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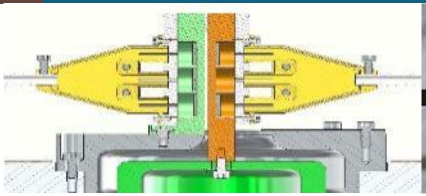
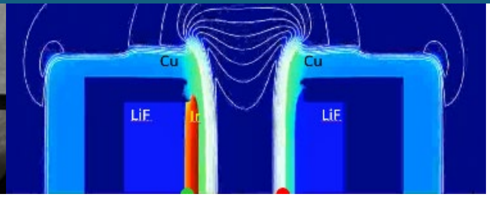
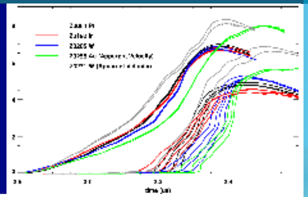
Sandia National Laboratories

SAND2021-3238C

Update on multi-megabar shockless compression at Sandia's Z machine (2021)







PRESENTED BY

Jean-Paul Davis and Justin L. Brown

APS March Meeting 2021
15-19 March 2021 ONLINE
Session M23: Materials in Extremes: Novel Experiments

U.S. DEPARTMENT OF ENERGY   NNSA

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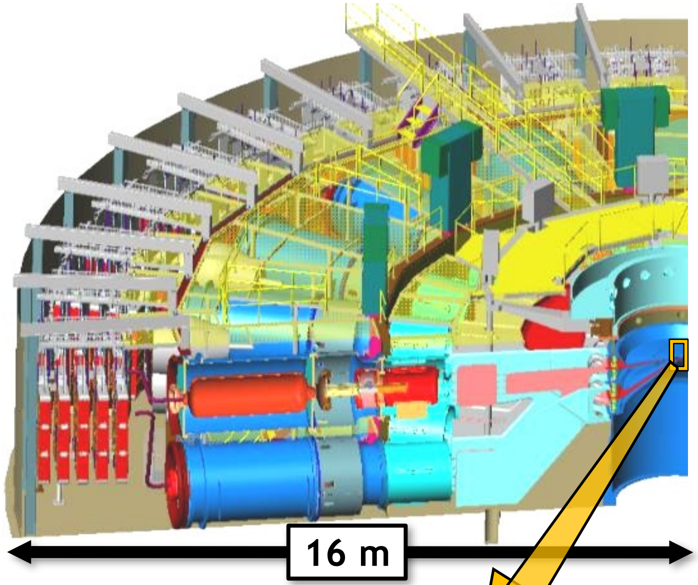
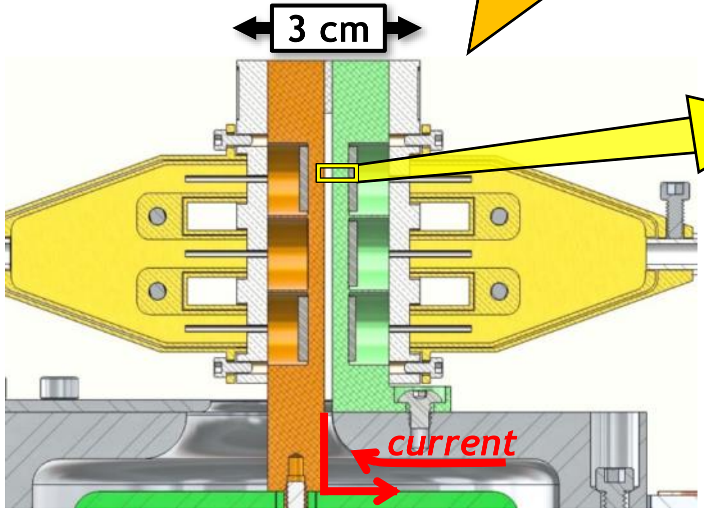
Stripline short-circuit loads on the Z pulsed-power machine can produce planar shockless compression of solids to 400+ GPa

- current pulse of 7-26 MA delivered to load (target)
- controllable pulse shape, rise time 100-1500 ns
- stripline = parallel flat-plate electrodes shorted at one end, identical loading of sample pairs
- magnetic $\boldsymbol{J}\times\boldsymbol{B}$ force induces ramped stress wave in electrode material
- stress wave propagates into ambient material, de-coupled from magnetic diffusion front

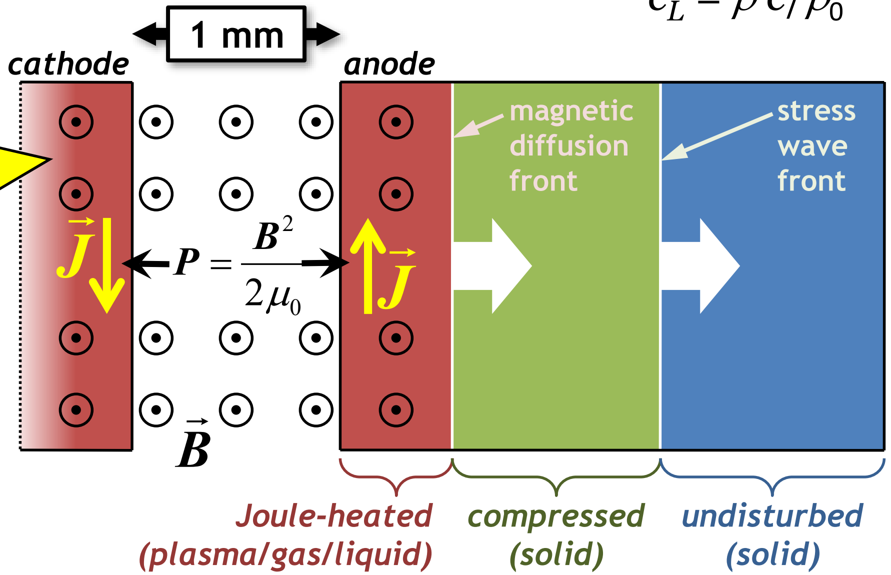


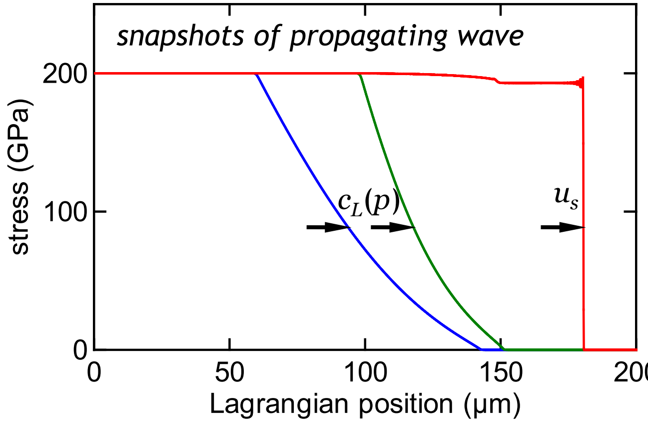


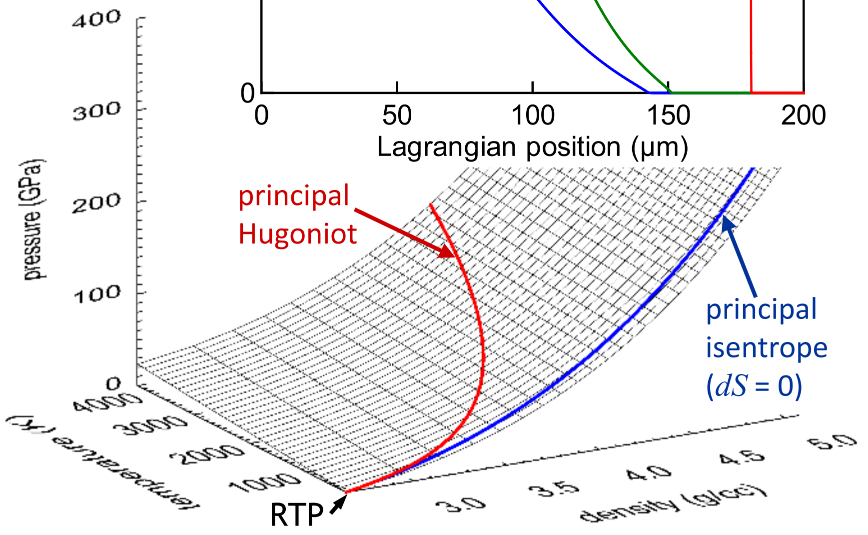
- sound speed c increases with pressure (normal materials)
- ramp steepens into a shock

