

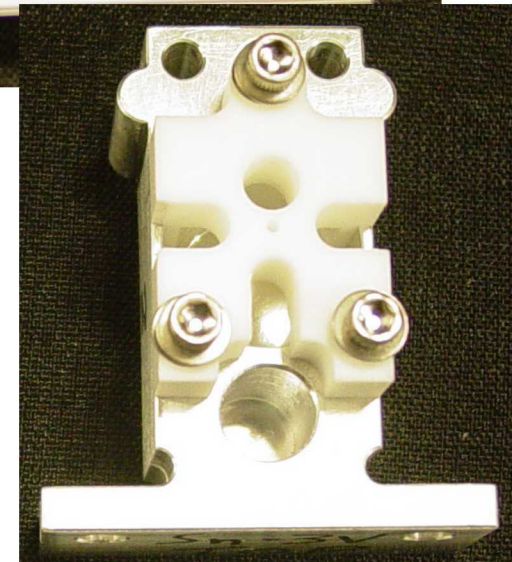
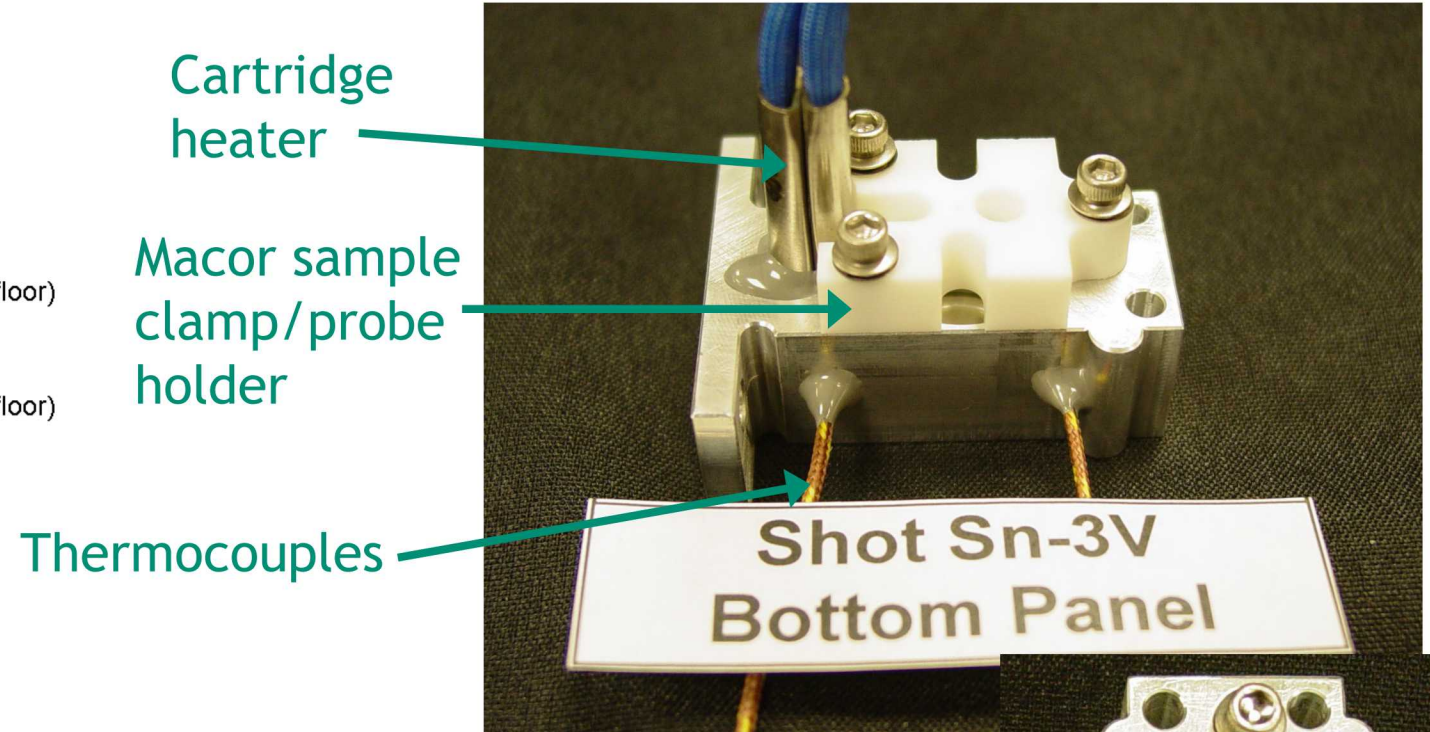
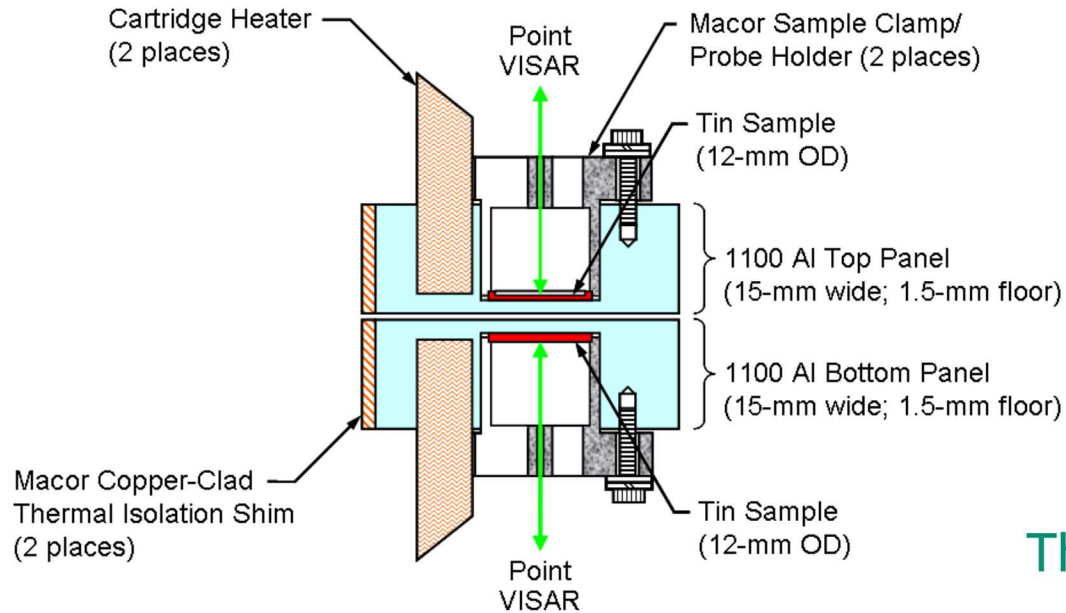


# Preheat of stripline loads on Veloce

Jack Wise, Jean-Paul Davis, Dan Dolan, Clint Hall, Dennis Hayes

Kinetics of phase transformations in metals under dynamic compression kickoff meeting, Nov. 26-28, 2018

## 2 Preheat experiments were conducted on Tin in 1999



Holes were bored at the bottom of the panels for cartridge heaters

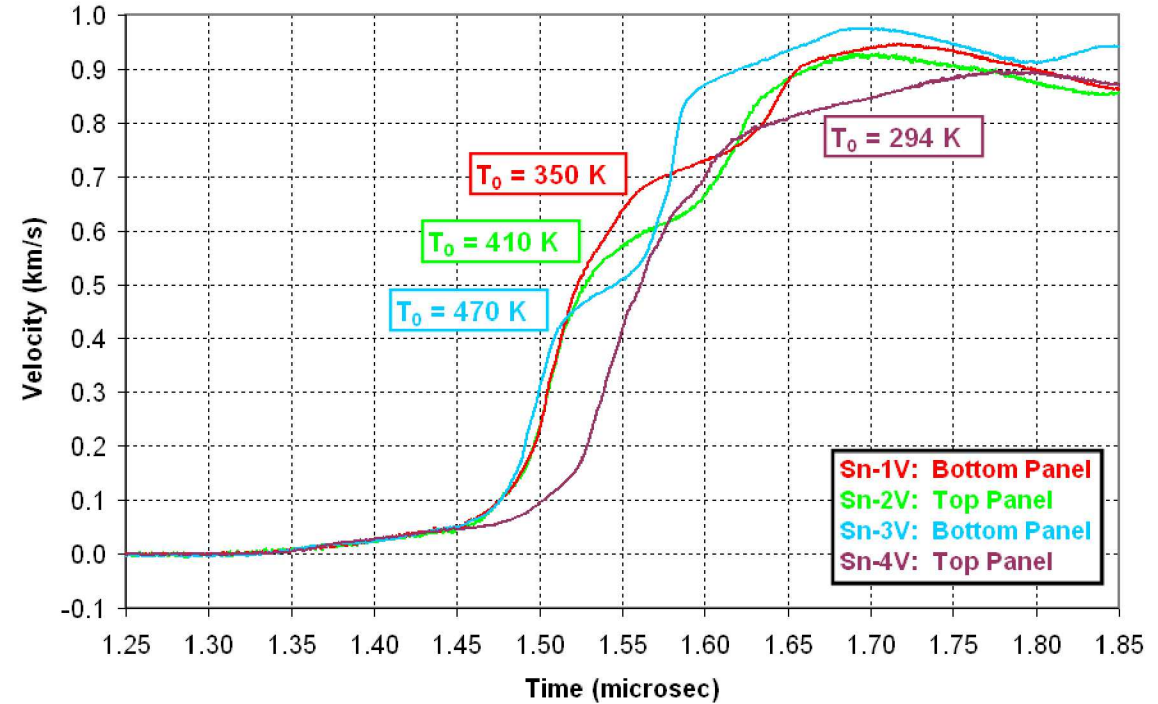
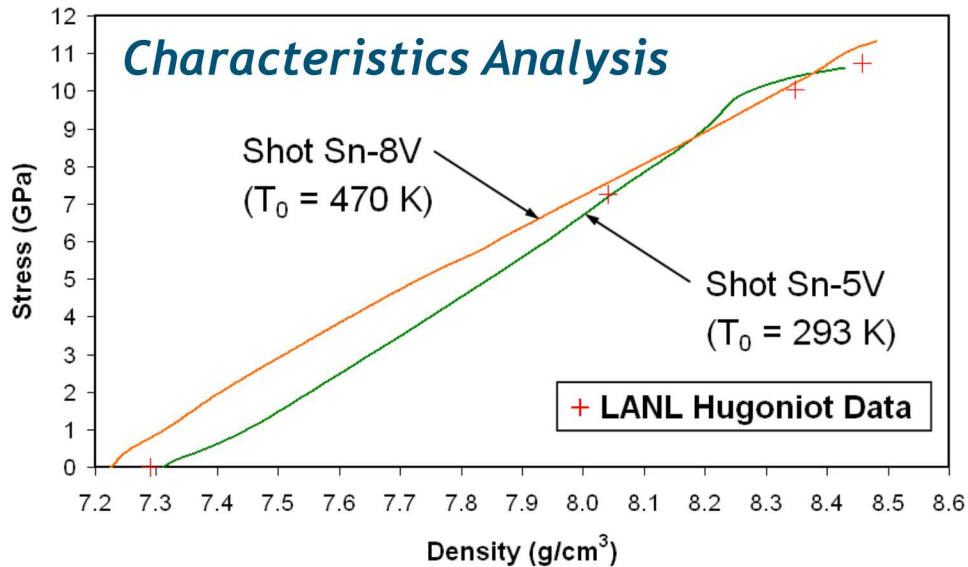
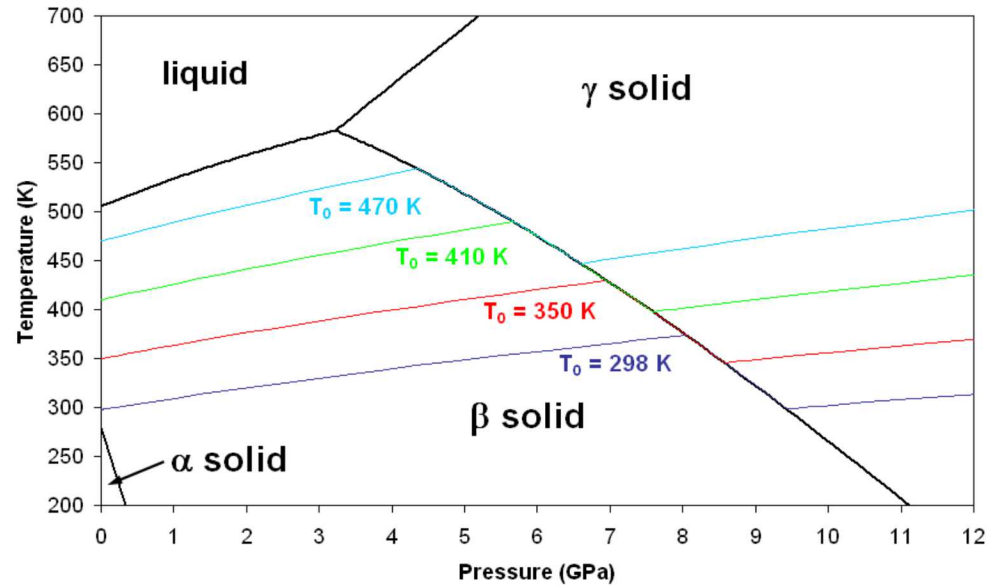
Macor was used to press the sample in position and hold the VISAR probes

