equation of state

Backward Integration

- The Lagrangian hydrodynamic equations along with a guess of the equation of state are backward integrated to obtain the drive profile at the sample-impactor interface:

$$\frac{\delta[P(\rho)]}{\delta x} = -\rho_0 \frac{\delta u}{\delta t}$$

$$\frac{1}{\rho_0} \frac{\delta u}{\delta x} = \frac{\delta \left[\frac{1}{\rho} \right]}{\delta t}$$

Forward Propagation

- The drive state can then be propagated forward to the sample-window interface to obtain the *in-situ* particle velocity (the particle velocity that would have been present at that location had there not been a release interface)

Lagrangian Sound Speed and EOS

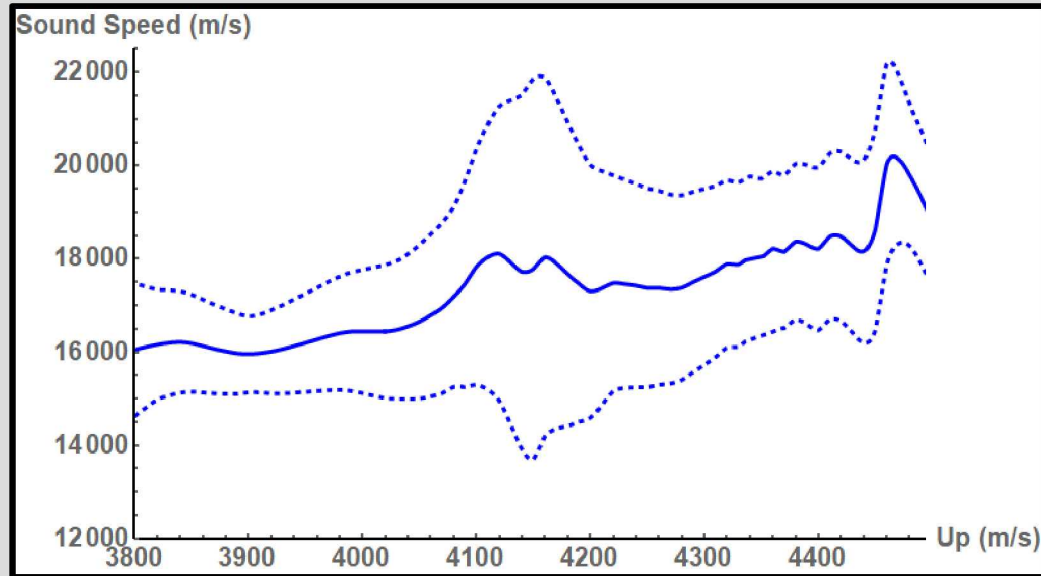
- A sound speed can then be directly calculated from $\Delta x / \Delta t$ measurements
- A P- ρ EOS is formed from the sound speed:

$$\frac{1}{\rho_f} = \frac{1}{\rho_s} - \int_{u_{ps}}^{u_{pf}} \frac{du_p}{\rho_0 C_L}$$

$$P_f = P_s + \int_{u_{ps}}^{u_{pf}} \rho_0 C_L du_p$$

Lagrangian sound speed is determined, and used to calculate the equation of state

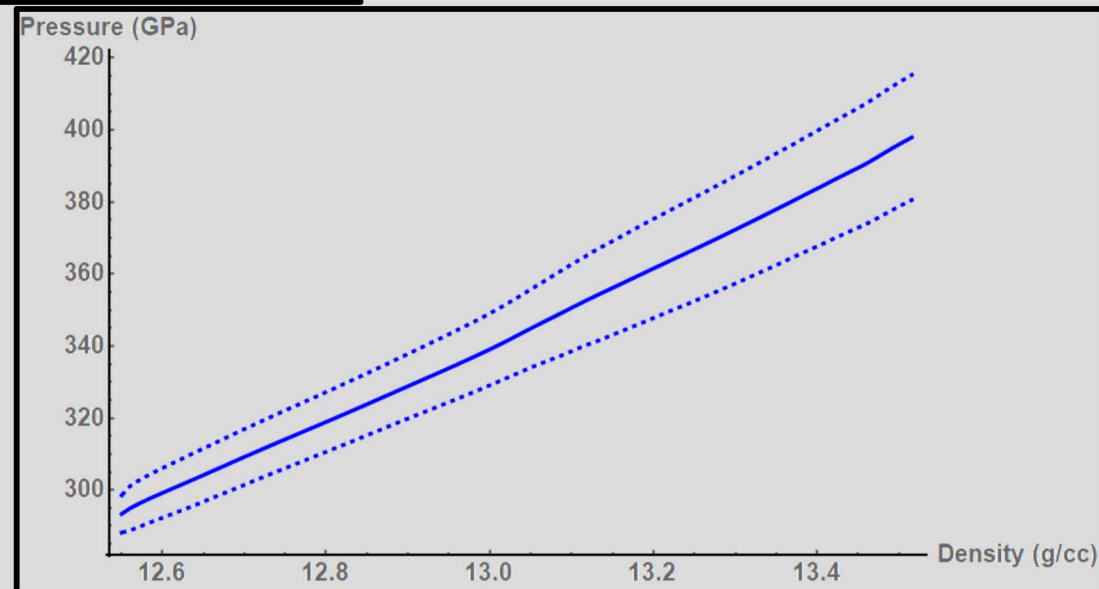
Sound Speed



$$\frac{1}{\rho_f} = \frac{1}{\rho_s} - \int_{u_{ps}}^{u_{pf}} \frac{du_p}{\rho_0 C_L}$$

$$P_f = P_s + \int_{u_{ps}}^{u_{pf}} \rho_0 C_L du_p$$

Equation of State



An iterative backward-integration forward Lagrangian analysis is used to build the equation of state

Backward Integration

- The Lagrangian hydrodynamic equations along with a guess of the equation of state are backward integrated to obtain the drive profile at the sample-impactor interface:

$$\frac{\delta[P(\rho)]}{\delta x} = -\rho_0 \frac{\delta u}{\delta t}$$

$$\frac{1}{\rho_0} \frac{\delta u}{\delta x} = \frac{\delta \left[\frac{1}{\rho} \right]}{\delta t}$$

Forward Propagation

- The drive state can then be propagated forward to the sample-window interface to obtain the *in-situ* particle velocity (the particle velocity that would have been present at that location had there not been a release interface)

Lagrangian Sound Speed and EOS

- A sound speed can then be directly calculated from $\Delta x / \Delta t$ measurements
- A P- ρ EOS is formed from the sound speed:

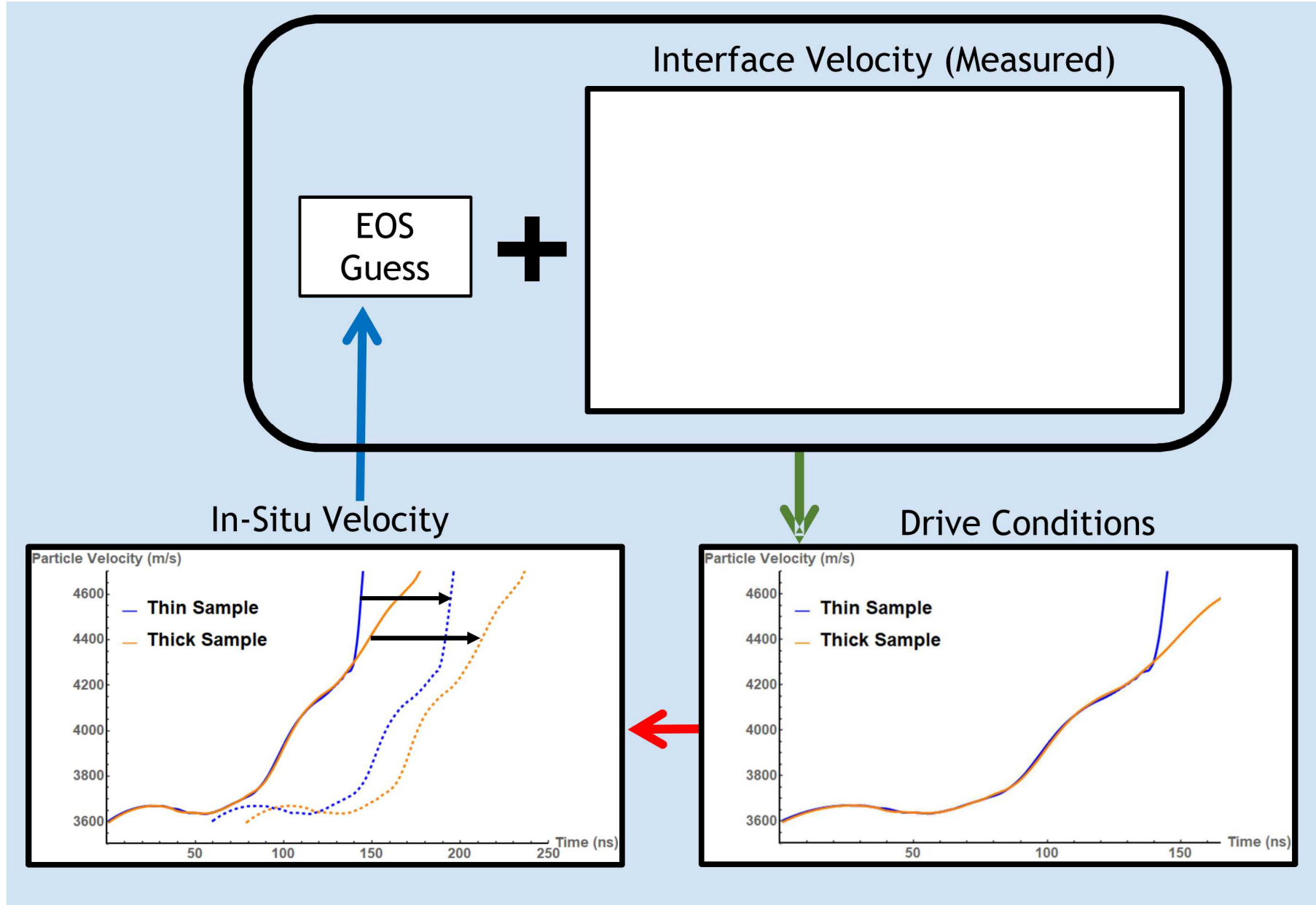
$$\frac{1}{\rho_f} = \frac{1}{\rho_s} - \int_{u_{ps}}^{u_{pf}} \frac{du_p}{\rho_0 C_L}$$

$$P_f = P_s + \int_{u_{ps}}^{u_{pf}} \rho_0 C_L du_p$$

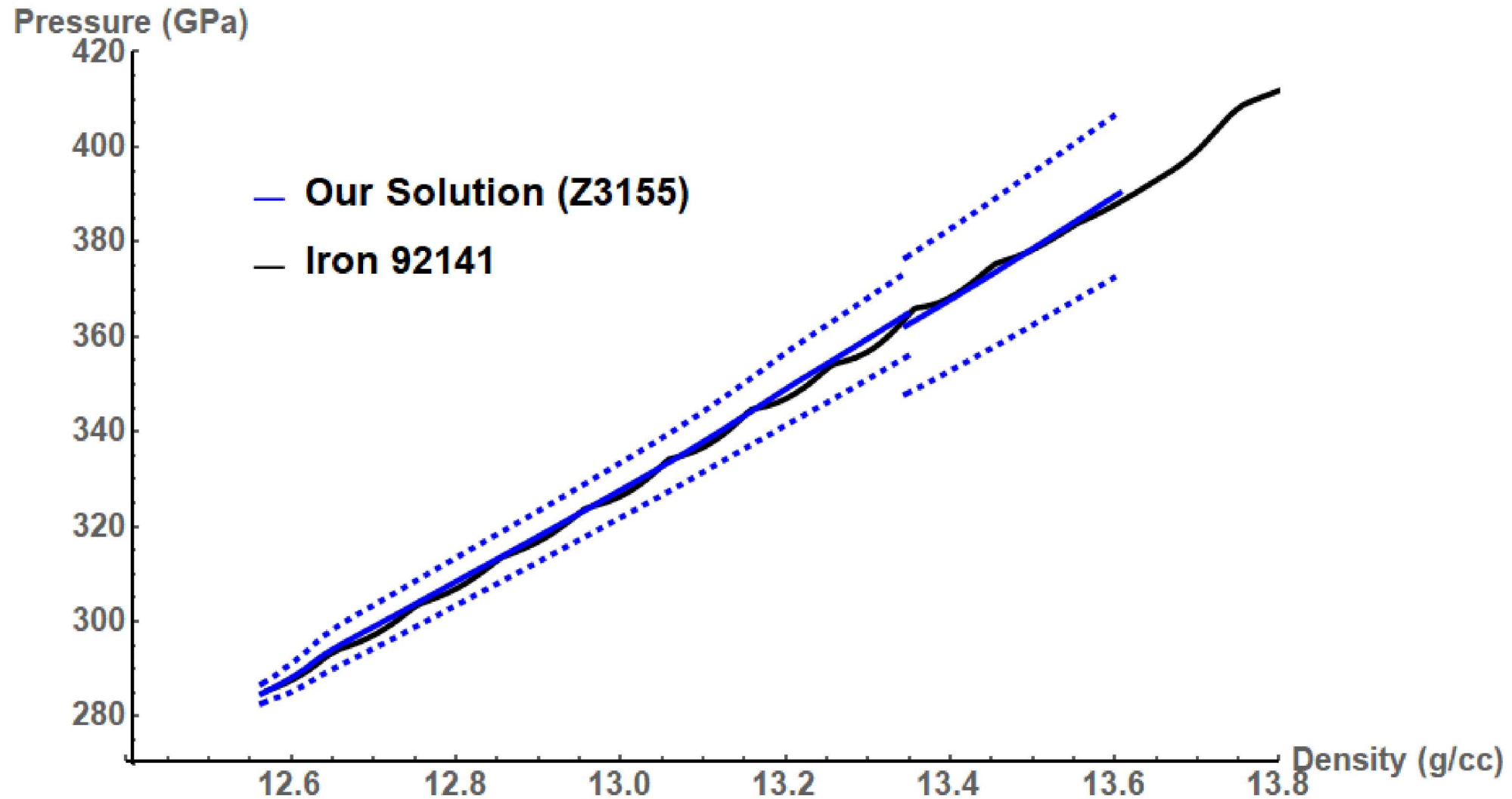
Iterate

- The process is then repeated with this new EOS
- This iterative process continues until the new EOS matches the solution from the previous iteration