$$c^2 = (\partial P/\partial \rho)_s$$

$$c_L = \rho\, c/\rho_0$$



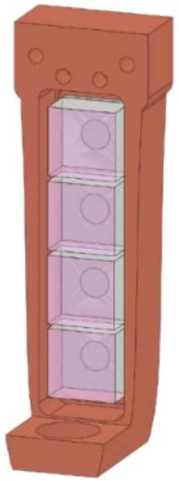


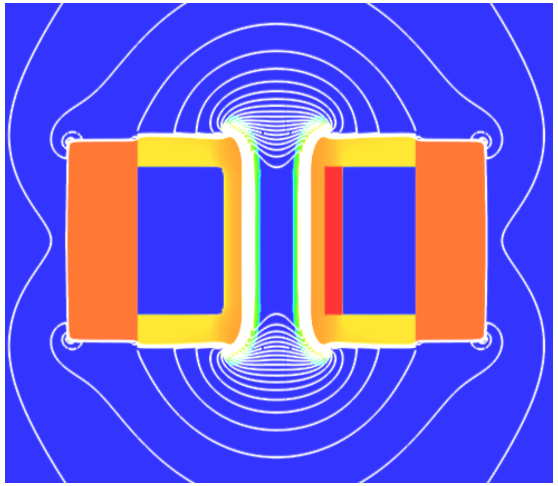


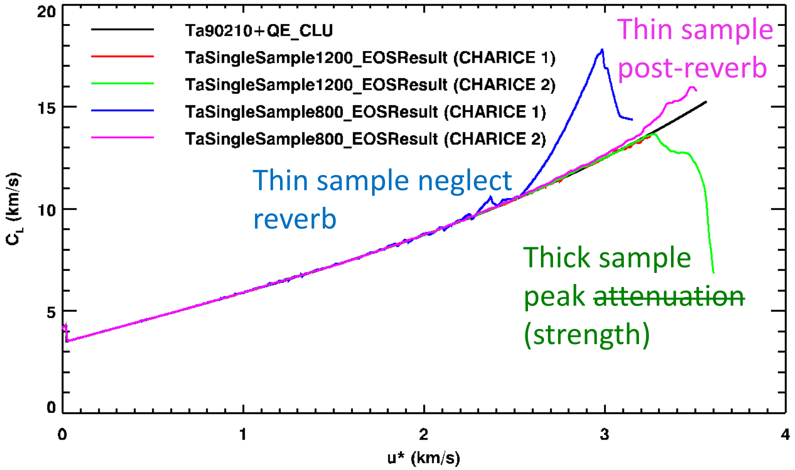
Focus today on two different analyses of one data set

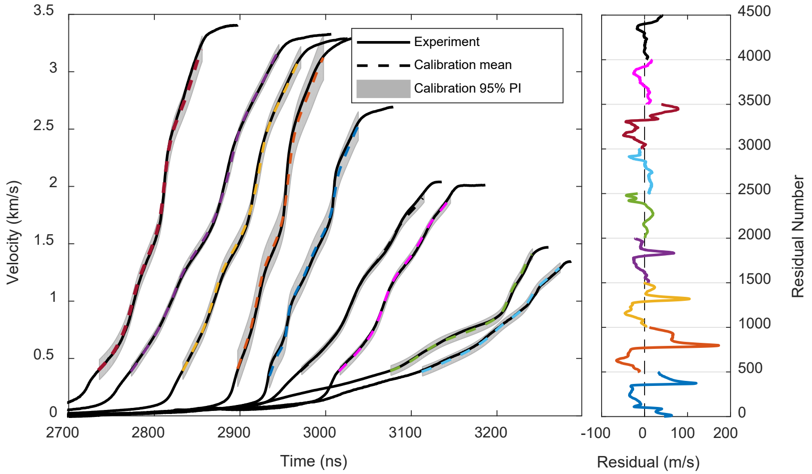
Last time (2019): experiment design choices, approaches to analyzing velocimetry data

- Electrode thickness, square samples, LiF windows, 2-D MHD drive correction
- Single-sample iterative Lagrangian analysis (**ILA**), post-reverberation characteristics mapping
- Bayesian calibration to infer EOS parameters with uncertainties, sensitivity analysis