- Thermal isolation for the probes

A Macor shim flash coated with copper was used between the panels and the connection to the machine

- Thermal isolation from the panels
- Flash coating provides initial electrical pathway for powerflow

## Preheat data on tin



2 velocity profiles (1 and 0.75mm thick) were measured for 4 different initial temperatures

- Slope of phase boundary is evident in data

Temperature limit is  $\sim 200$ C due to the dielectric



# Preheat of stripline loads on Z

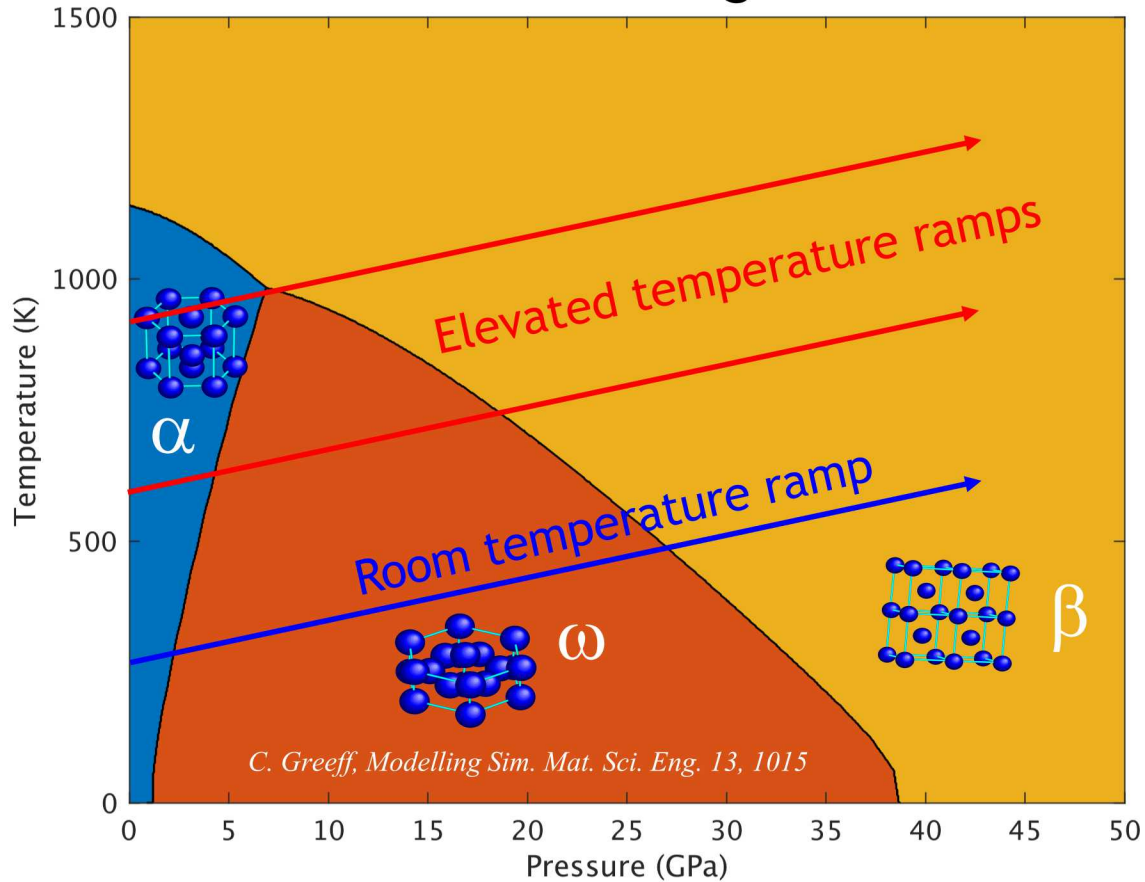
Justin Brown, Jack Wise, Morris Kaufman, Randy Hickman, Jim Williams

Kinetics of phase transformations in metals under dynamic compression kickoff meeting, Nov. 26-28, 2018

# A preheat system was designed to study the phase transition kinetics of shocklessly compressed Zr



## Zr Phase Diagram



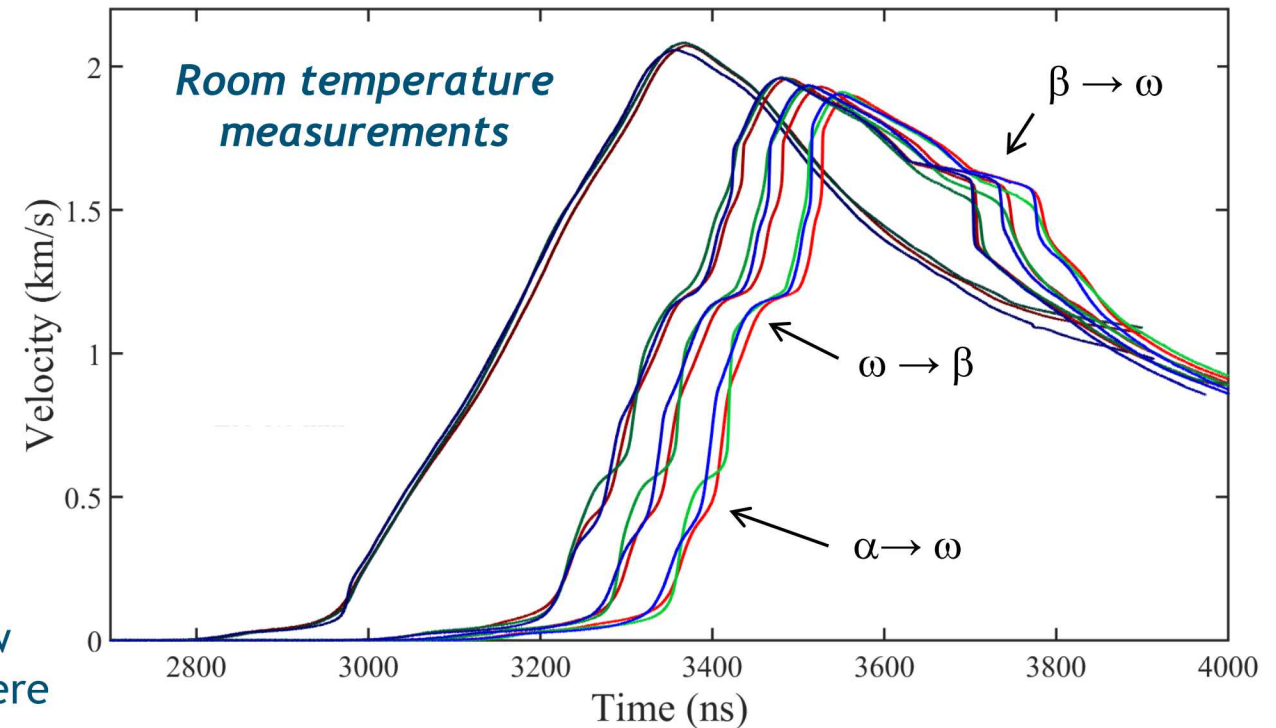
Material	Hf	Fe	Al	V	O	N	C	Density (g/cm <sup>3</sup> )
Zr <sub>0</sub> high purity	35	<50	<20	<50	<50	<20	22	6.499 ± 0.005
Zr <sub>1</sub> low purity	350	125	<20	<25	390	15	70	6.503 ± 0.003
Zr <sub>11</sub> very low purity	14 000	2400	...	...	1200	80	270	6.556 ± 0.007

High, mid, and low purity Zr samples were used

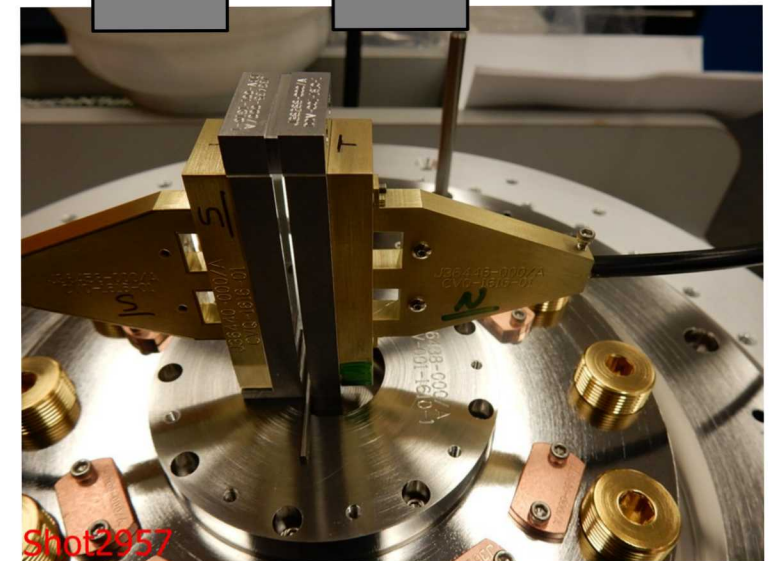
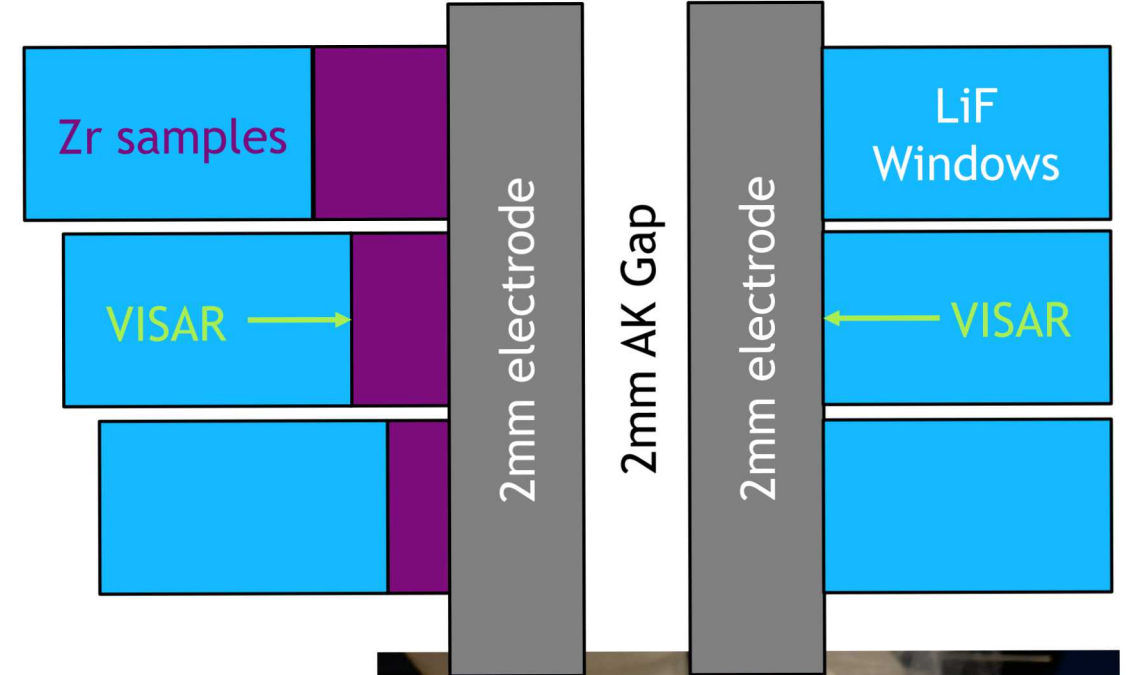
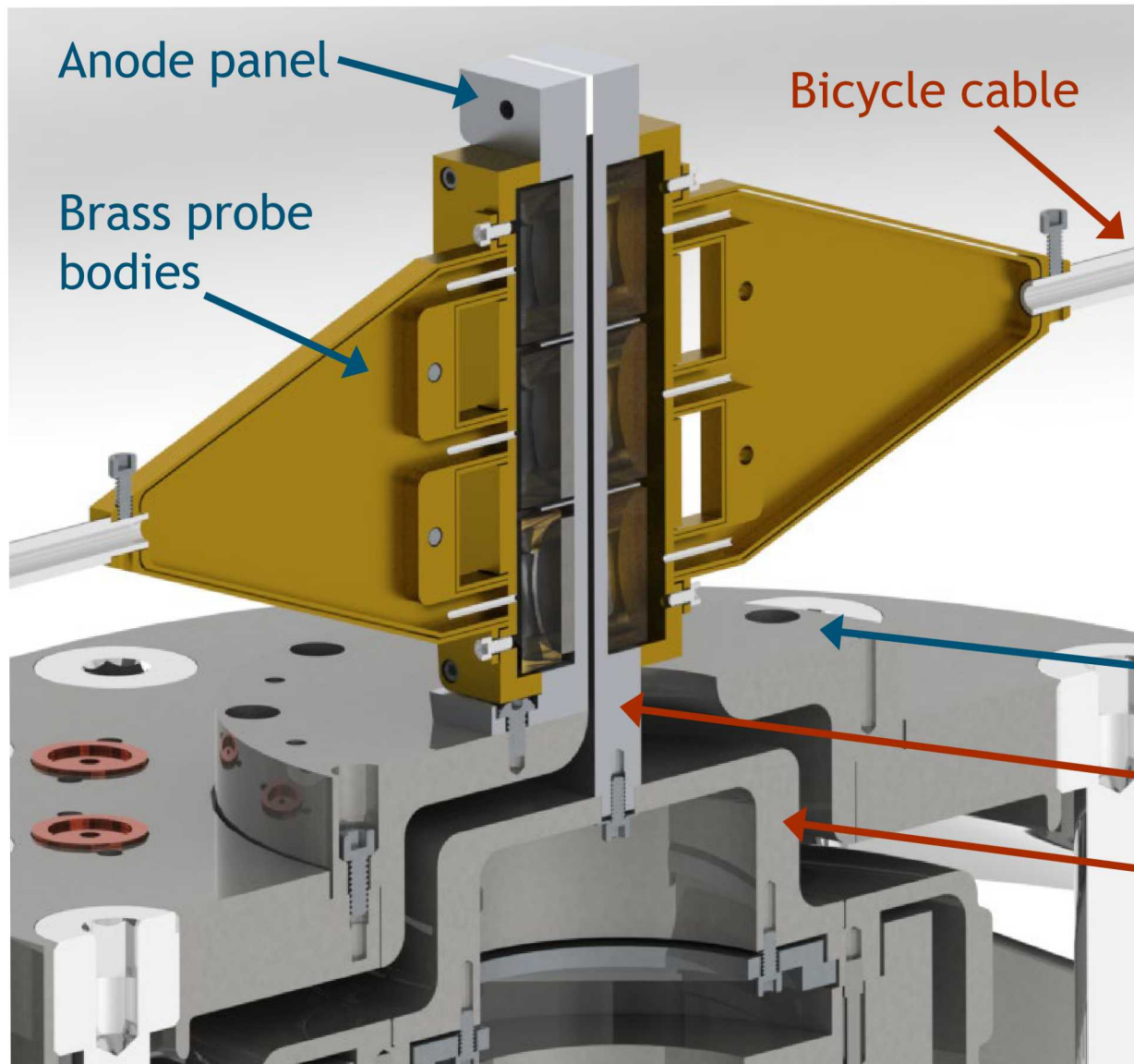
## Design Requirements:

- 20mm wide stripline load
- Peak pressures ~65 GPa
- Preheat samples up to 1000 K
- 1% uniformity

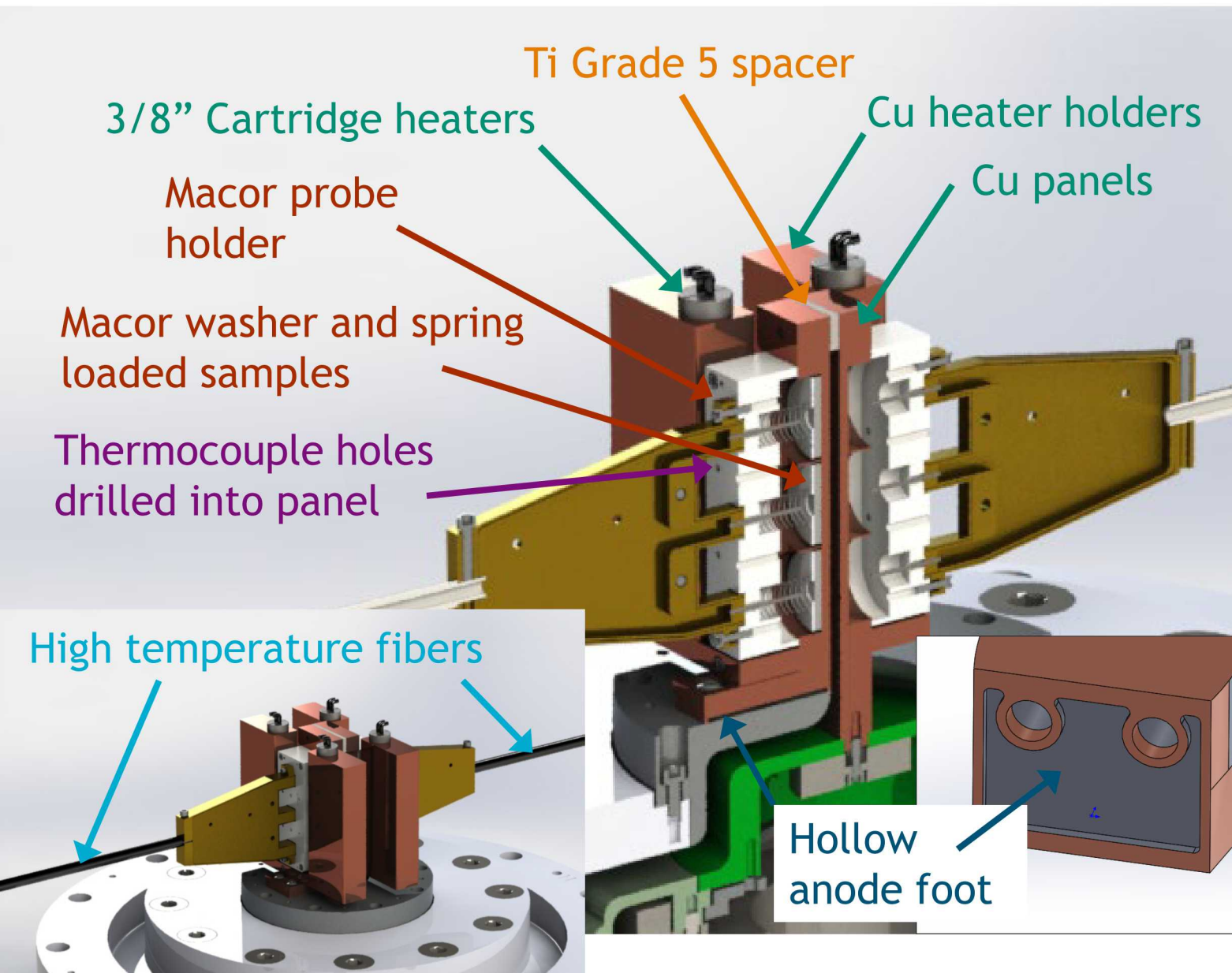
Resistive Preheat



# Review of standard (room temperature) stripline setup



## Changes implemented for preheat



Cu blocks attach to electrodes at the bottom of the panel

- Thermal load path does not go through the panels = better uniformity

Macor provides thermal insulation between the panels/samples and the VISAR probes

Ti spacer is a low thermal conductivity metal which reduces heat flow between the panels, improving uniformity

Material was removed from anode foot to limit thermal contact as much as possible

- Priority was placed on power flow (electrical considerations) so there is not perfect thermal isolation

Holes for 8 thermocouples on each panel were drilled into each panel

- Monitor thermal gradients along height and width

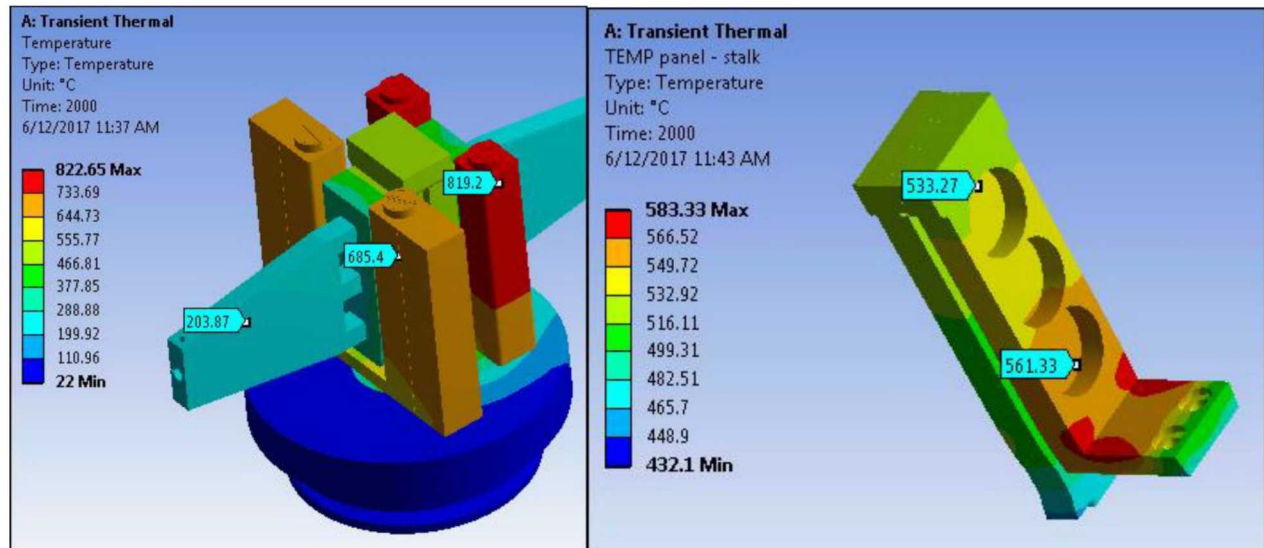
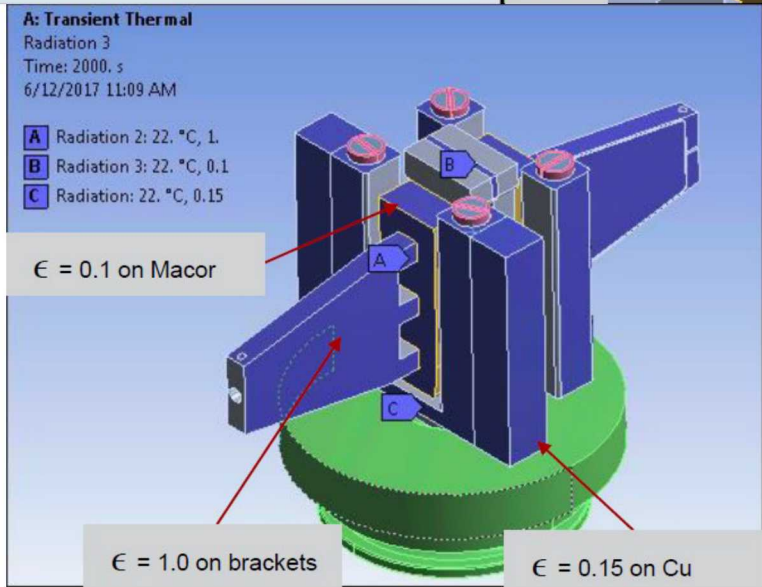
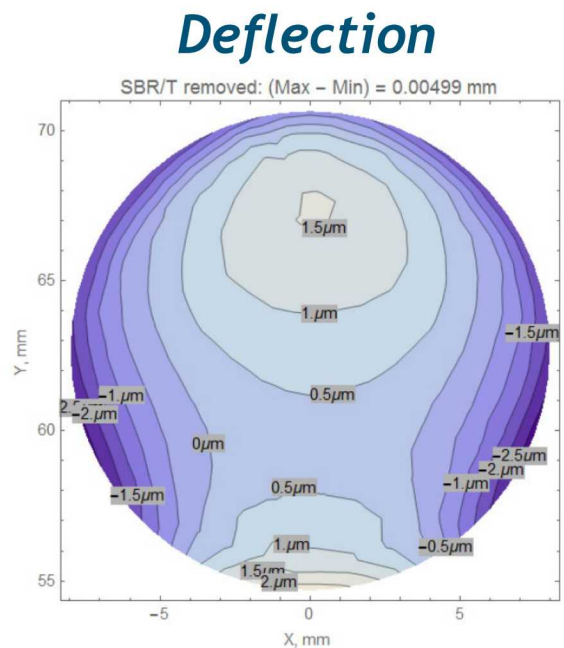
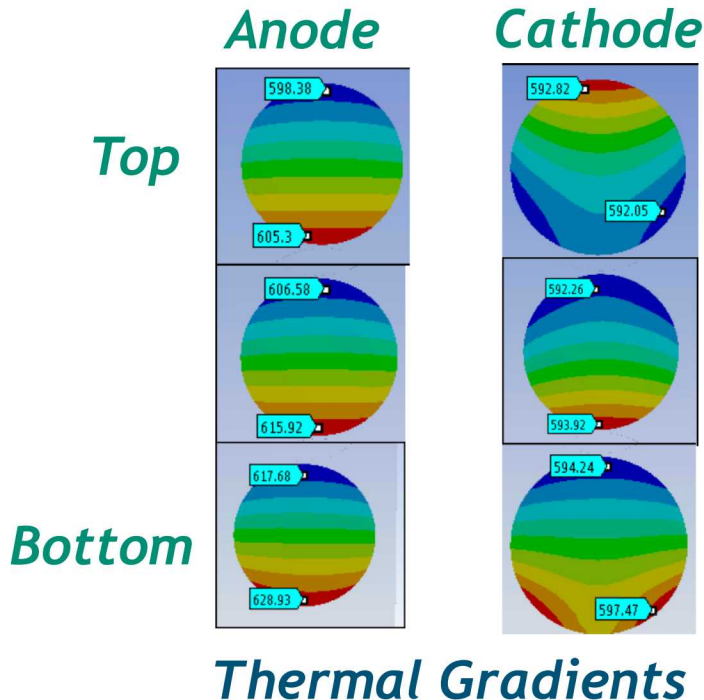
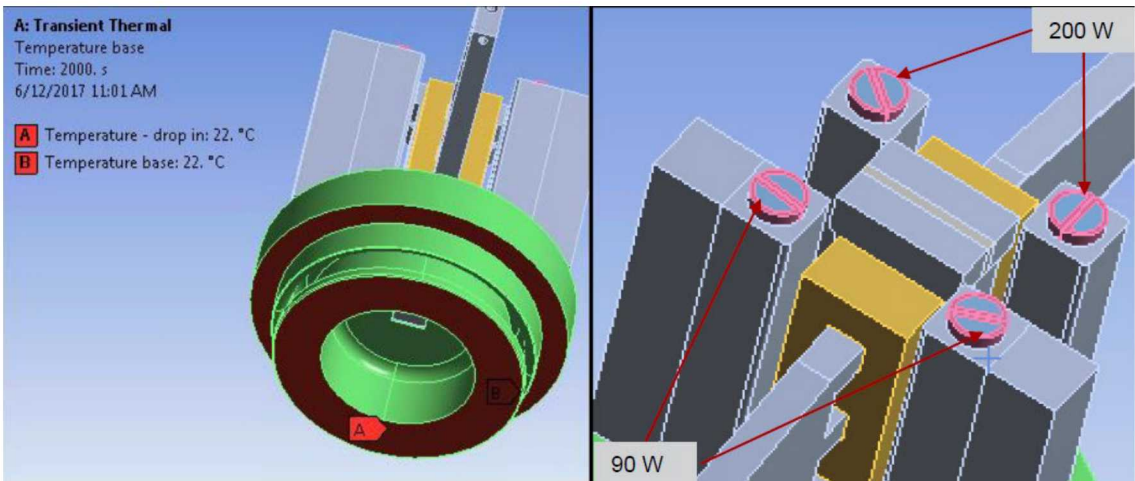
High temperature fibers