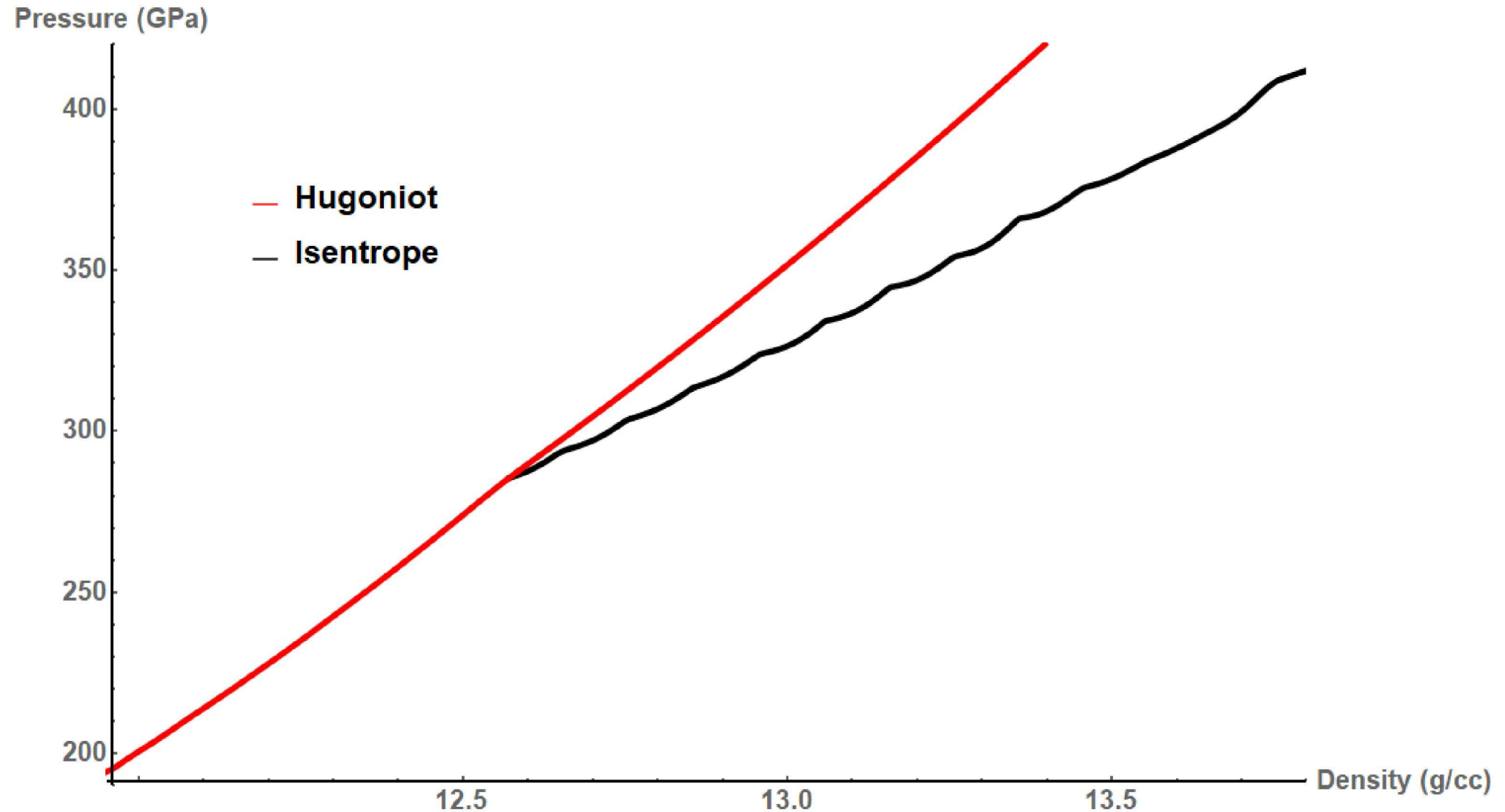
An iterative backward-integration forward Lagrangian analysis is used to build the equation of state