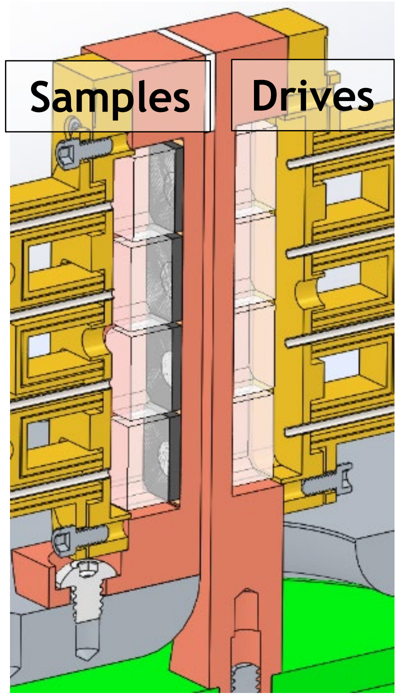


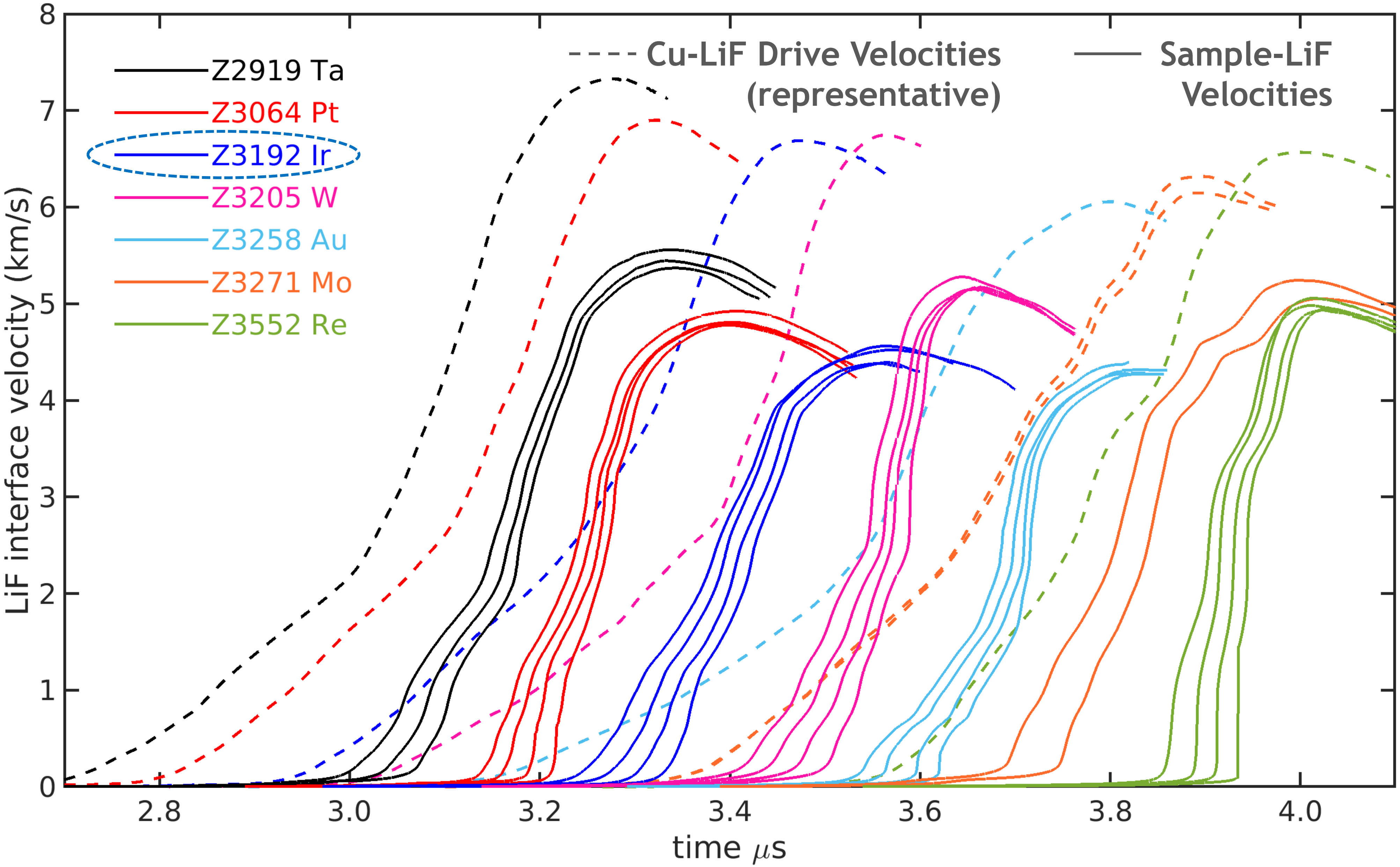


Today: comparing ILA and Bayesian calibration (**BC**)

- Analyze four measurements from one experiment on iridium (Ir)
- Interaction between sample strength and window release limits ILA below peak pressure
- Parameterize EOS for BC using arbitrary reference isentrope in B(P)

Processed velocimetry data from multi-megabar ramp-compression experiments on seven different transition metals are awaiting analysis

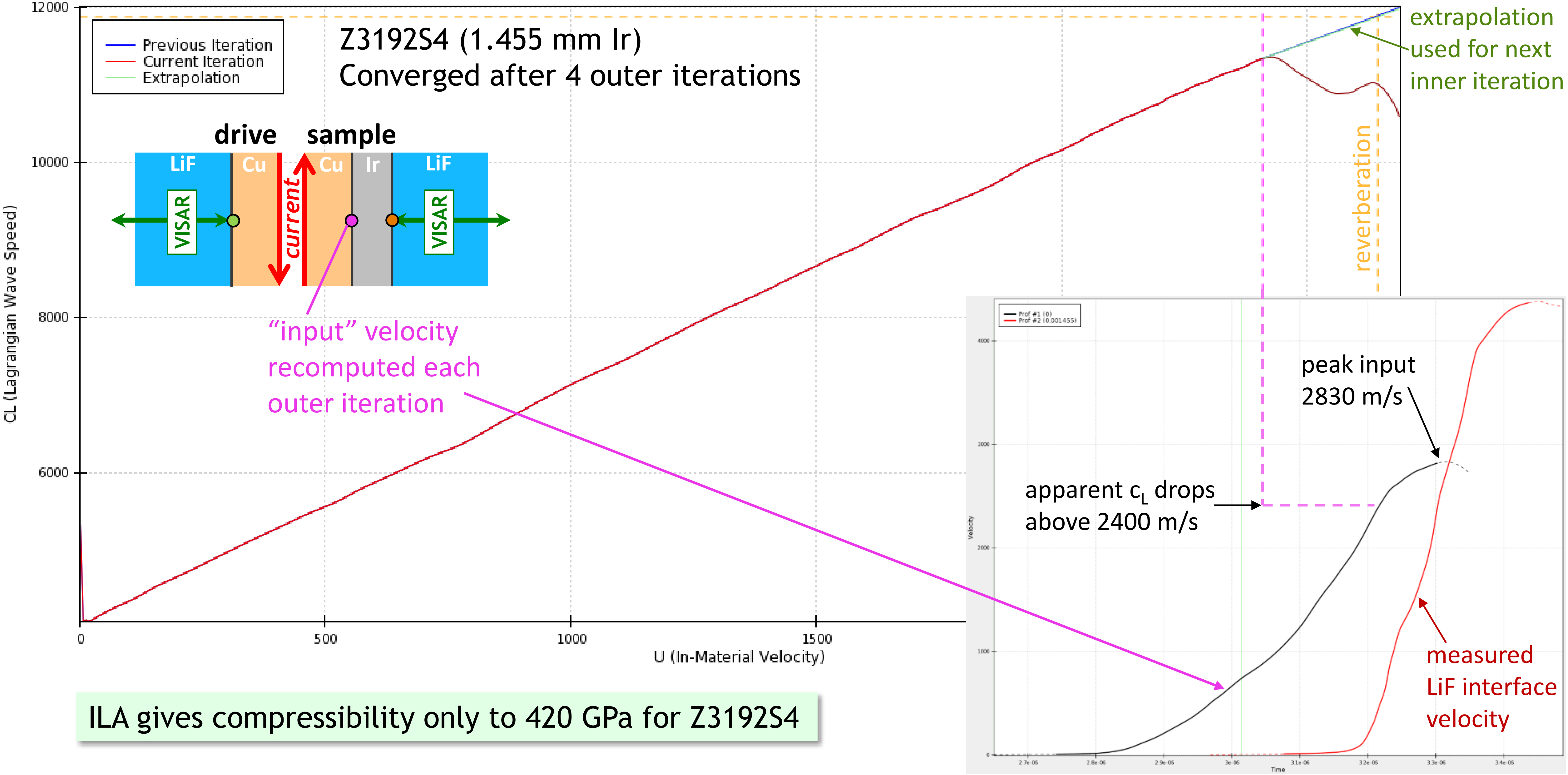




Why these metals?

- Standards for dynamic & static experiments
- No structural phase transitions

Single-sample ILA of thick Ir sample loses validity ~15% below peak velocity



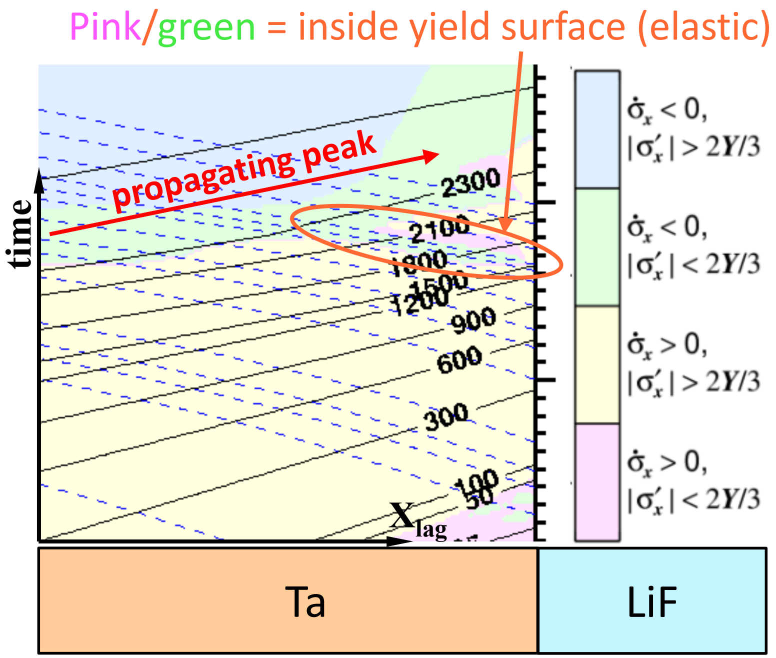
ILA gives compressibility only to 420 GPa for Z3192S4