All free surface measurements

# Extensive thermo-mechanical simulations were performed to inform this design



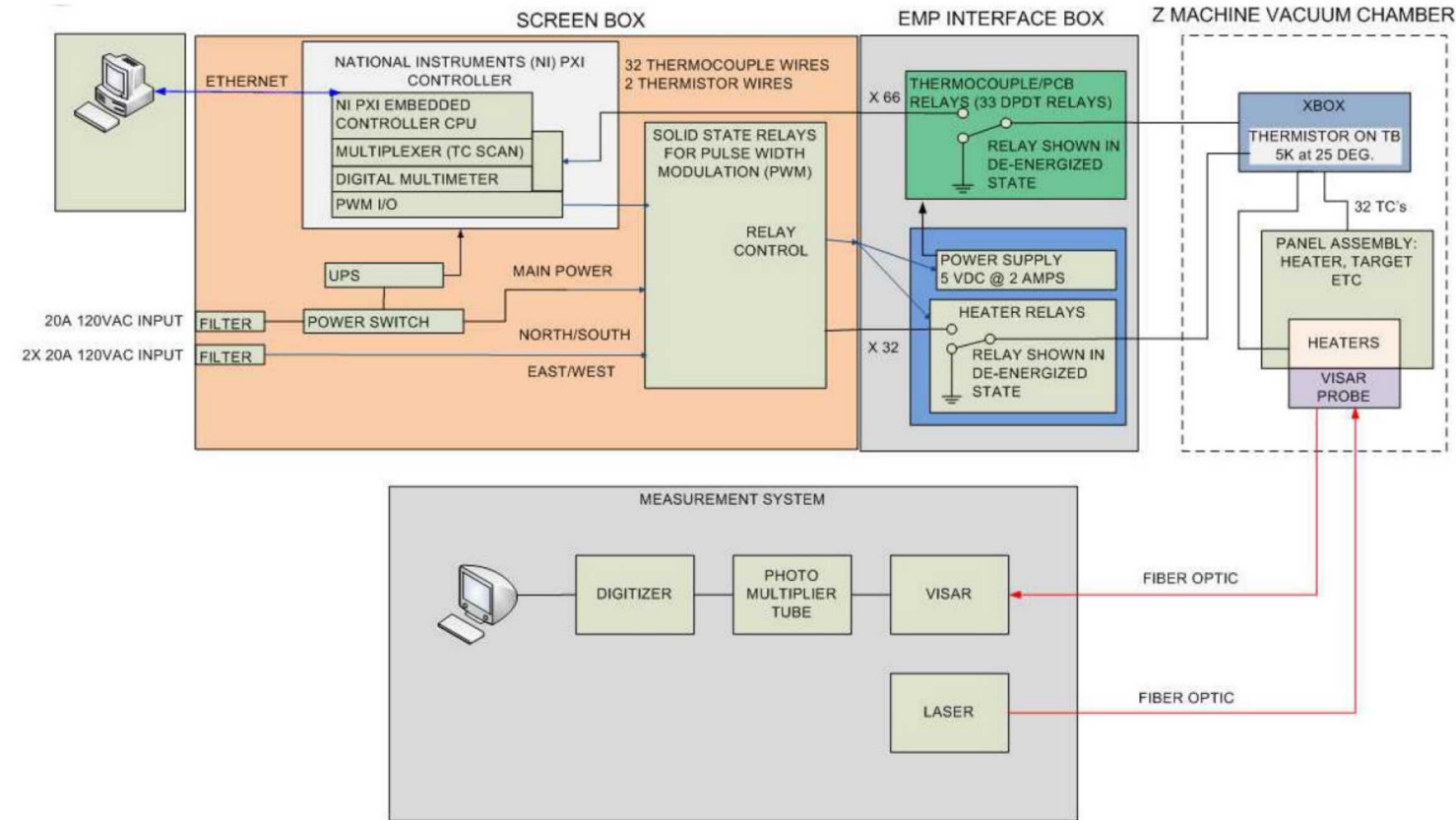
## Boundary Conditions



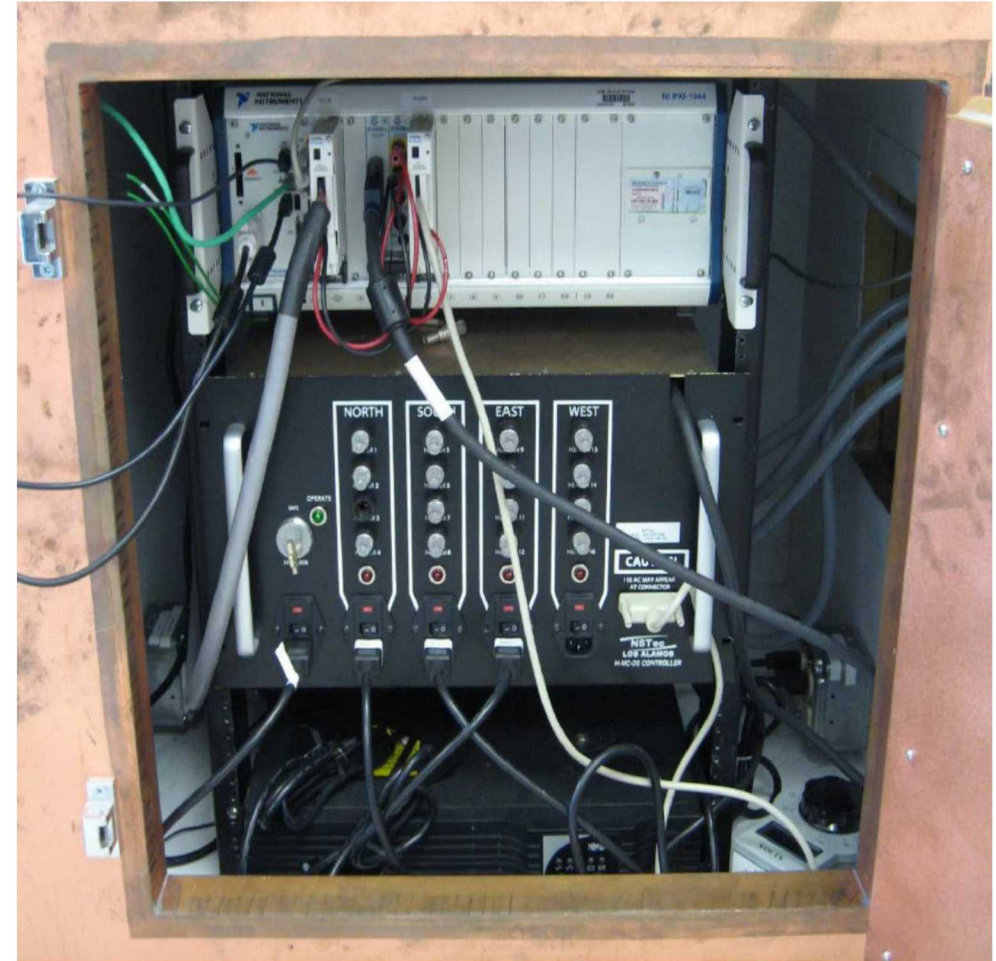
A custom controller is used to control the heaters and monitor TC output



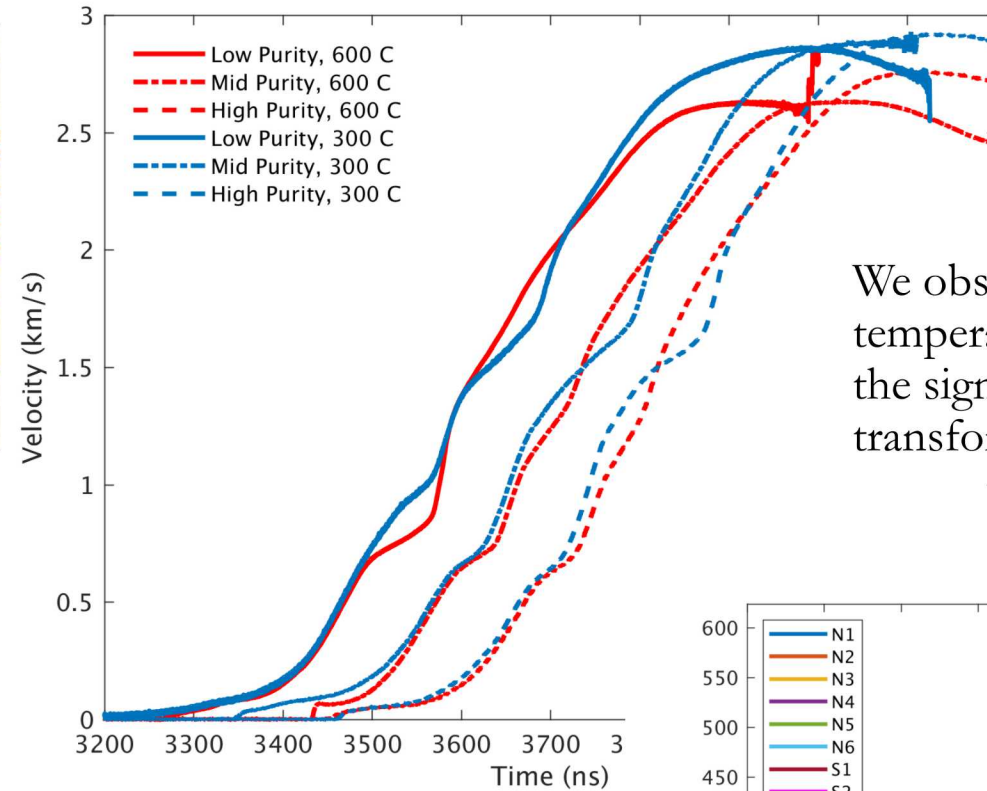
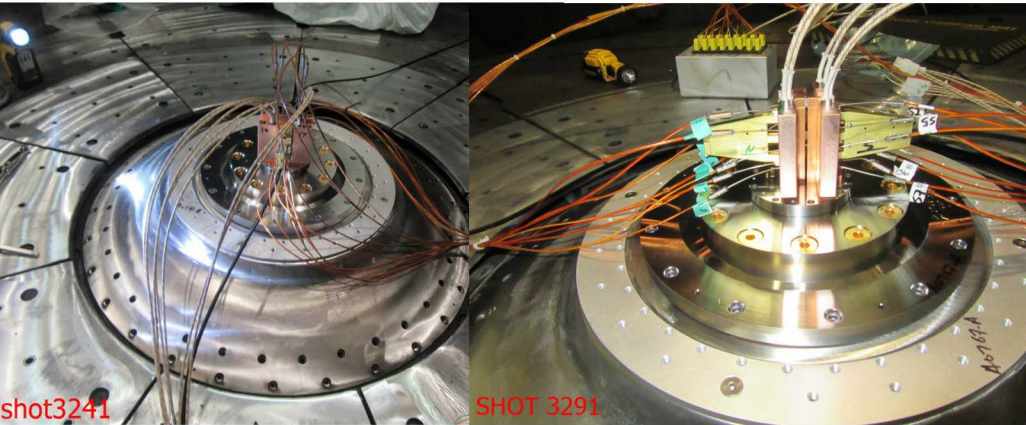
## Preheat + VISAR block diagram