Results from our previous experiment agree well with current EOS tables

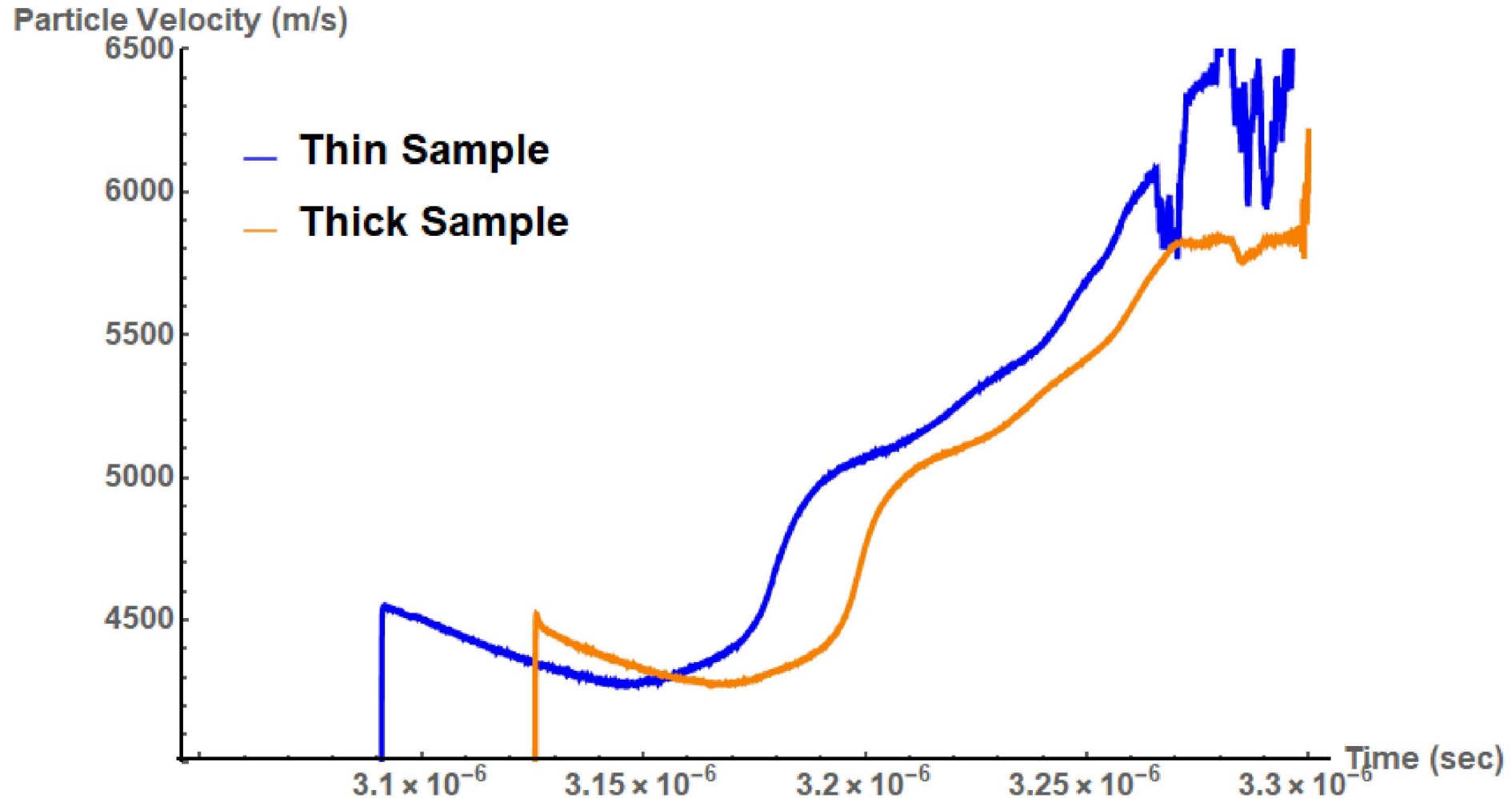


This framework typically assumes a steady shock front before the ramp



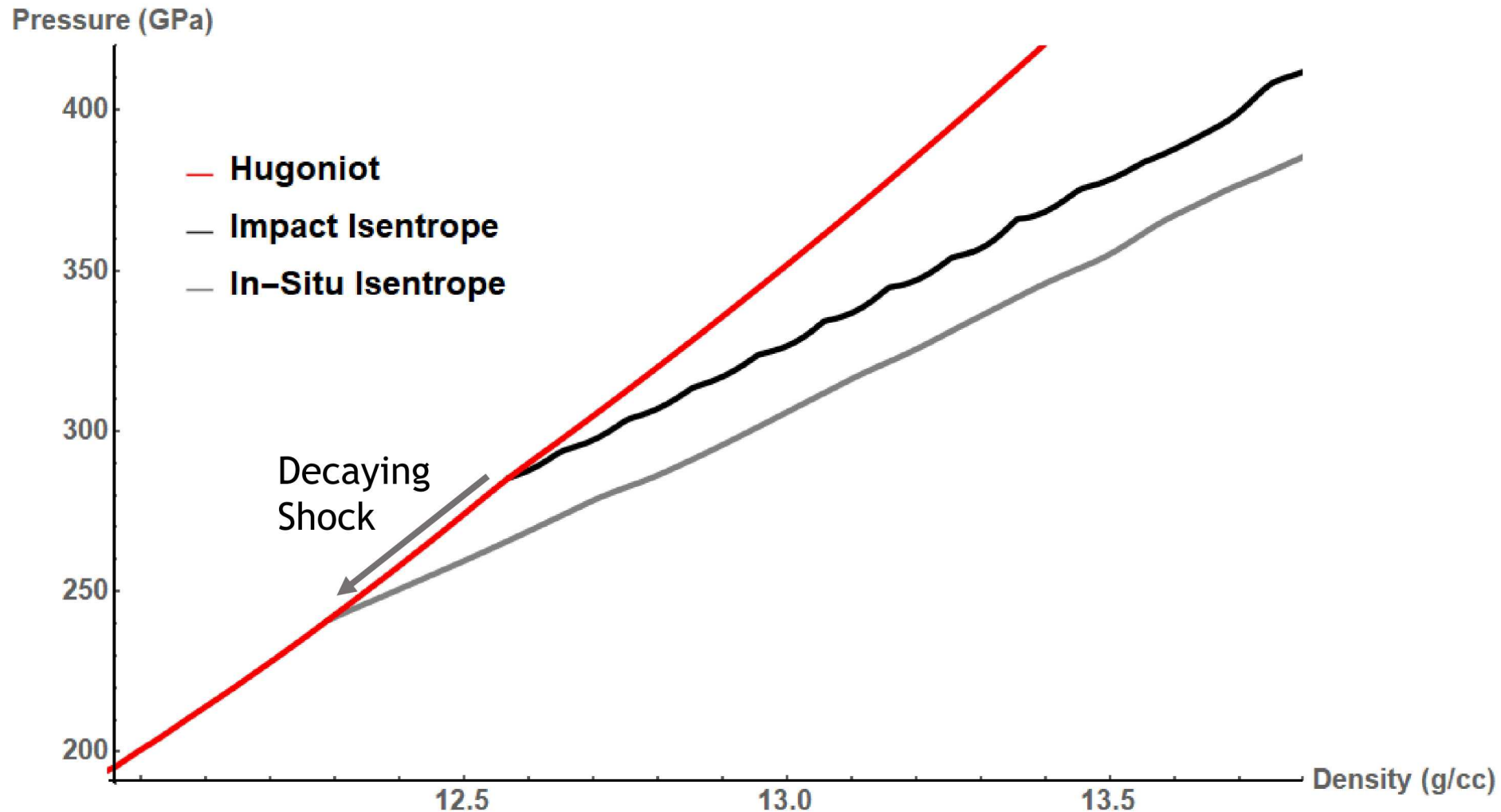
This framework typically assumes a steady shock front before the ramp

- Our most recent experiment experienced noticeable decay on the initial shock state



The experiment is no longer constrained along a single isentrope

- Instead, a range of isentropes are covered based on the Lagrangian position of the sample

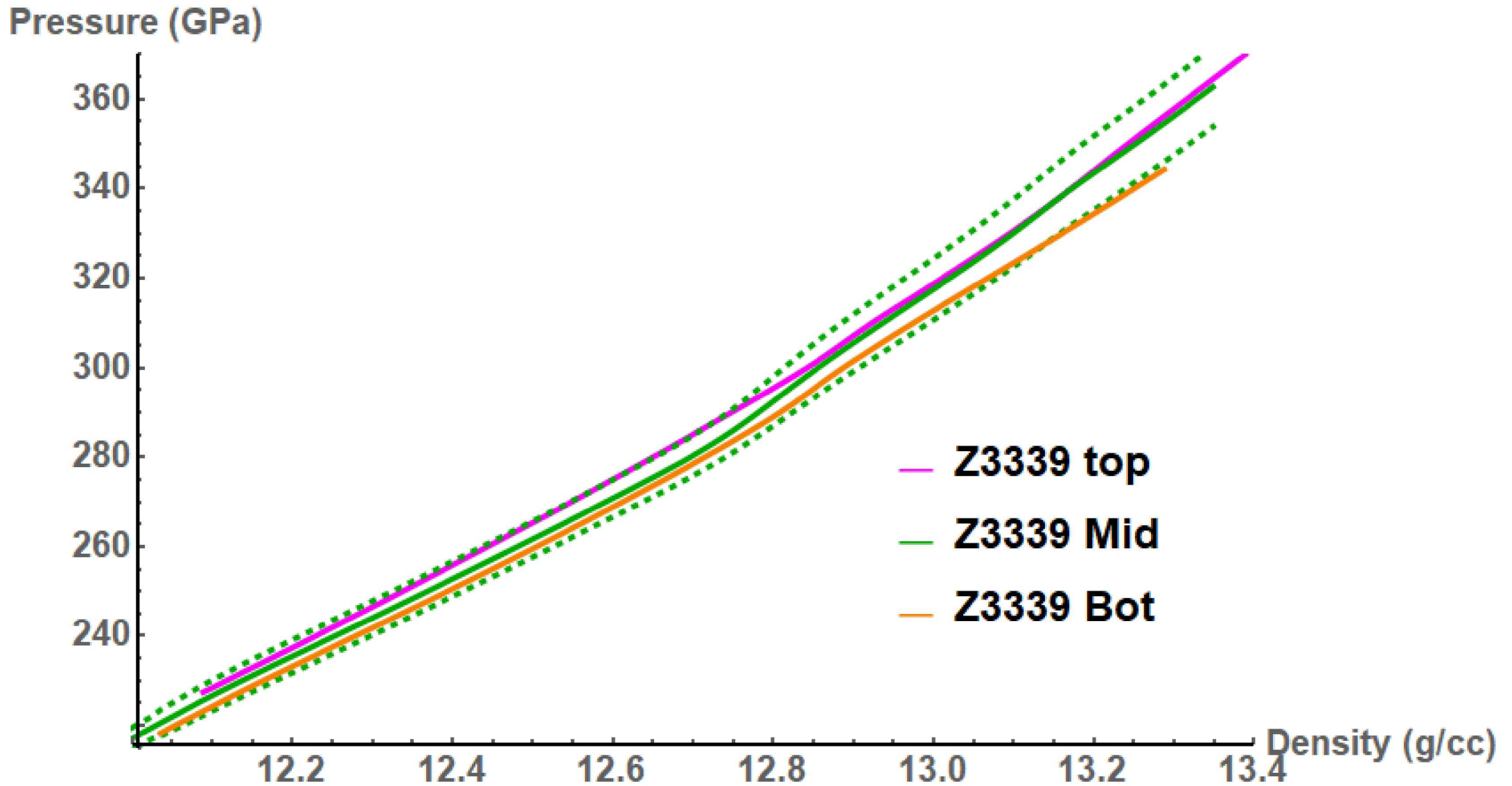


With modifications to the standard analysis, we analyzed the data from the three sample pairs in Z3339