Characteristics-based window correction in ILA cannot account for local elastic release response of sample as peak reflects from LiF

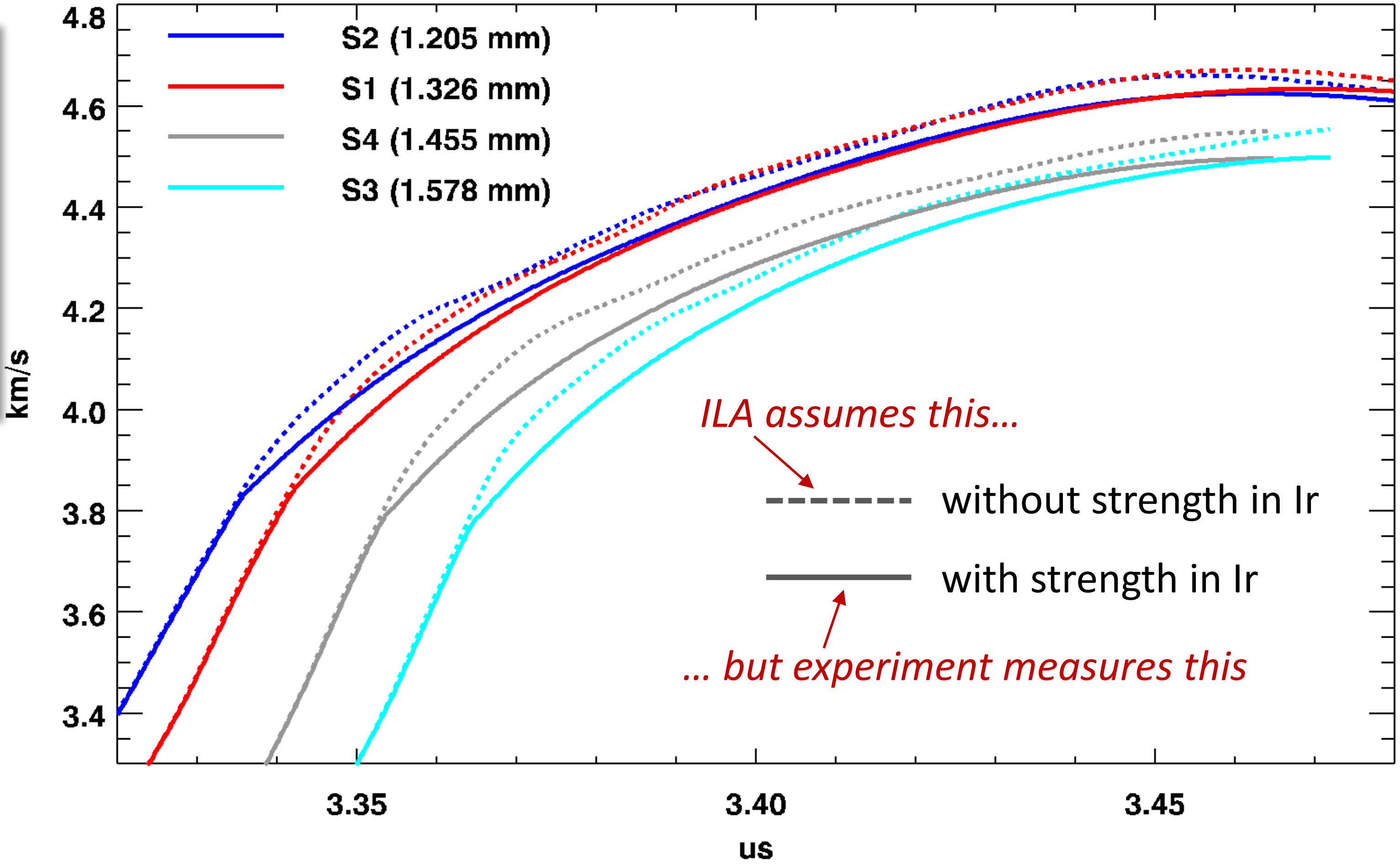
Example: simulation of Ta/LiF

Line contours of Riemann invariants

- Representative of characteristics
- Peak input velocity > 2300 m/s
- Characteristics from input velocity > 1500 m/s traverse elastic region before reaching window



Simulated Ir/LiF interface velocities for Z3192



Onset of error depends on pulse shape and sample thickness

- occurs at lower pressure for thick sample because ramp is steeper
- thinner samples (with post-reverberation method!) good to higher P

Bayesian calibration of EOS parameters fits a hydro-code model to velocimetry measurements from multiple independent samples of material

1. Set up and parameterize set of 1-D MHD simulations corresponding to set of measurements
   - Define uncertain parameters and their prior distributions (mean and standard deviation)
   - Experimental (B-field drive, thickness, timing) and material-model parameters (velocity is not a parameter)
2. Generate training data by Latin Hyper-cube Sampling (LHS) from the prior distributions
   - Ideally ~1000 simulation sets per uncertain parameter
   - Output is velocity residual (simulation − experiment) waveforms as a function of input parameters
3. Construct Gaussian Process (GP) emulator from the LHS training data
4. Use Markov Chain Monte Carlo (MCMC) to sample posterior distributions from GP
   - Use a GP emulator because MCMC is a serial operation and hydro-code is too slow

$$\mathrm{V}(\mathrm{t}) = \eta(t, \boldsymbol{\theta}) + \epsilon(t)$$

- $\mathrm{V}(\mathrm{t})$ → Observed velocity
- η → Hydro-code simulator
- $\boldsymbol{\theta}$ → All the uncertain parameters in the simulation
- $\epsilon(t)$ → Experimental uncertainty

Brown et al., *Journal of the Royal Statistical Society Series C*, **67**, 4 (2018)

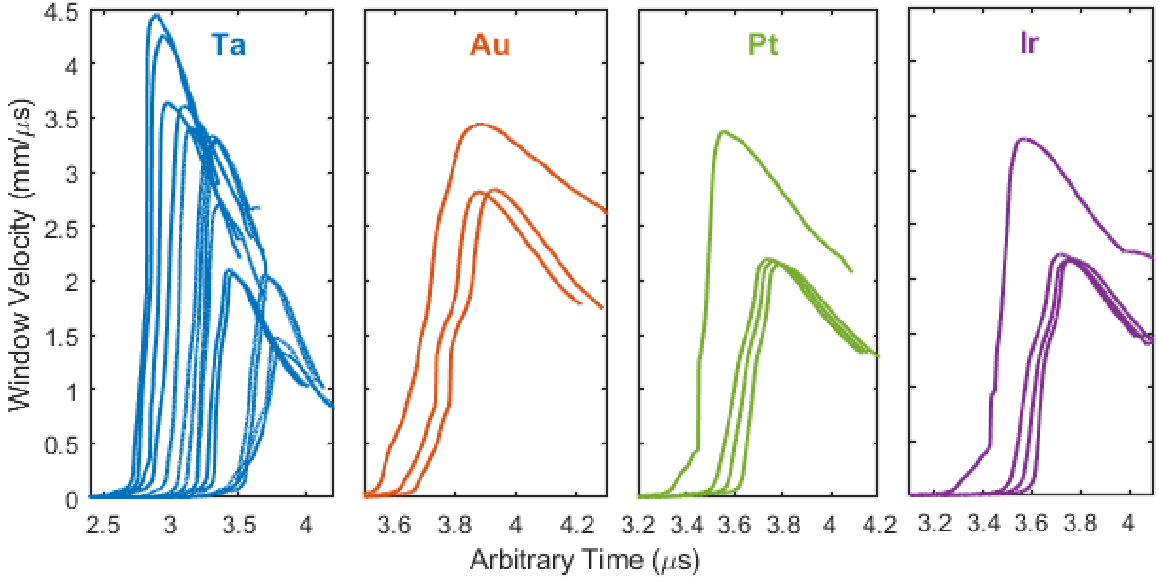
Typically use strength model with fixed parameters that have been calibrated to separate high-pressure ramp-and-release experiments