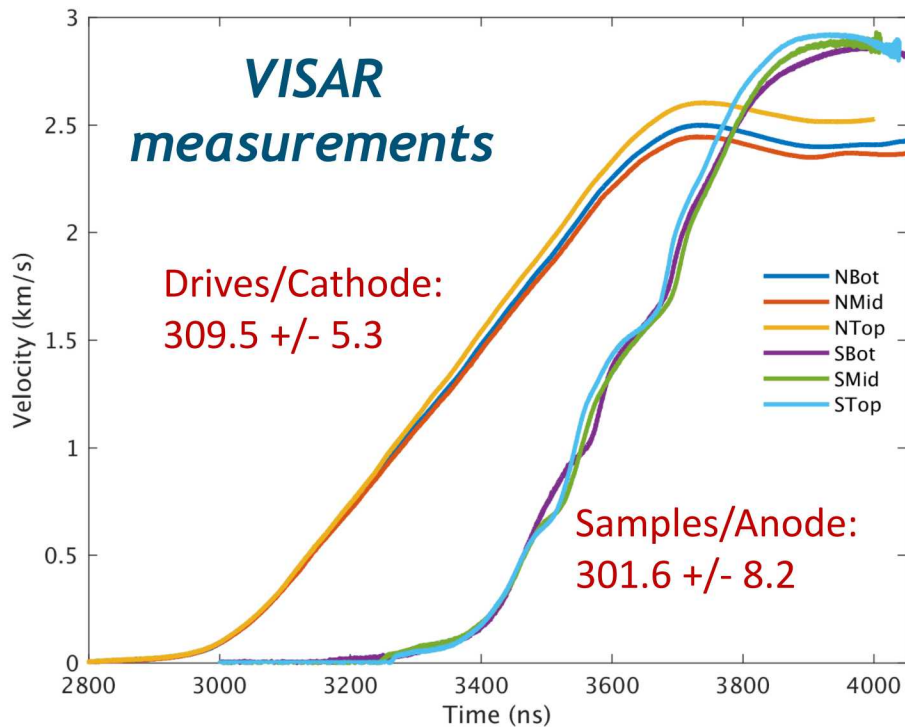
## Controller in the screenbox



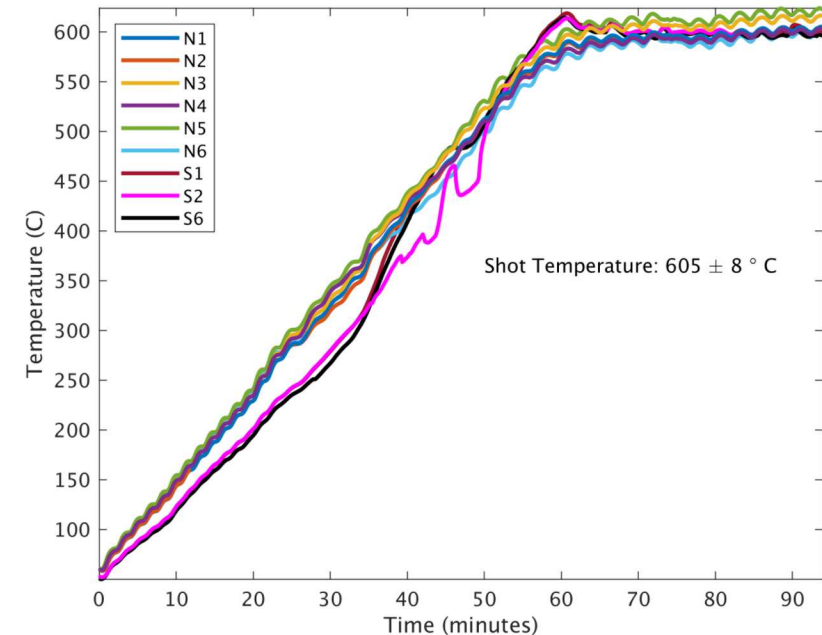
# We have performed 2 preheat experiments on Zr



We observe significant effects of temperature and impurity level on the signature of the phase transformations



More scatter in the thermocouple measurements than desired, but these are consistent with K-type TC error ( $\sim 0.75\%$ )

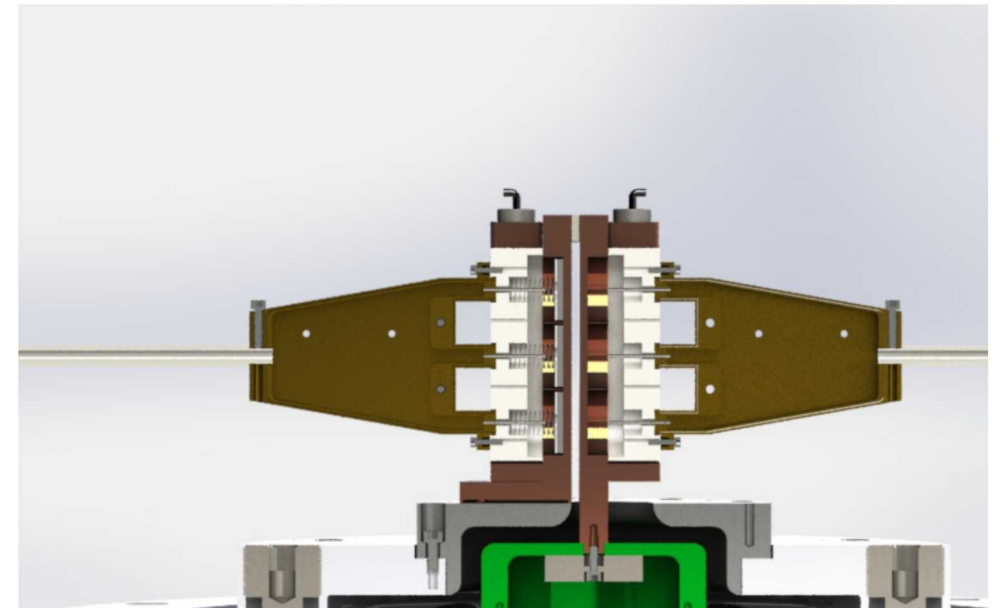
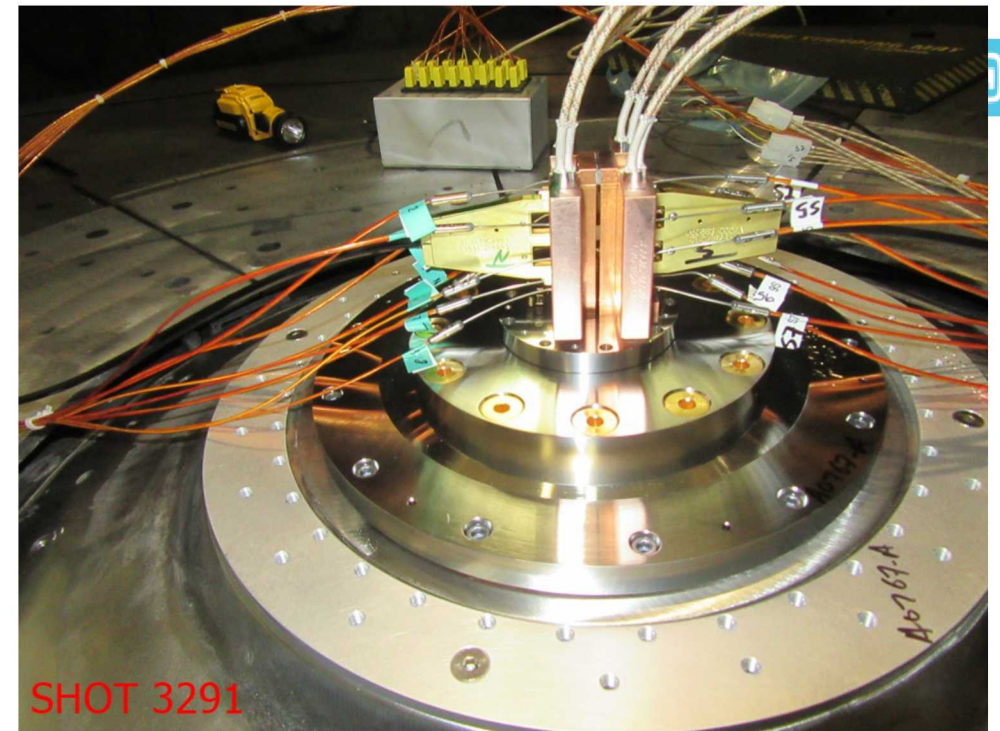


A resistive preheat system has been developed for stripline loads on Z

- Maximum design temperature: 600C

Preheated shockless compression experiments have been performed on Zr

- Initial temperatures of  $\sim 300$  and 600C
- Appears to be a significant effect of temperature on the phase transition kinetics



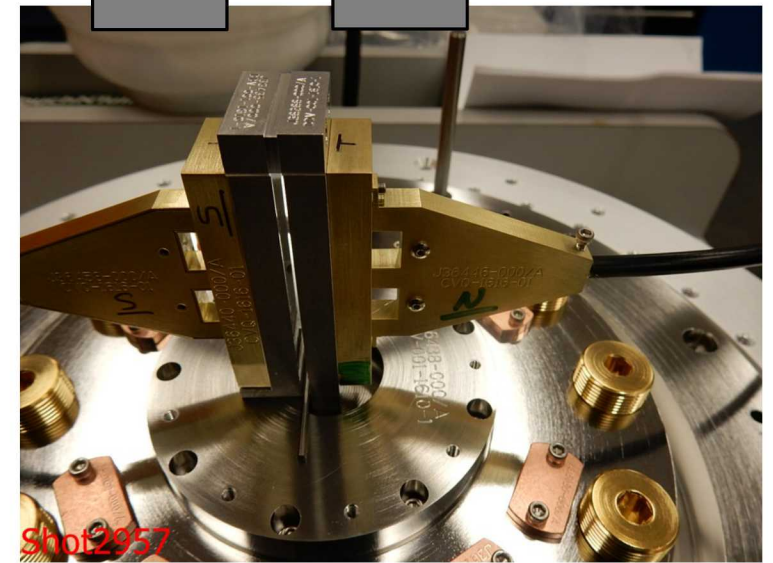
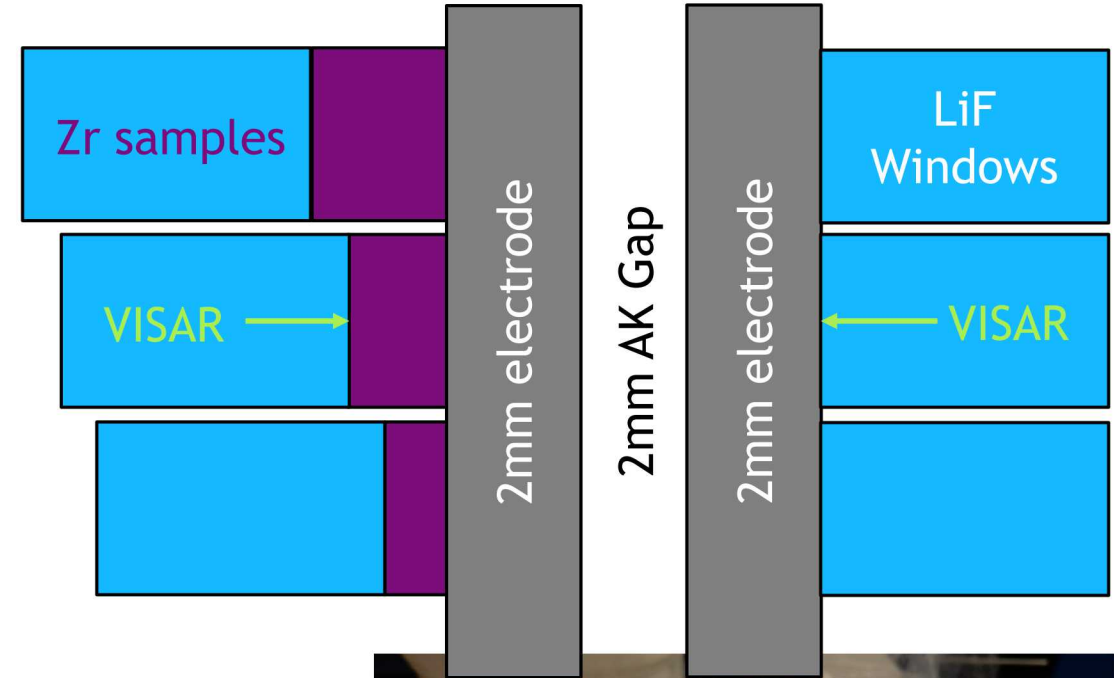
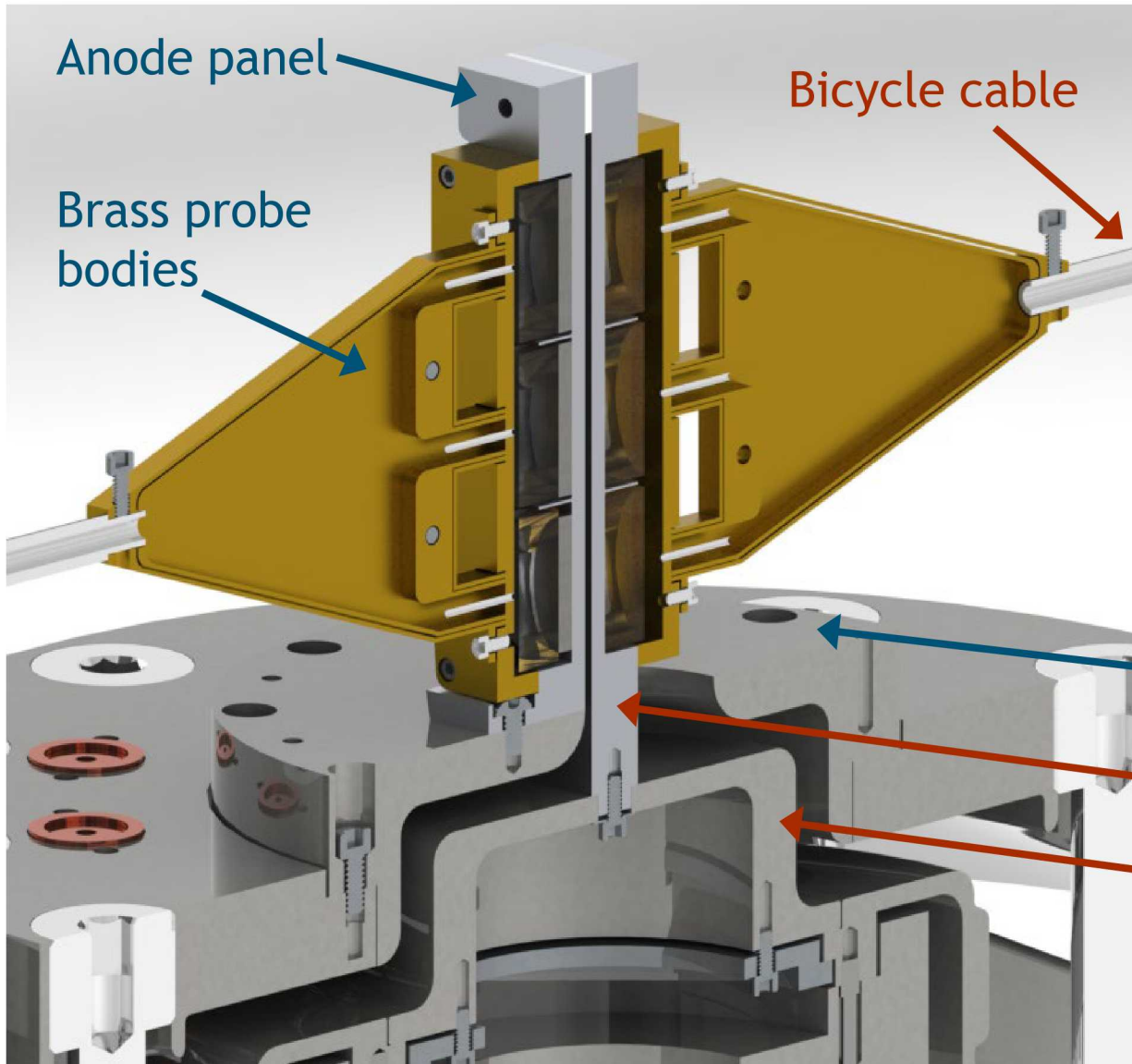