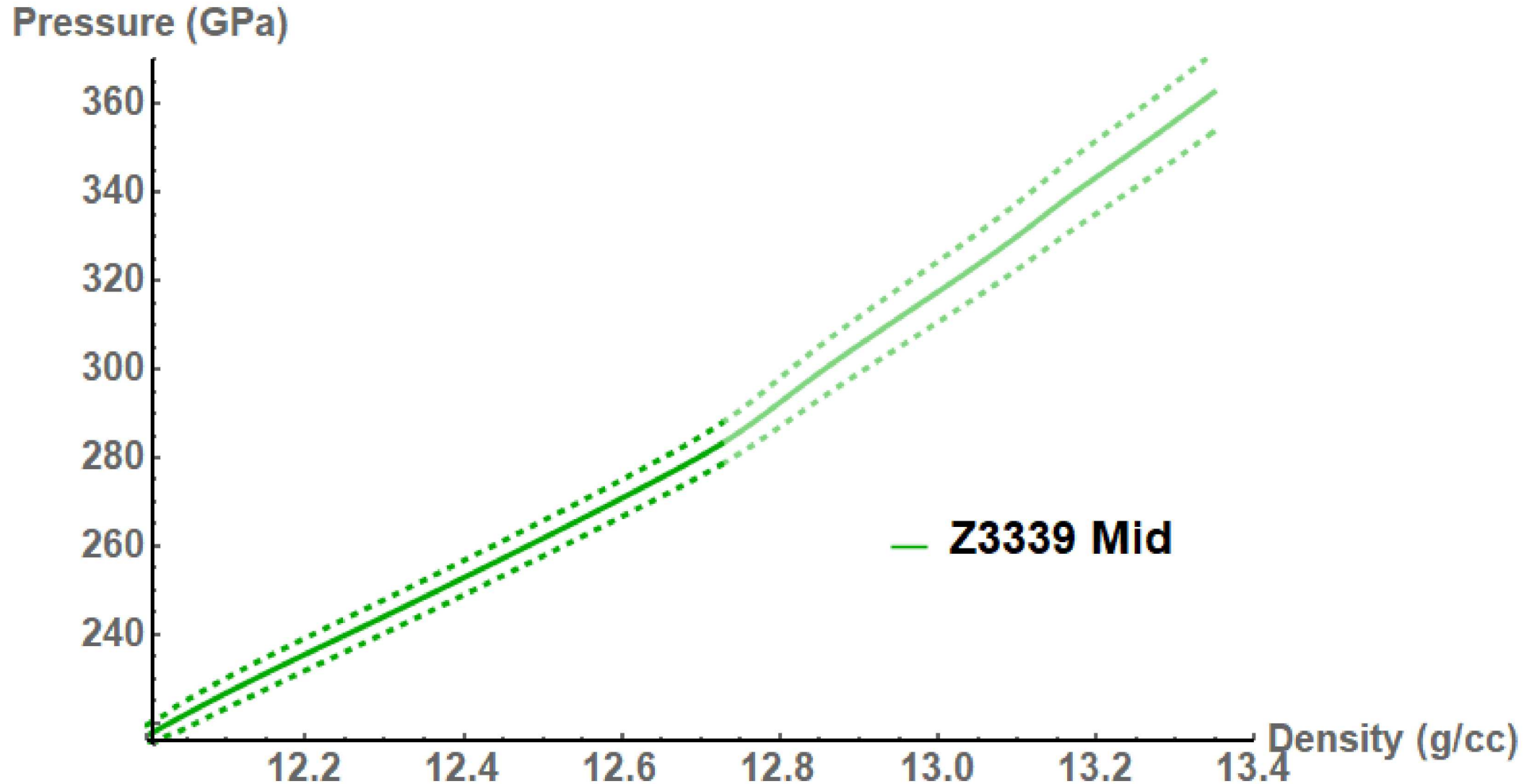
Modifications primarily include:

- The shock-front, and associated boundary condition, varies as a function of Lagrangian position, based on the observed shock states at impact and the two sample-window interfaces.
- Instead of inputting a single isentrope EOS as the 'guess' into the iterative process, a range of isentropes covering the conditions defined by the variable shock state must be provided or generated by the user.

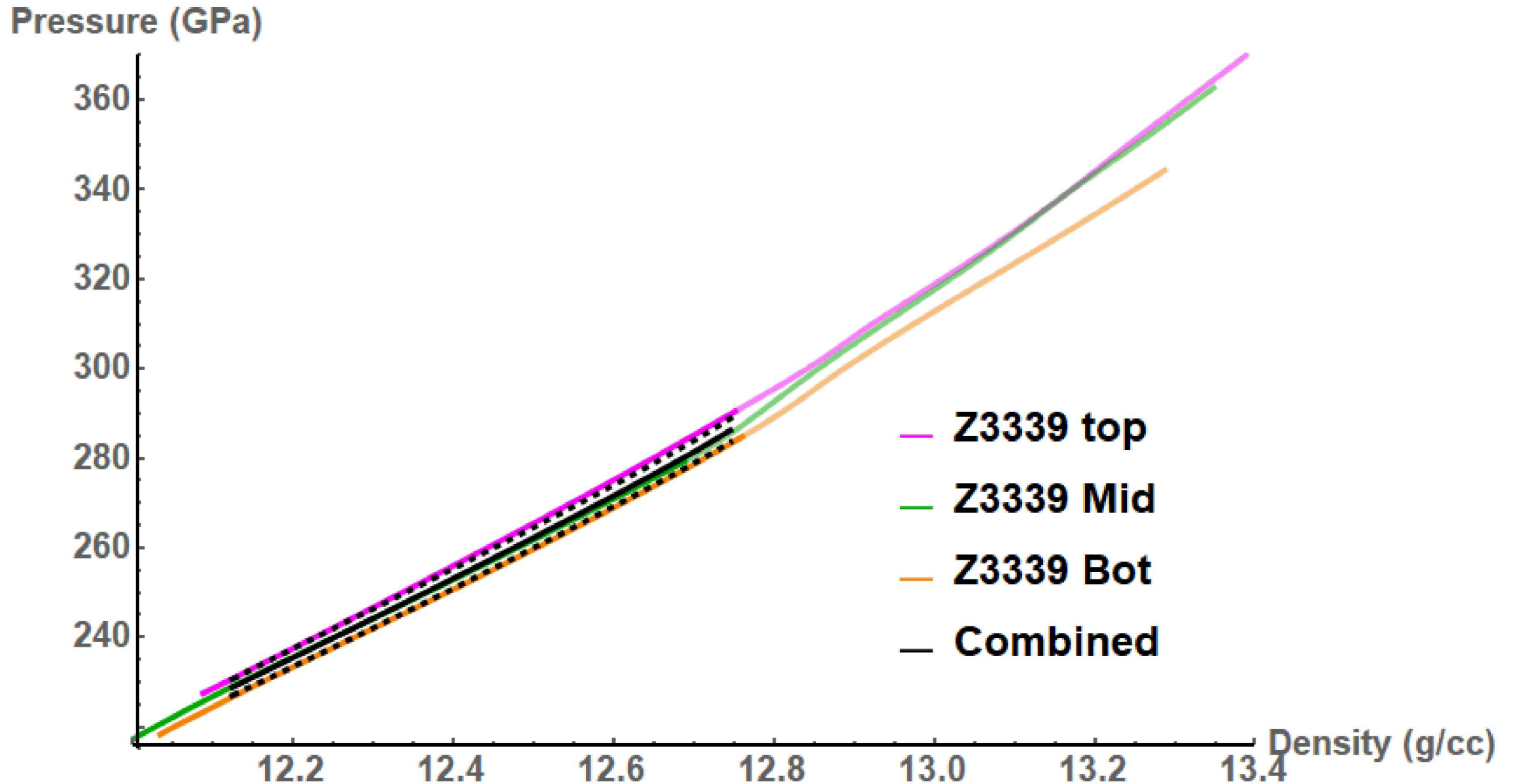
With modifications to the standard analysis, we analyzed the data from the three sample pairs in Z3339