Uni-axial strain ramp-compression response convolves EOS and strength

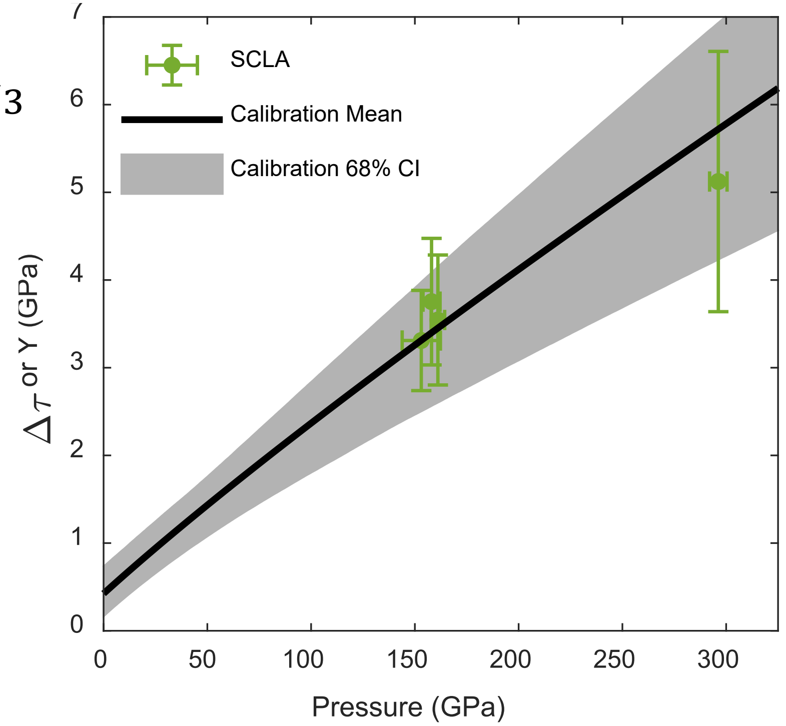
- Deviatoric stress from pressure-dependent yield stress
- Thermal pressure increment due to plastic work

Specially-designed experiments capture release from peak velocity

- High-pressure yield stress extracted from peak region insensitive to EOS
- Calibrate a simplified pressure-hardening model to data at multiple pressures

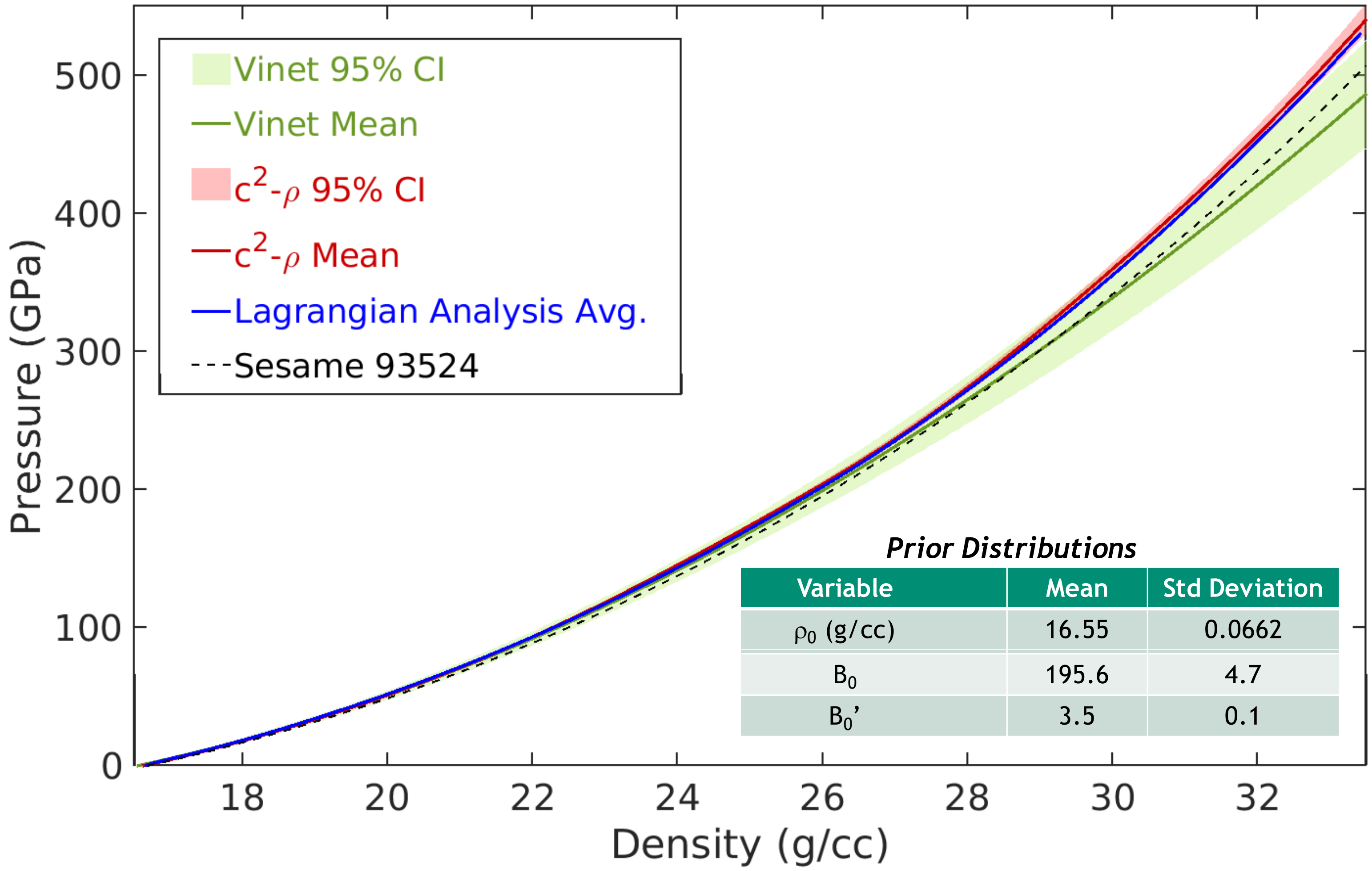


$$\frac{Y}{Y_0} = 1 + AP\left(\frac{\rho_0}{\rho}\right)^{1/3}$$



Brown et al., *J. Dyn. Behav. Mater.* (2020). https://doi.org/10.1007/s40870-020-00256-6

Inferred probability distributions can depend strongly on priors…



Prior Distributions

Variable	Mean	Std Deviation
ρ_0 (g/cc)	16.55	0.0662
B_0	195.6	4.7
B_0’	3.5	0.1

c^2-ρ = R-T isotherm is interpolation on ~10 knots in c^2 (ρ) space

(more on this in a couple slides)

Lagrangian Analysis = transfer-function mapping, no iteration (not ILA)