# Ramp loading of Zr

Justin Brown, Carl Greeff, Nenad Velisavljevic

Kinetics of phase transformations in metals under dynamic compression kickoff meeting, Nov. 26-28, 2018

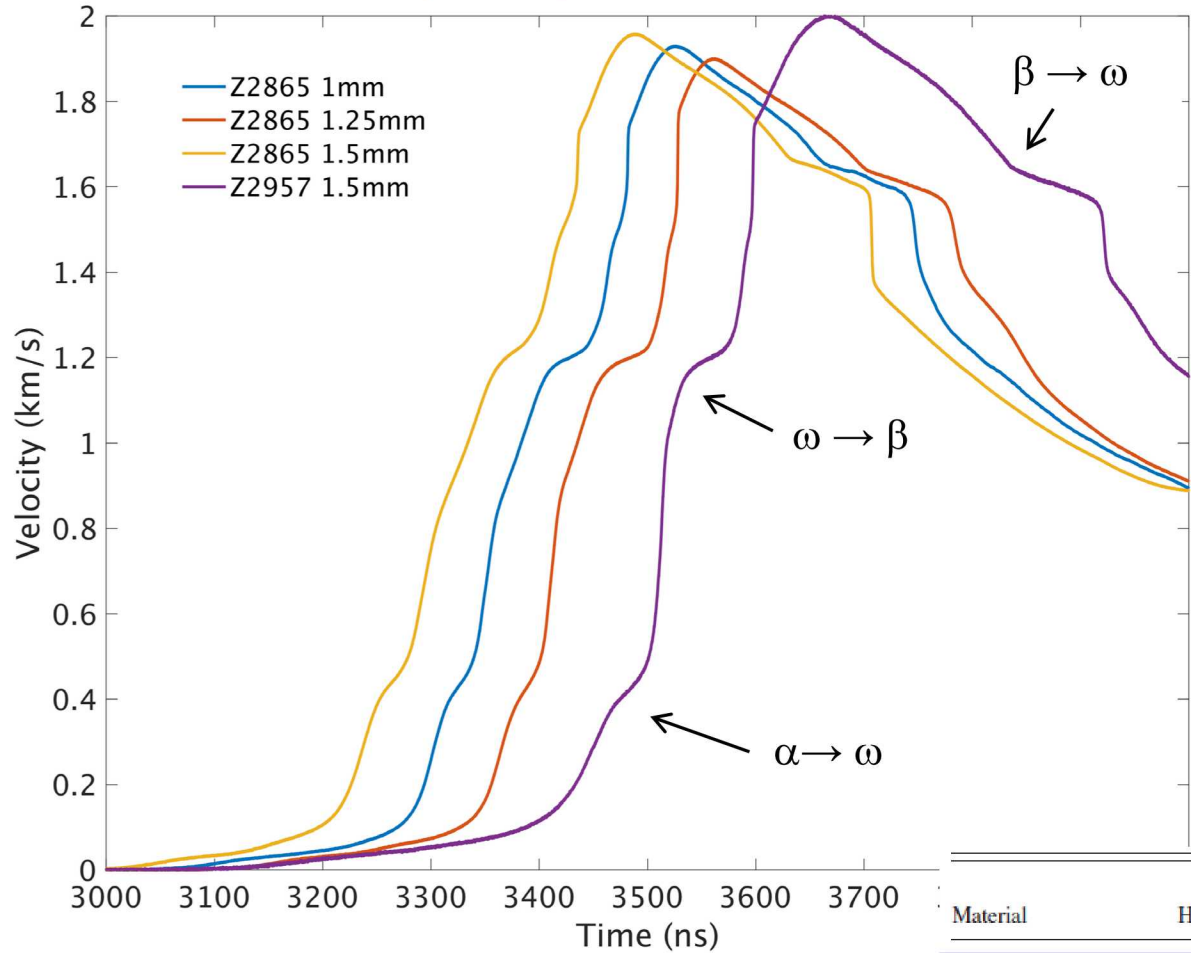
# Review of standard (ambient temperature) stripline setup



# 4 room temperature Zr experiments were conducted resulting in 4 velocity history measurements for each impurity level



## Mid purity measurements



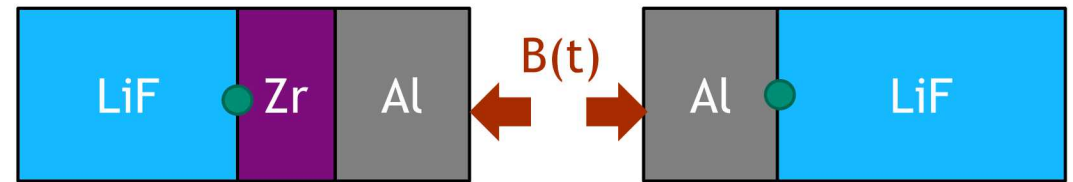
First 3 experiments contained a single impurity level and 3 different thickness samples.

- All 3 shots had identical machine configurations.

Last experiment contained all 3 impurity levels and had a modified pulse shape.

Each measured velocity has a corresponding drive measurement

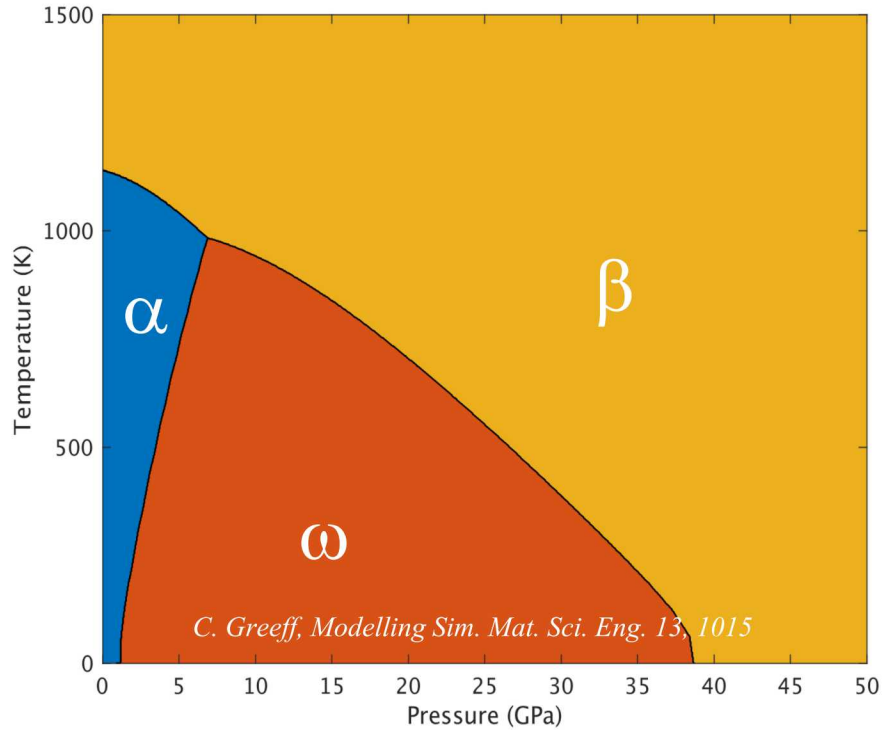
- This configuration is ideal for running 1D simulations
- Drive measurement is used to “unfold” the magnetic pressure



Material	Hf	Fe	Al	V	O	N	C	Density (g/cm <sup>3</sup> )
Zr <sub>0</sub> high purity	35	<50	<20	<50	<50	<20	22	6.499 ± 0.005
Zr <sub>I</sub> low purity	350	125	<20	<25	390	15	70	6.503 ± 0.003
Zr <sub>II</sub> very low purity	14 000	2400	...	...	1200	80	270	6.556 ± 0.007

Bayesian calibration was performed to estimate kinetic parameters for each set of experiments

**Assumption: EOS is fixed during the calibration!**

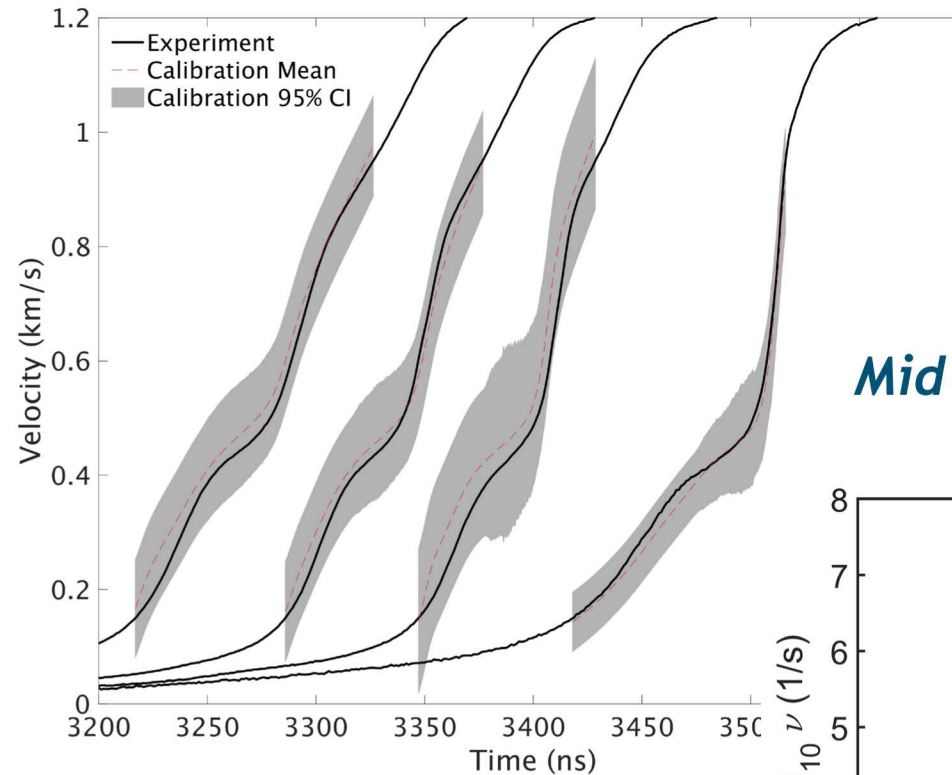


**Assumption: Greeff kinetic model:**

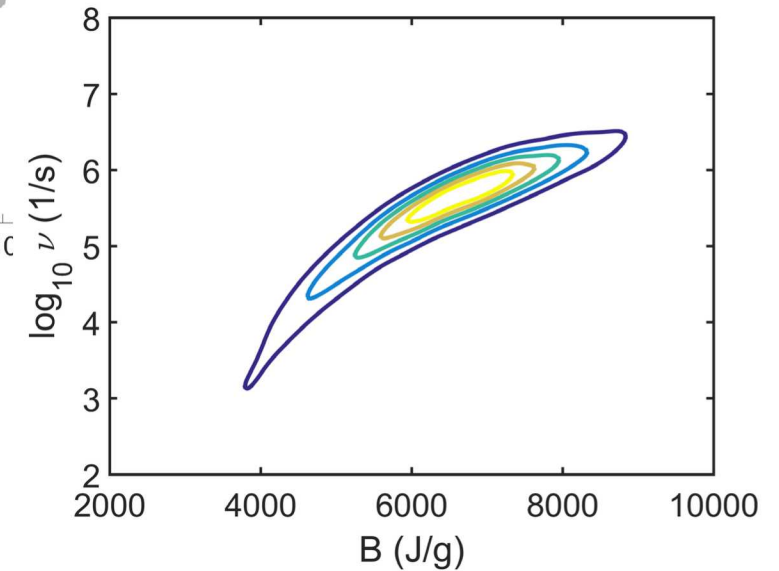
$$\dot{\lambda}_i = \sum_{j \neq i} (\lambda_j R_{ji} - \lambda_i R_{ij}) \quad R_{ij} = \theta (G_i - G_j) \frac{v_{ij}}{B_{ij}} (G_i - G_j) \exp \left[ \frac{(G_i - G_j)^2}{B_{ij}^2} \right]$$