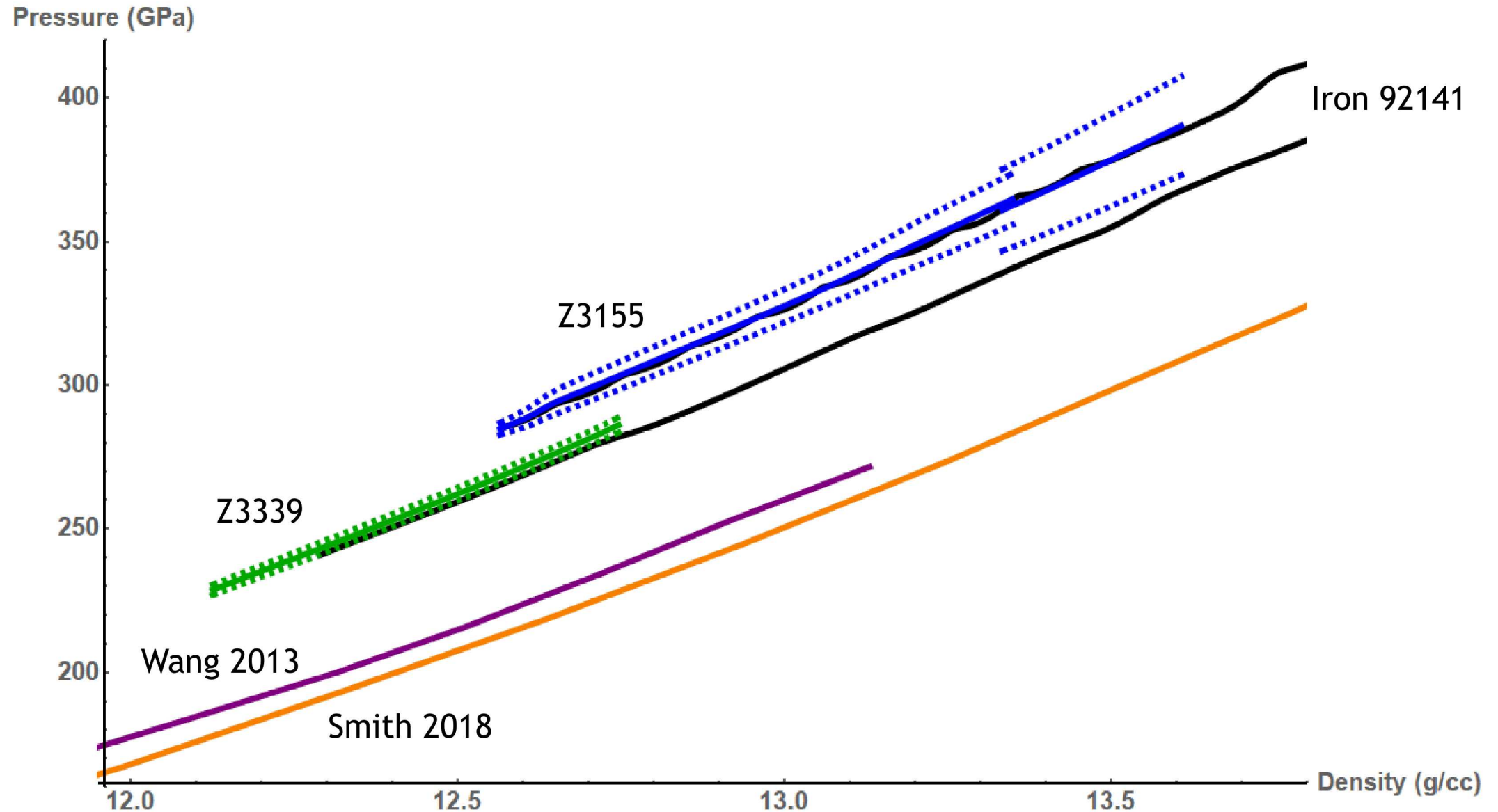
However, the latter half of these data sets are not adequately converging



We combine the relevant data from all three sample pairs



Our two data sets both agree well with the iron 92141 sesame EOS table



Equation of state information is often incorporated into research via parameters to analytic models

- Various analytic models
 - Birch-Murnaghan, Vinet, Mie-Gruneisen, etc.
- Planetary modeling codes
 - BurnMan
- Fit parameters for the existing liquid data:

$$P = \frac{3}{2} K_0 \left(\left(\frac{\rho}{\rho_0} \right)^{\frac{7}{3}} - \left(\frac{\rho}{\rho_0} \right)^{\frac{5}{3}} \right) \left[1 - \frac{3}{4} (4 - K_0') \left(\left(\frac{\rho}{\rho_0} \right)^{\frac{2}{3}} - 1 \right) \right]$$

$$P_{th} = \gamma_{vib} \rho \int_{300}^T C_{v,vib} dT + \gamma_e \rho \int_{300}^T C_{ve} dT$$