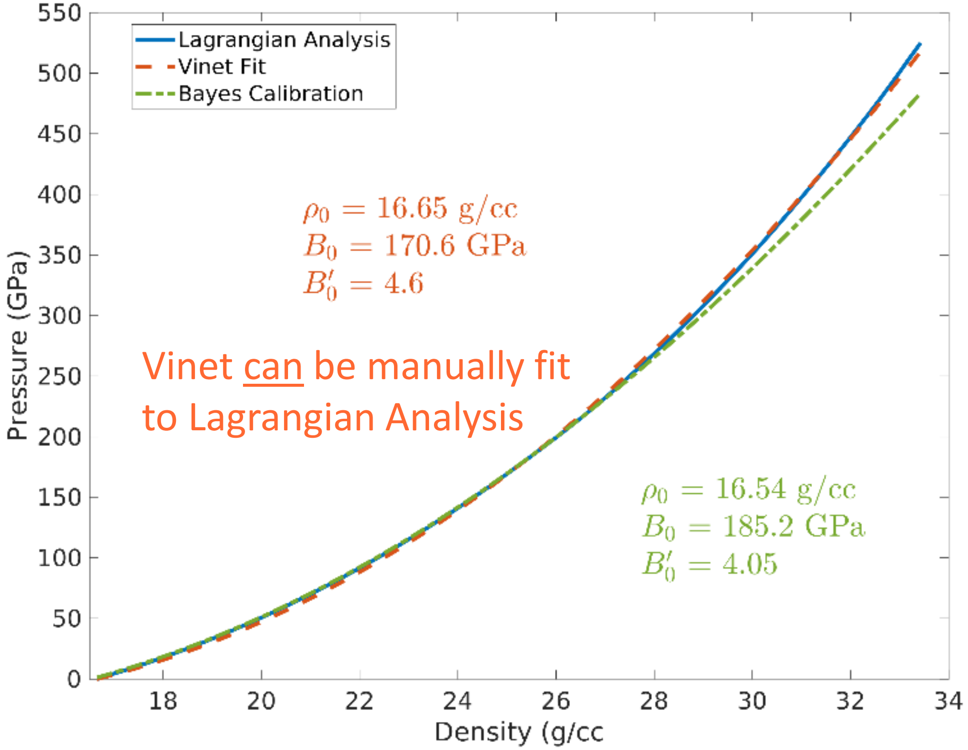
Vinet R-T isotherm

$$P(V,T) = \frac{3B_0}{X^2} Z \exp(\eta_0 Z) + \alpha_0 B_0 (T - T_{ref})$$

$$X = \left(\frac{V}{V_0}\right)^{1/3}, \quad Z = (1 - X), \quad \eta_0 = \frac{3}{2}(B_0' - 1)$$

Calibrate 2 (3 w/ ρ_0) reference curve params

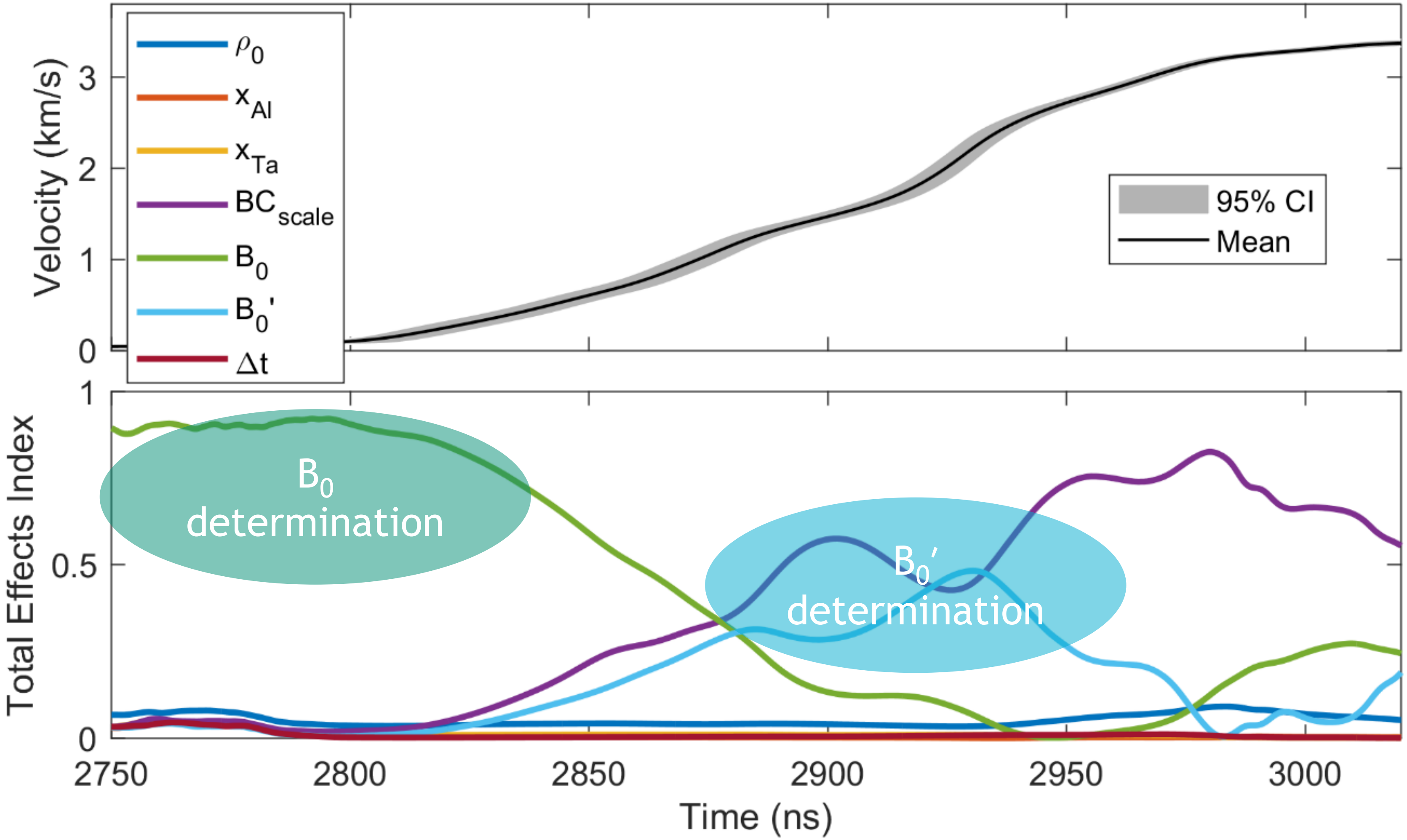
Keep 2 thermal params (c_v, α) fixed



… and on sensitivity of velocity to each parameter

Global variance-based sensitivity analysis (Sobol)

- Gives an indication of which parameters are identifiable within the calibration



Prior Distributions

Variable	Mean	Std Deviation
ρ_0 (g/cc)	16.55	0.0662
Electrode Thickness (mm)	2.0054	0.0015
Sample Thickness (mm)	1.5002	0.0015
B-Field Scaling	1.0	0.004
Δt (ns)	0	0.2
B_0	195.6	4.7
B_0’	3.5	0.1

Very sensitive

Not sensitive

No high-pressure information is feeding into the calibration!