**2 calibration parameters**



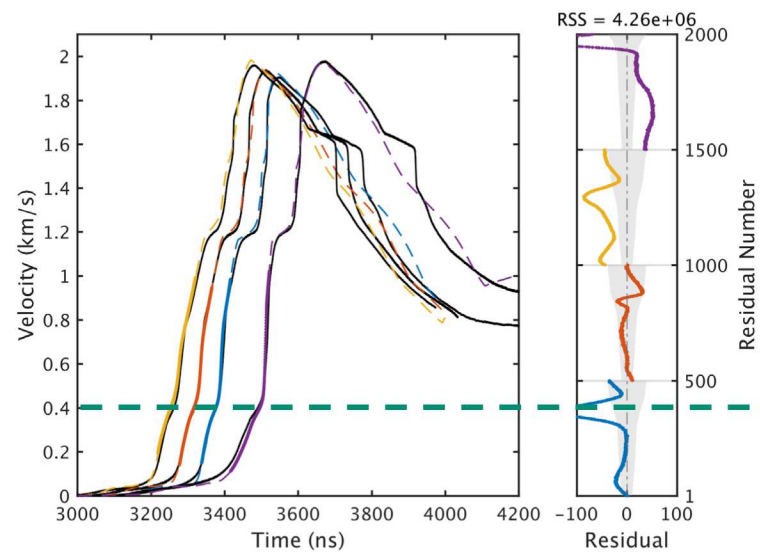
**Mid purity calibration**



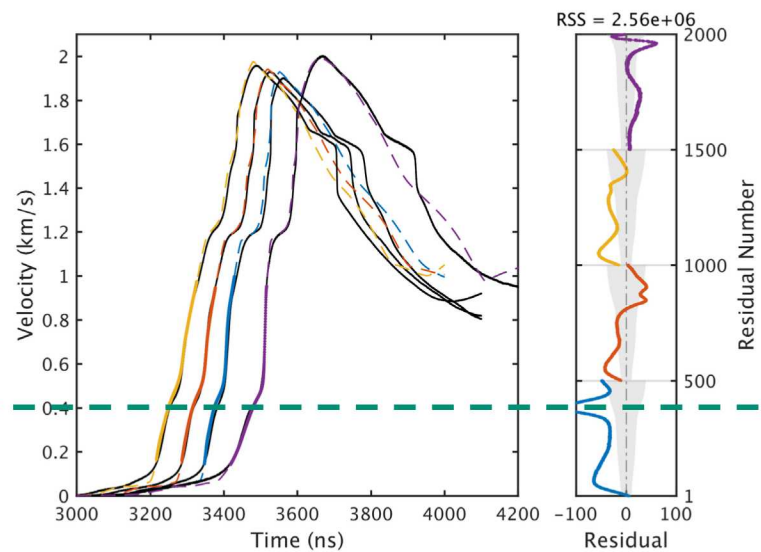
# Bayesian calibration results in quantifiable differences between the kinetic model parameters



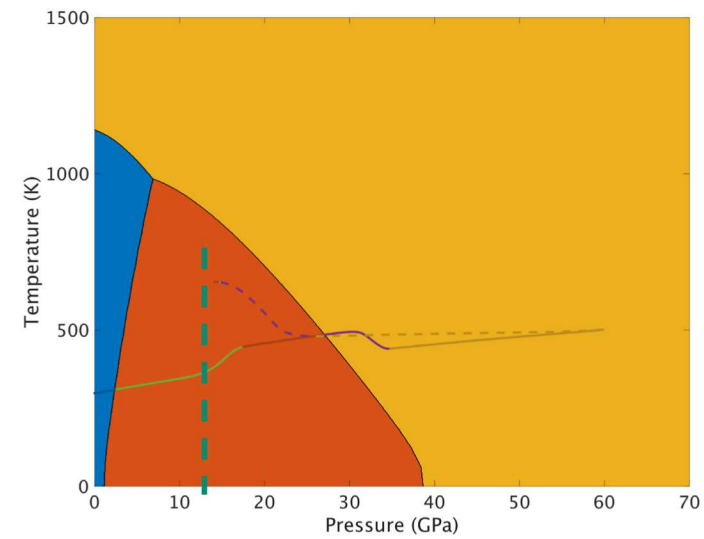
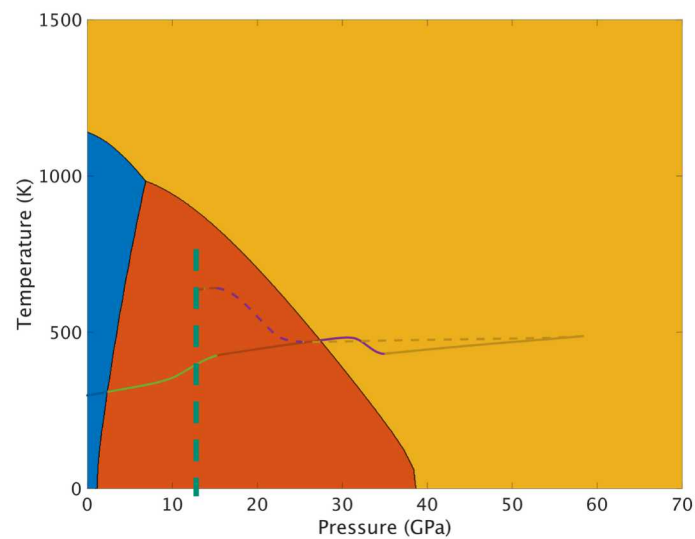
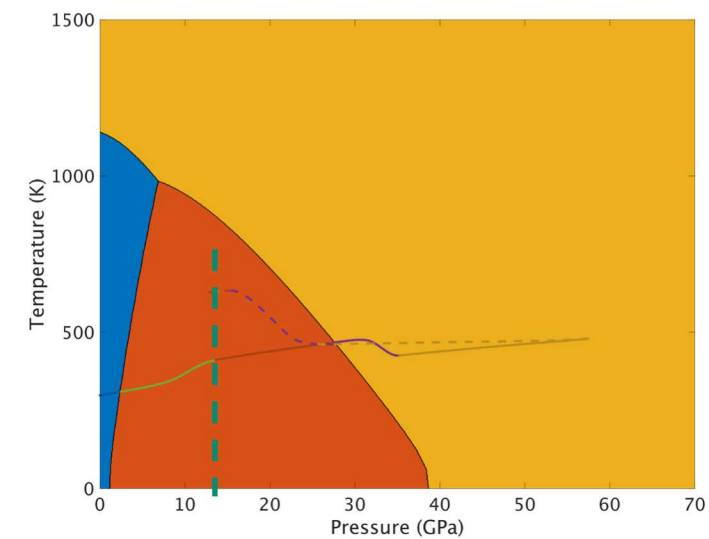
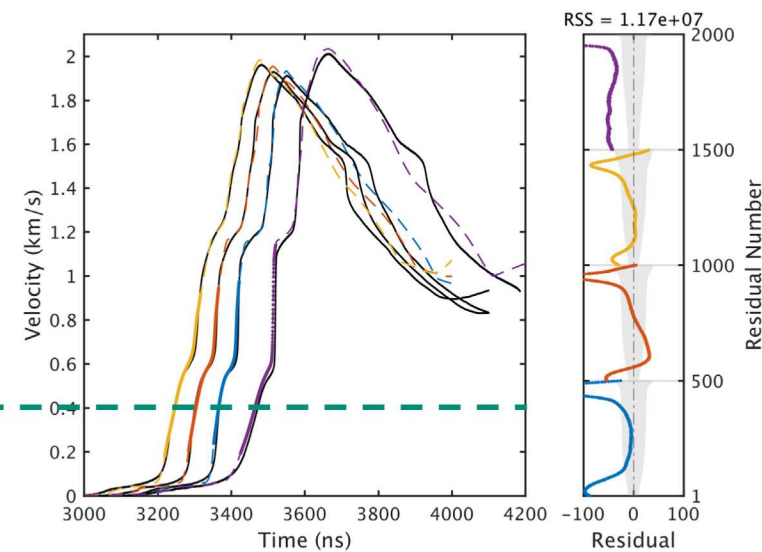
## High Purity