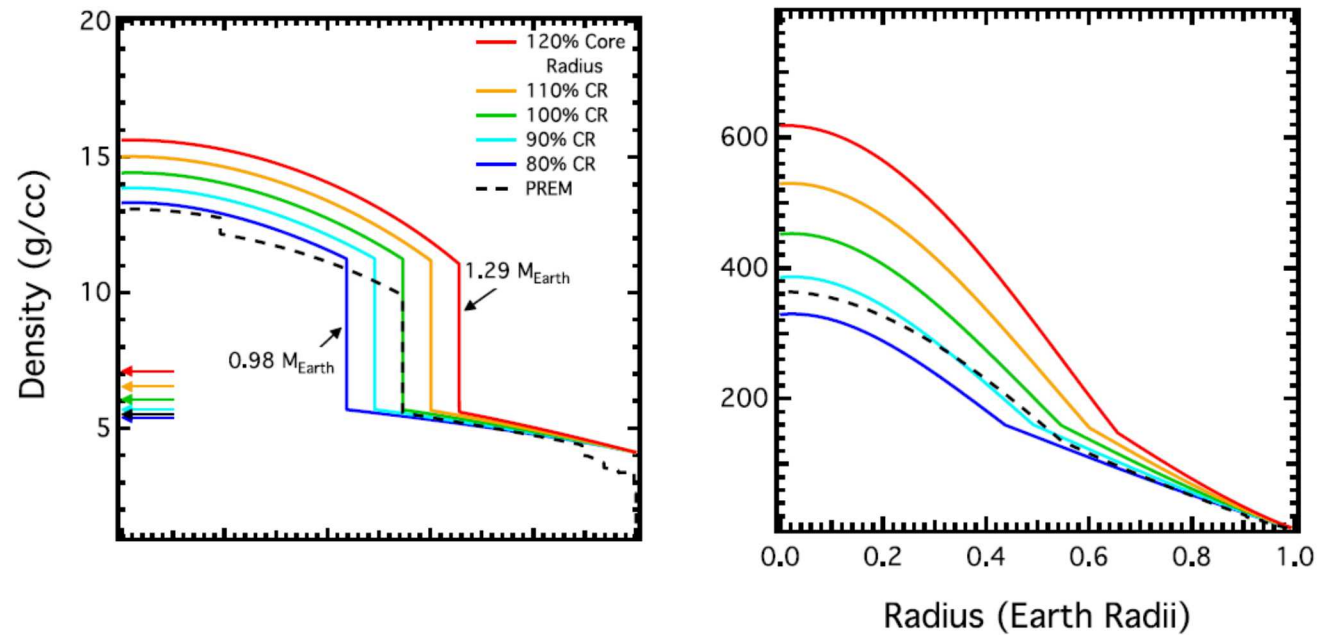
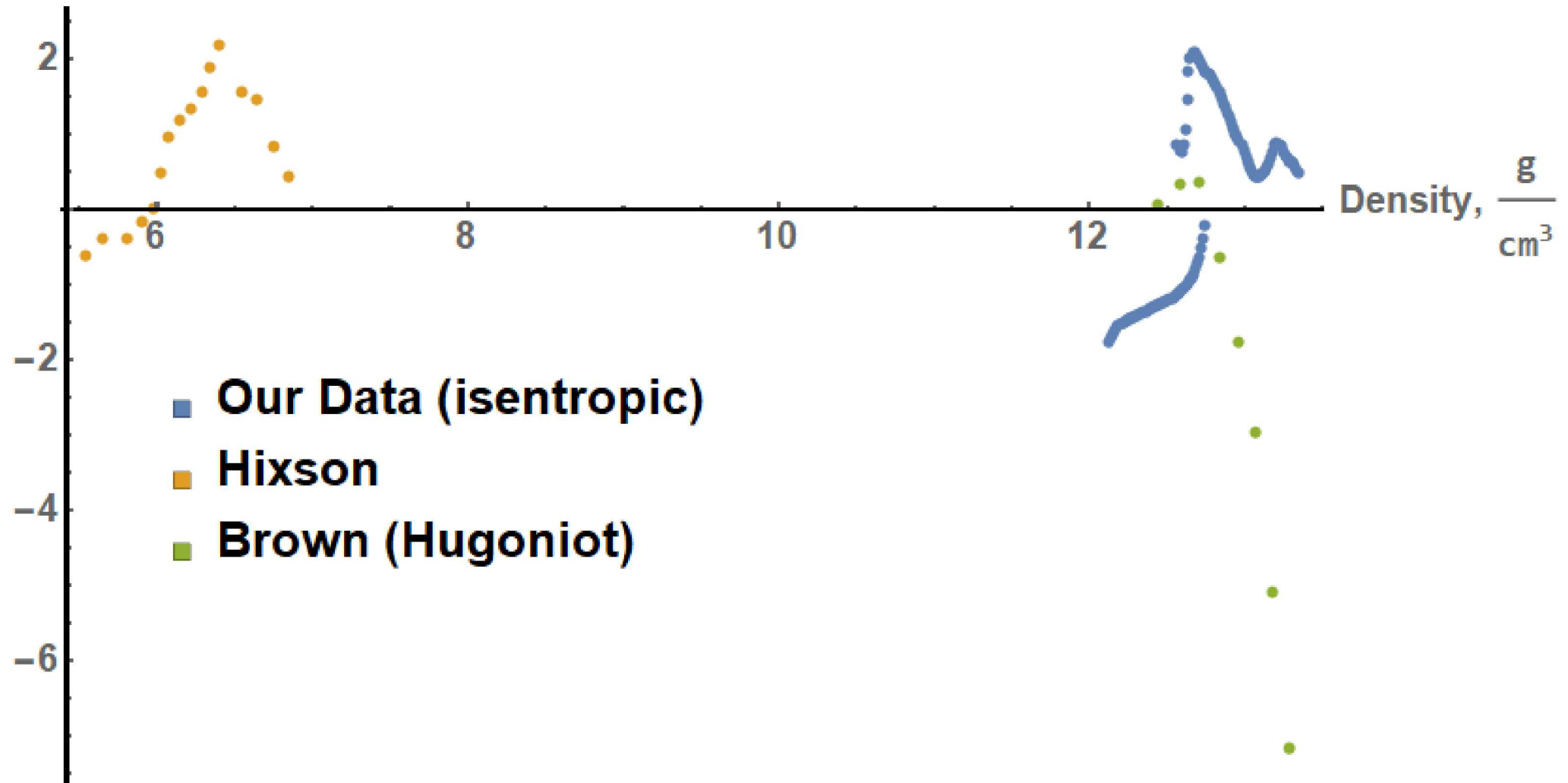


Figure 2. Density and pressure profiles for a two-layer (pure liquid Fe core and MgSiO₃-bridgmanite mantle) one $R_{\oplus}$ planet as a function of planetary radius for a variable core radius. PREM is shown in the black-dashed line for comparison. Average planet densities for each model are shown as arrows of same color scheme as density/pressure profiles. Figures 2–5 are all plotted on the same scale for comparison.

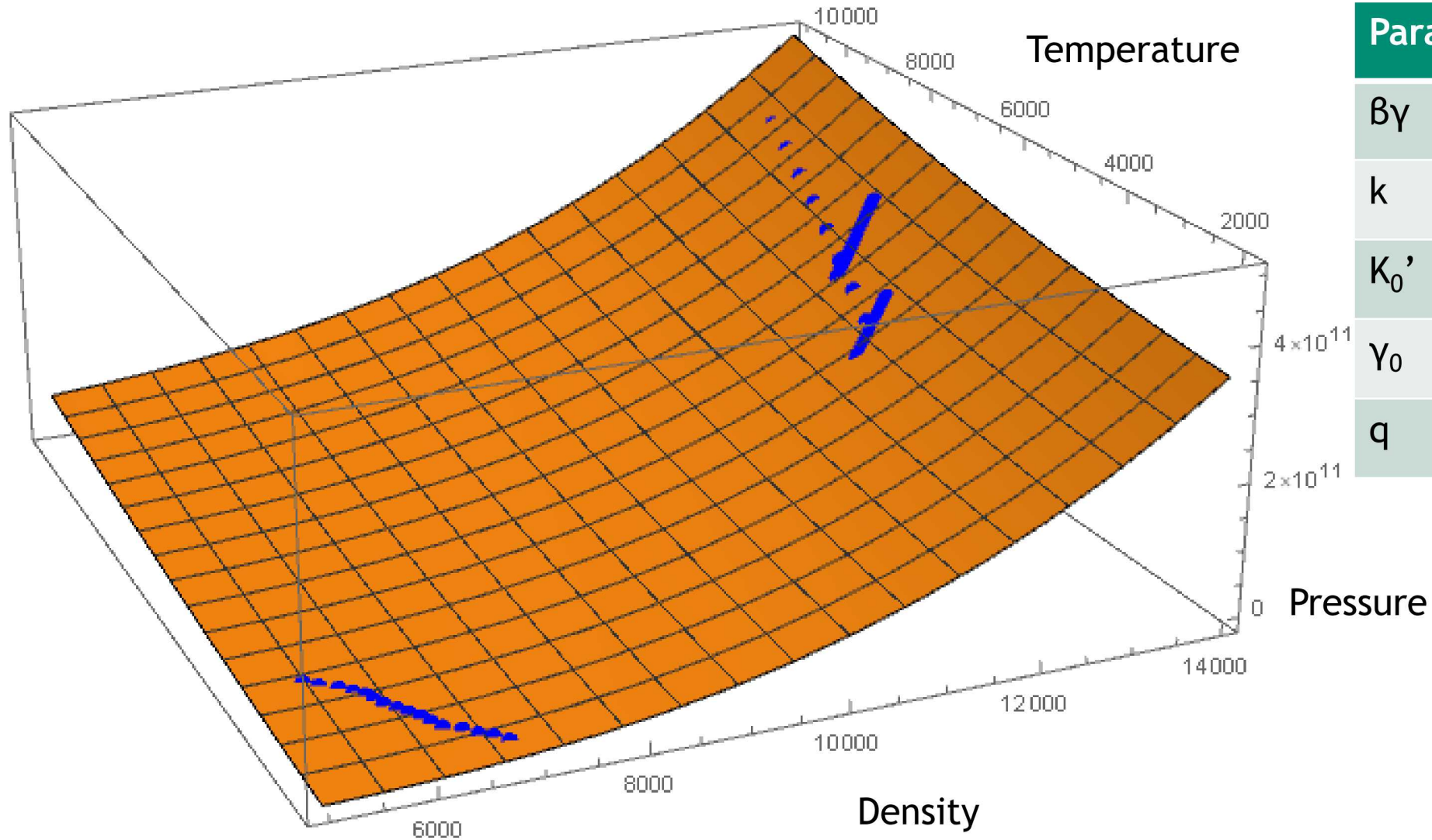
Unterborn, C. T., Dismukes, E. E., & Panero, W. R. (2016). Scaling the Earth: a sensitivity analysis of terrestrial exoplanetary interior models. *The Astrophysical Journal*, 819(1), 32.