Brown et al., *Journal of the Royal Statistical Society Series C*, 2018

An arbitrary reference EOS curve localizes sensitivity

$B_i = c_i B_i^{REF}, \; i = 1,2,\ldots,15$

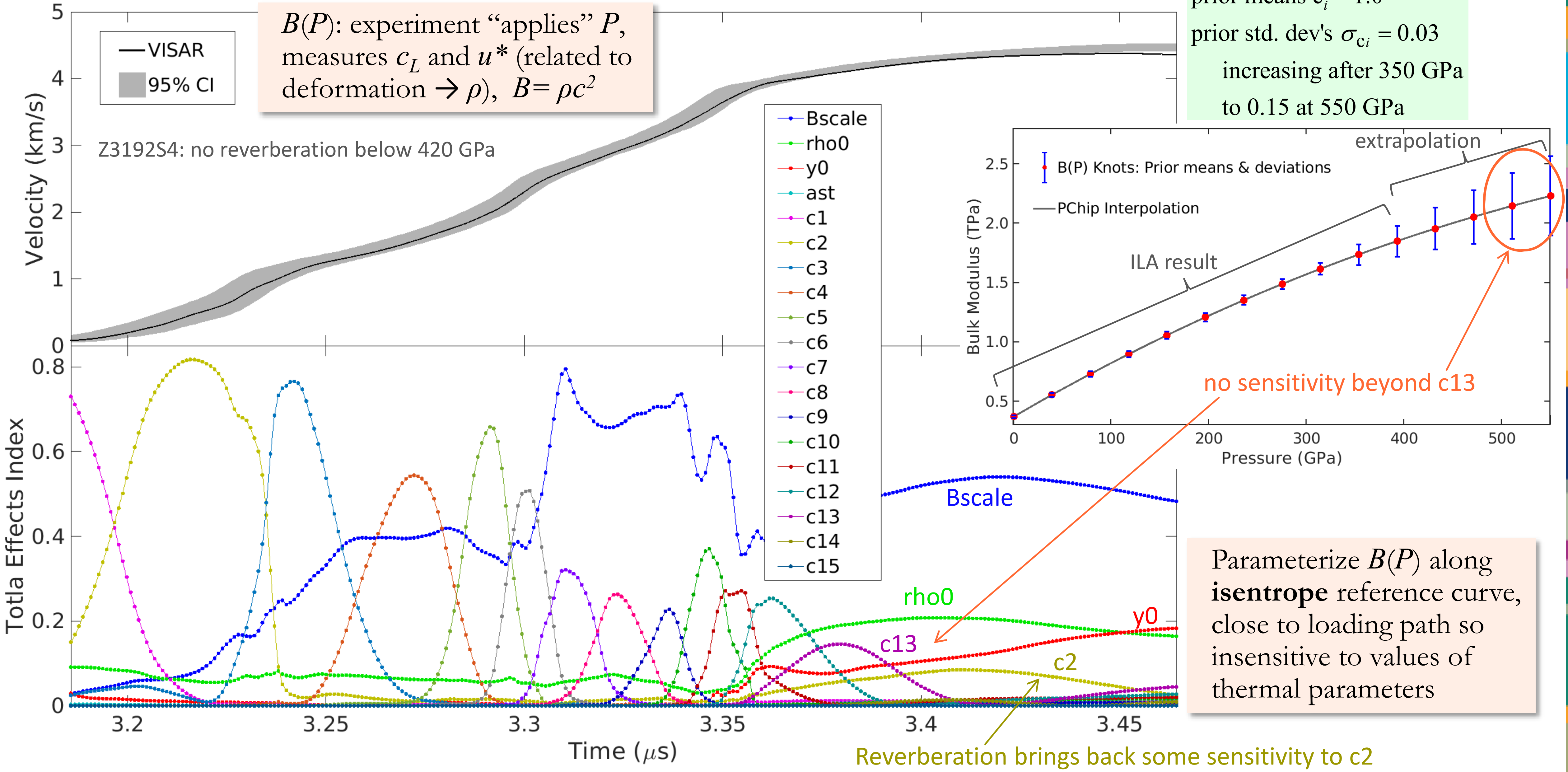
prior means $c_i = 1.0$

prior std. dev's $\sigma_{c_i} = 0.03$

increasing after 350 GPa

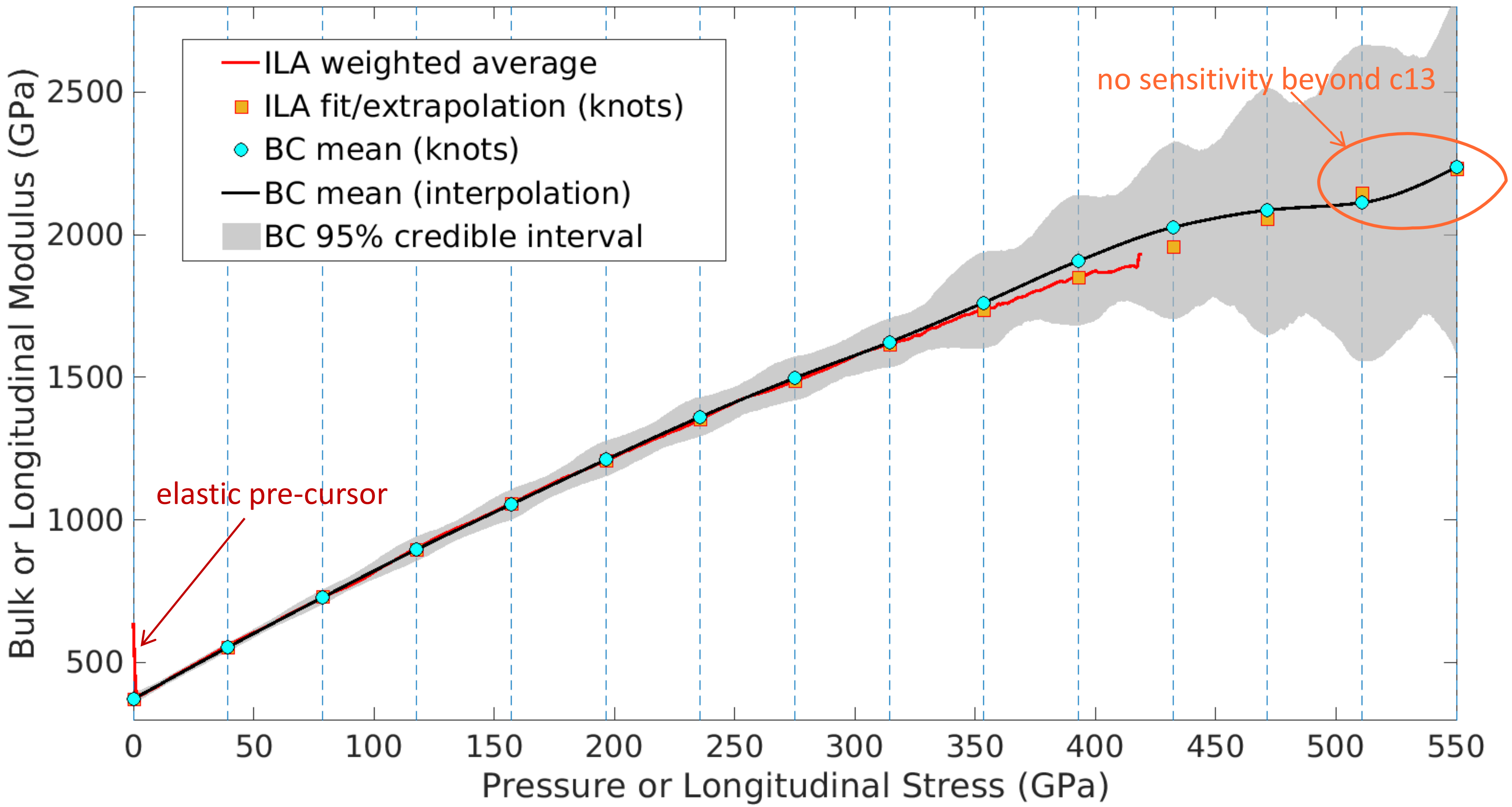
to 0.15 at 550 GPa

$B(P)$: experiment "applies" P, measures c_L and u^* (related to deformation → ρ), $B = \rho c^2$