Our fit matches most of the existing experimental data to within 2 GPa

Pressure Difference, GPa

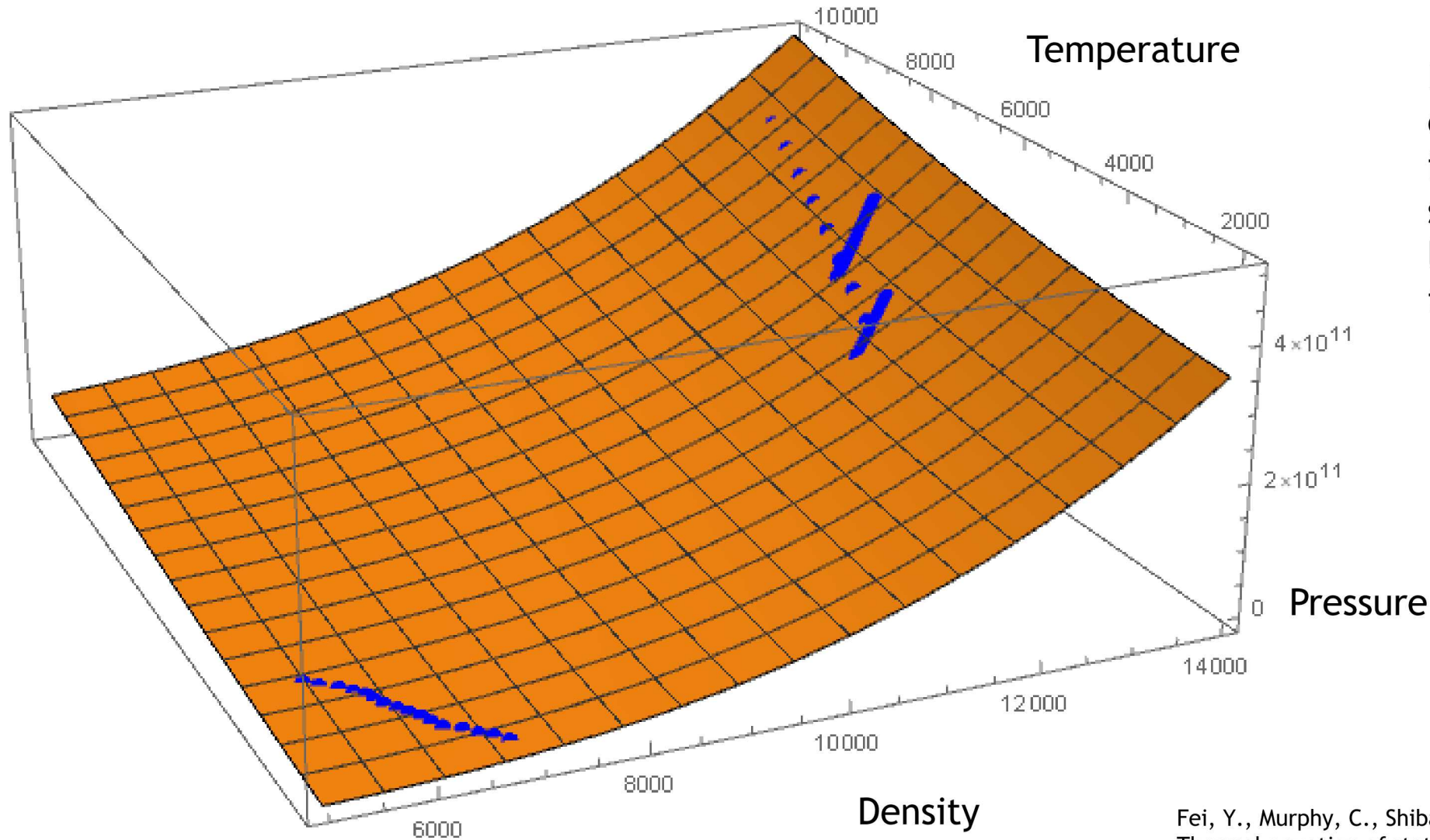


Thus we obtain an EOS surface for liquid iron



Parameter	Value
$B\gamma$	$0.15 \pm .1$
k	0 ± 0.8
K_0'	5.1 ± 0.1
γ_0	1.03 ± 0.71
q	0.91 ± 0.43

Thus we obtain an EOS surface for liquid iron



In comparison to a similar curve generated for solid iron by Fei et al., our surface is ~ 10 GPa ($\sim 3\%$) lower at the conditions of the Earth's core.

Fei, Y., Murphy, C., Shibazaki, Y., Shaha, A., & Huang, H. (2016). Thermal equation of state of hcp-iron: Constraint on the density deficit of Earth's solid inner core. *Geophysical Research Letters*, 43(13), 6837-6843.

Conclusion:

- We have performed shock-ramp experiments on Sandia National Laboratories' Z Machine to evaluate the equation of state of liquid iron along an elevated isentrope near Earth core pressure and temperature conditions.
- The results agree well with the 92141 sesame table, validating its accuracy in this parameter region.
- We provide fit parameters for a new analytic EOS for liquid iron.

Future Plans:

- It would be even more beneficial to planetary models to get similar measurements on iron alloys

Sandia:

- **The many people of Z operations**
- **DICE team:** Randy Hickman, Nicole Cofer, Keith Hodge, and Josh Usher
- **MSTS:** Sheri Payne and Richard Hacking
- **Design Engineers:** Andrew Maurer, James Williams, Lynn Twyeffort, John Fisher
- **Managers:** Christopher Seagle, John Benage, and Dawn Flicker
- **SEERI Program:** Trish St. John and Kristy Martinez
- **Z Fundamental Science Program**