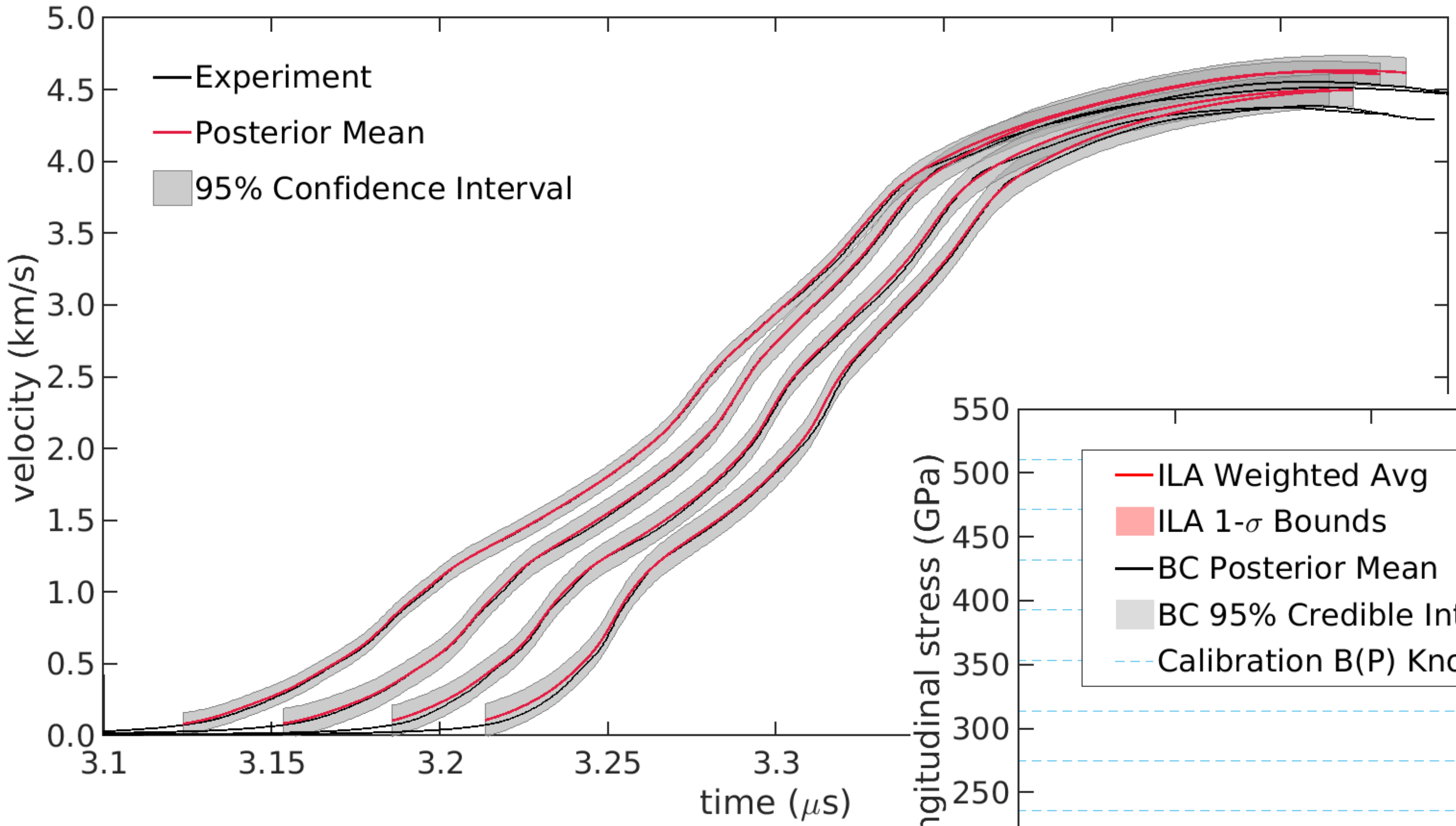


Parameterize $B(P)$ along **isentrope** reference curve, close to loading path so insensitive to values of thermal parameters

First-cut BC for Z3192 deviates from ILA above ~350 GPa



Posterior "coverage" of velocity suggests problem at highest pressures

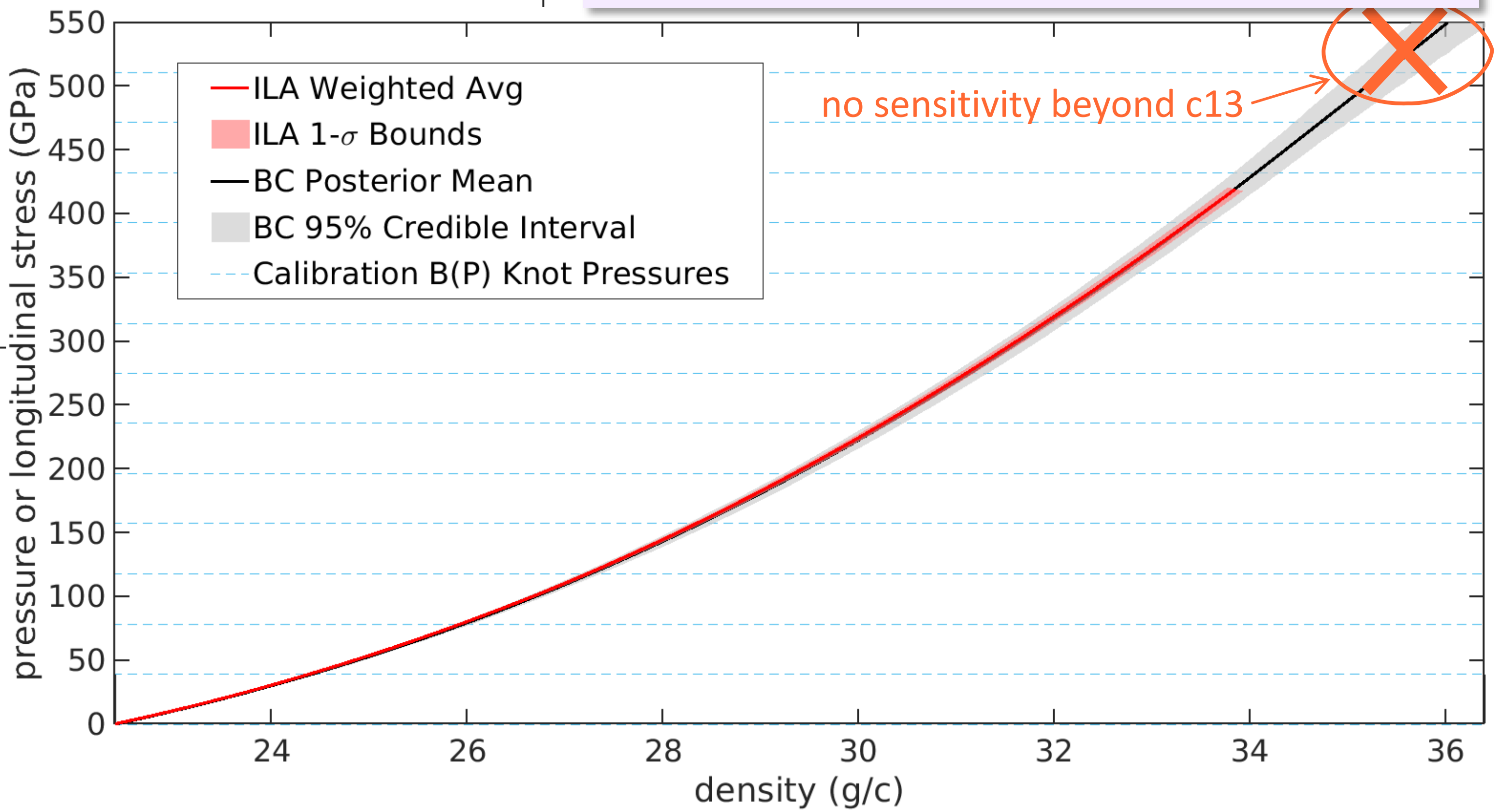


BC mean velocity overshoots peak

- $B(P)$ must increase more above 400 GPa?
- or, assumed strength much too low?

If allow inference of ρ_0 (same LHS data)

- match better < 3.5 km/s, worse ~4 km/s
- biases ρ_0 to 22.7 g/cc (prior 22.4 g/cc)



ILA 2-σ bounds < BC 95% CI

- ILA estimate is not conservative, BC is

Expected ILA (σ_x) to lie above BC (P)

SUMMARY

1. Analyzed shockless compression of Ir to > 400 GPa
2. Iterative Lagrangian Analysis (ILA) limited by sample strength effects on window interaction due to single-valued response assumed by characteristics mapping
3. Bayesian Calibration (BC) method using arbitrary B(P) reference isentrope **may**, with more work, be able to constrain compressibility of Ir at pressures > 400 GPa
4. Plenty more to do!
   - Investigate iterative transfer-function mapping as way to account for strength-window effect
   - Make additional high-pressure strength measurements to improve precision of EOS results
   - Apply best techniques found for Ir to data on the other six metals
   - Etc., etc.