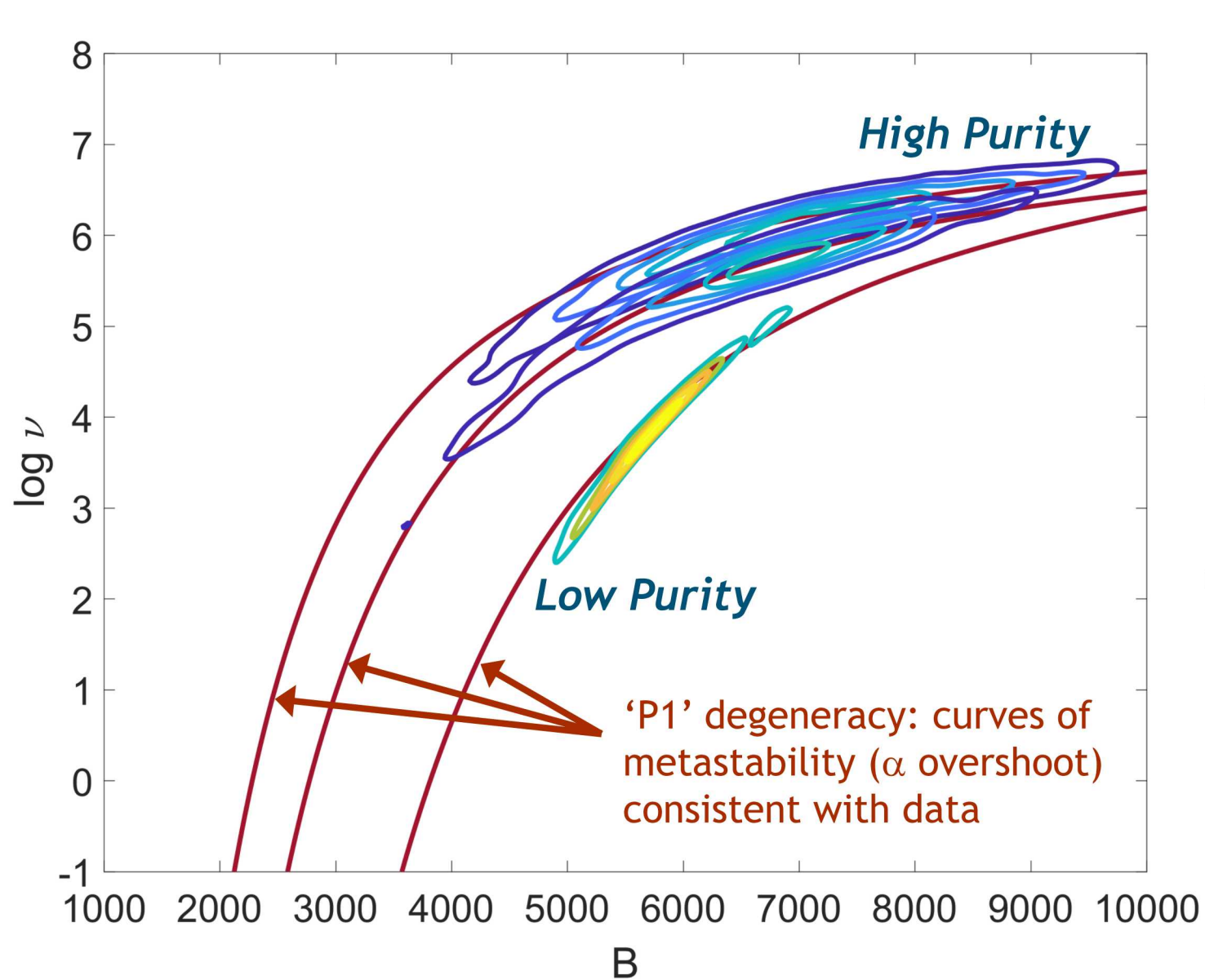
## Mid Purity



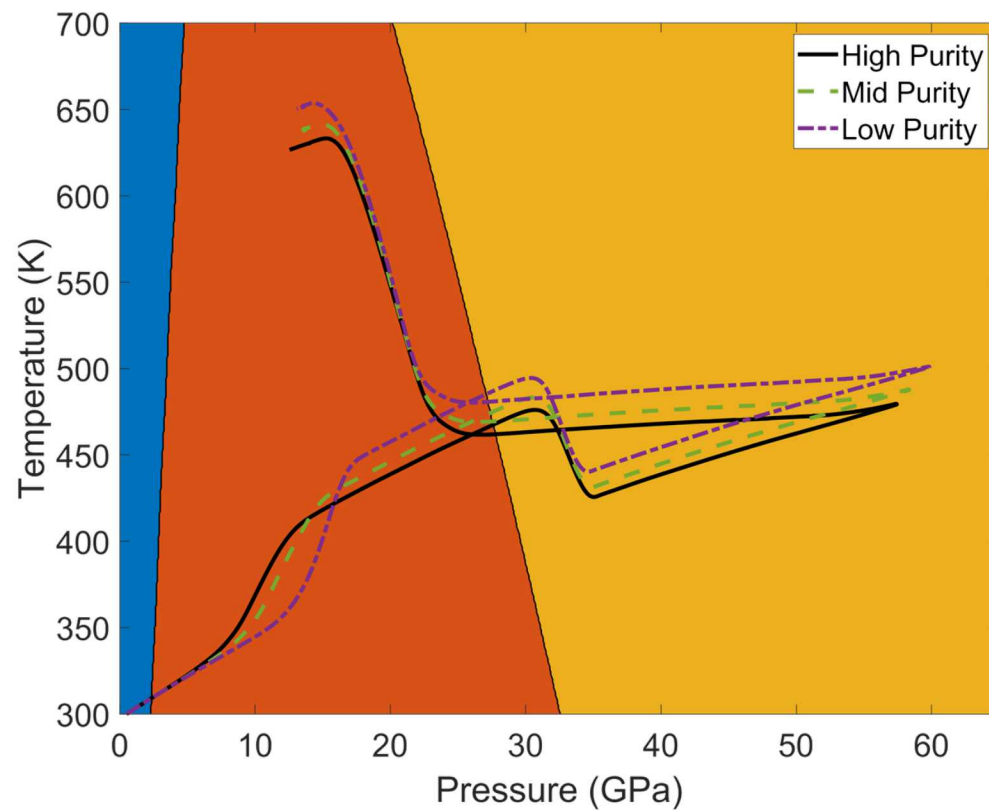
## Low Purity



## Summary of the Zr kinetic parameter calibration



$$R_{ij} = \theta (G_i - G_j) \frac{\nu_{ij}}{B_{ij}} (G_i - G_j) \exp \left[ \frac{(G_i - G_j)^2}{B_{ij}^2} \right]$$





Observe clear evidence of the expected phase transitions in the velocity data

- Phase transition signatures are influenced by the presence of impurities

We have coupled the data to simulations incorporating multi-phase EOS and phase transition kinetics models

- Can obtain excellent agreement with the data
- Cannot decouple EOS and kinetics from these experiments alone



# Ramp loading of Ga

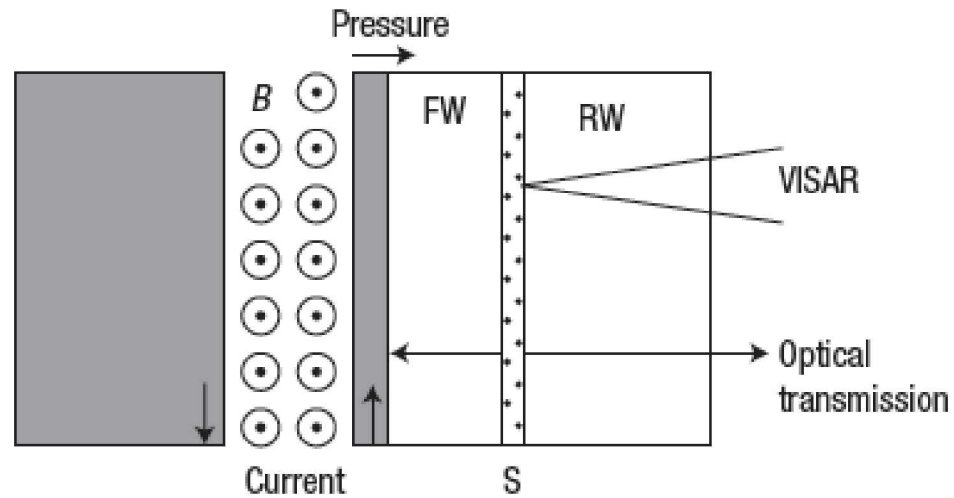
Justin Brown, Jon Belof, Brian Stoltzfus

Kinetics of phase transformations in metals under dynamic compression kickoff meeting, Nov. 26-28, 2018

# A review of Dolan's water experiments



LETTERS



*Dolan et al., Nature Physics 3(5), 2007*

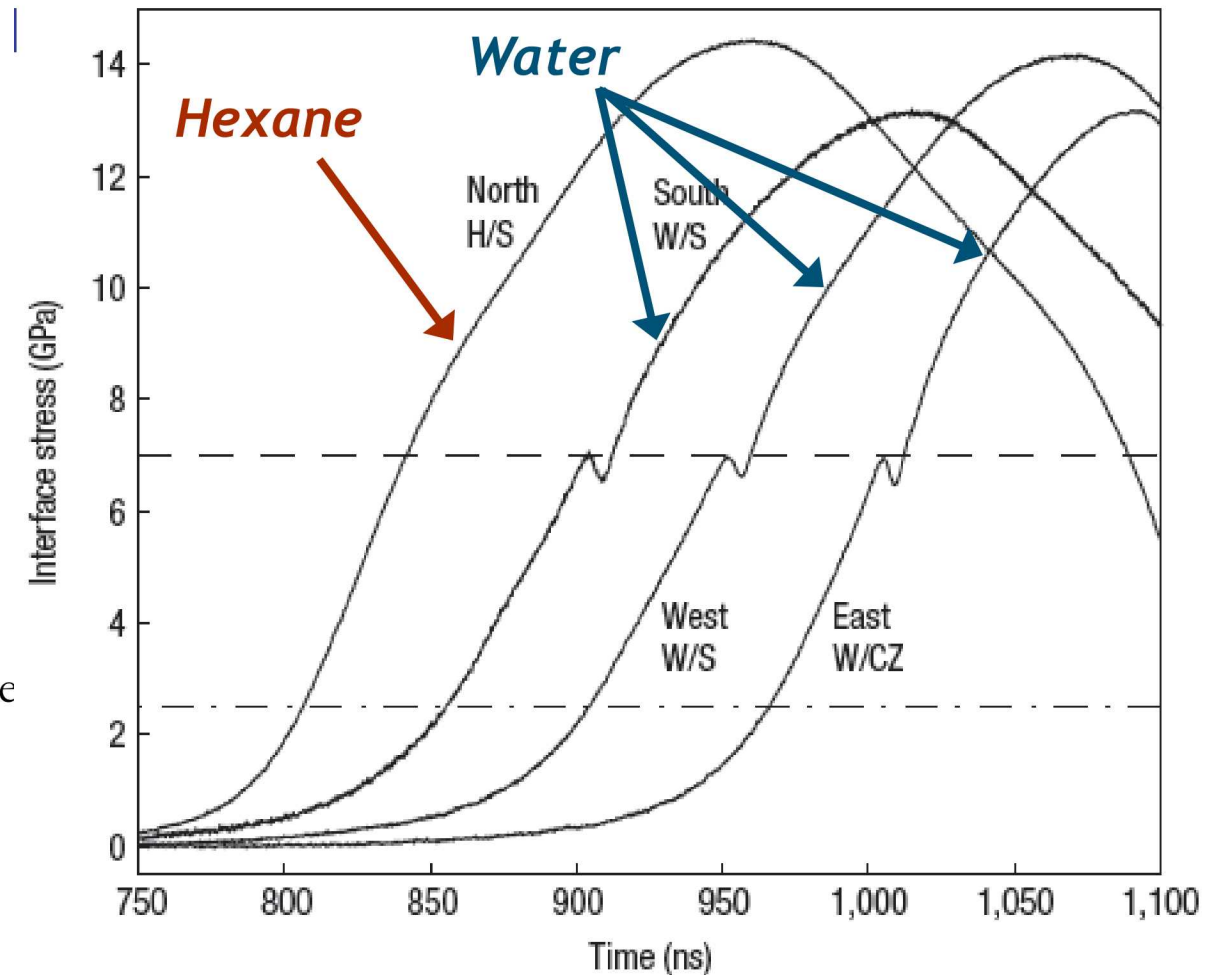
20  $\mu\text{m}$  liquid sample sandwiched between sapphire windows

Clear signature in the VISAR of the water freezing

- First-order phase transition within  $\sim 10$  ns
- Suspect homogeneous nucleation and a transient nucleation time

## A metastable limit for compressed liquid water

D. H. DOLAN\*, M. D. KNUDSON, C. A. HALL AND C. DEENEY



# LLNL recently developed a physics based kinetics model which can reproduce Dolan's water experiments



PHYSICAL REVIEW LETTERS **121**, 155701 (2018)

Editors' Suggestion

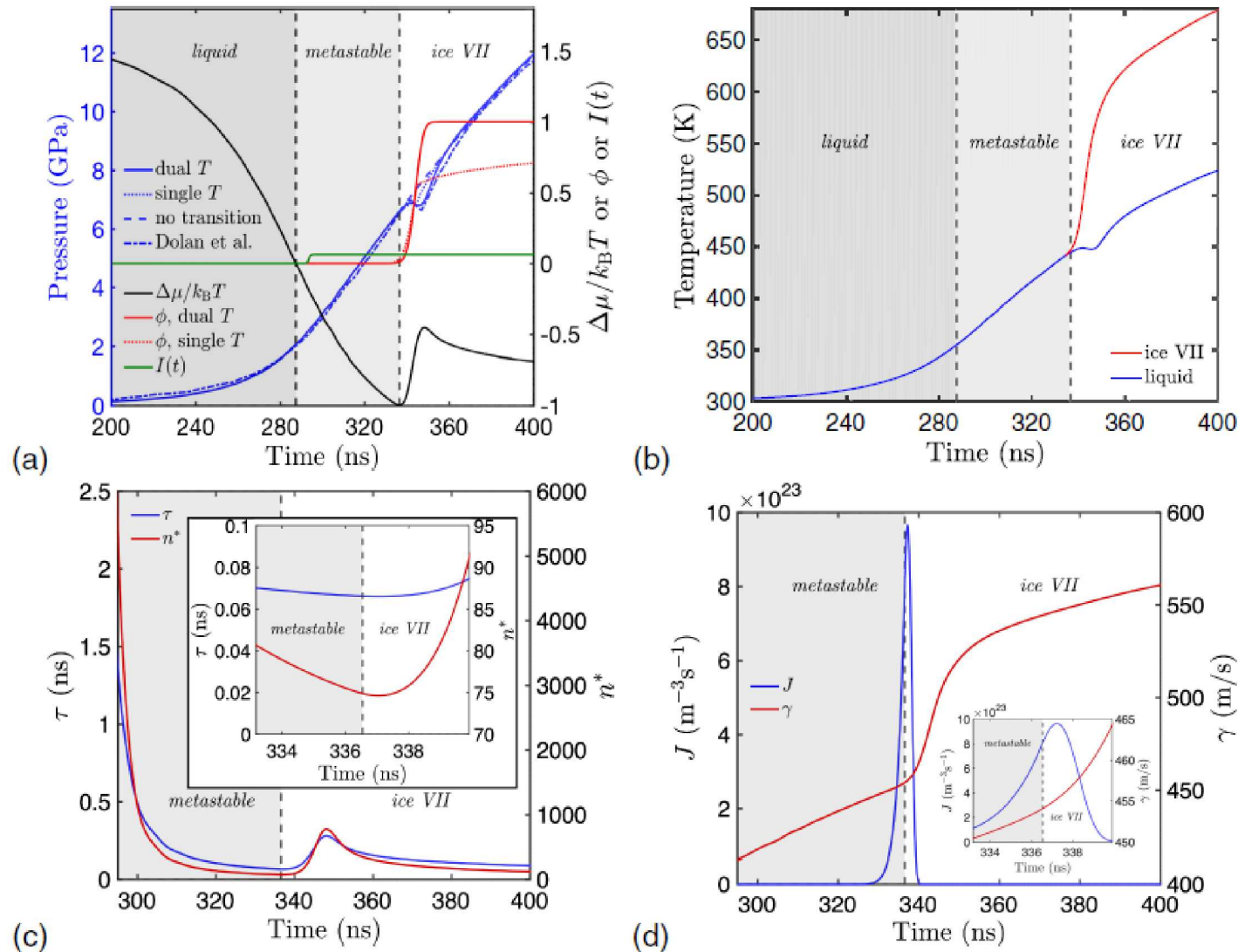
## Nanosecond Freezing of Water at High Pressures: Nucleation and Growth near the Metastability Limit

Philip C. Myint, Alexander A. Chernov, Babak Sadigh, Lorin X. Benedict, Burl M. Hall, Sebastien Hamel, and Jonathan L. Belof\*  
Lawrence Livermore National Laboratory, Livermore, California 94550, USA

### KJMA classical nucleation theory with 2 additions:

- Transient nucleation
- Induction time relates to time to cross a critical cluster size
- Only adjustable parameter in their model
- Separate liquid and solid temperatures
- Growth rate is faster than the rate of latent heat transport
- Heat released by solidification is absorbed by growing crystal, so liquid is cooler than a typical single temperature model

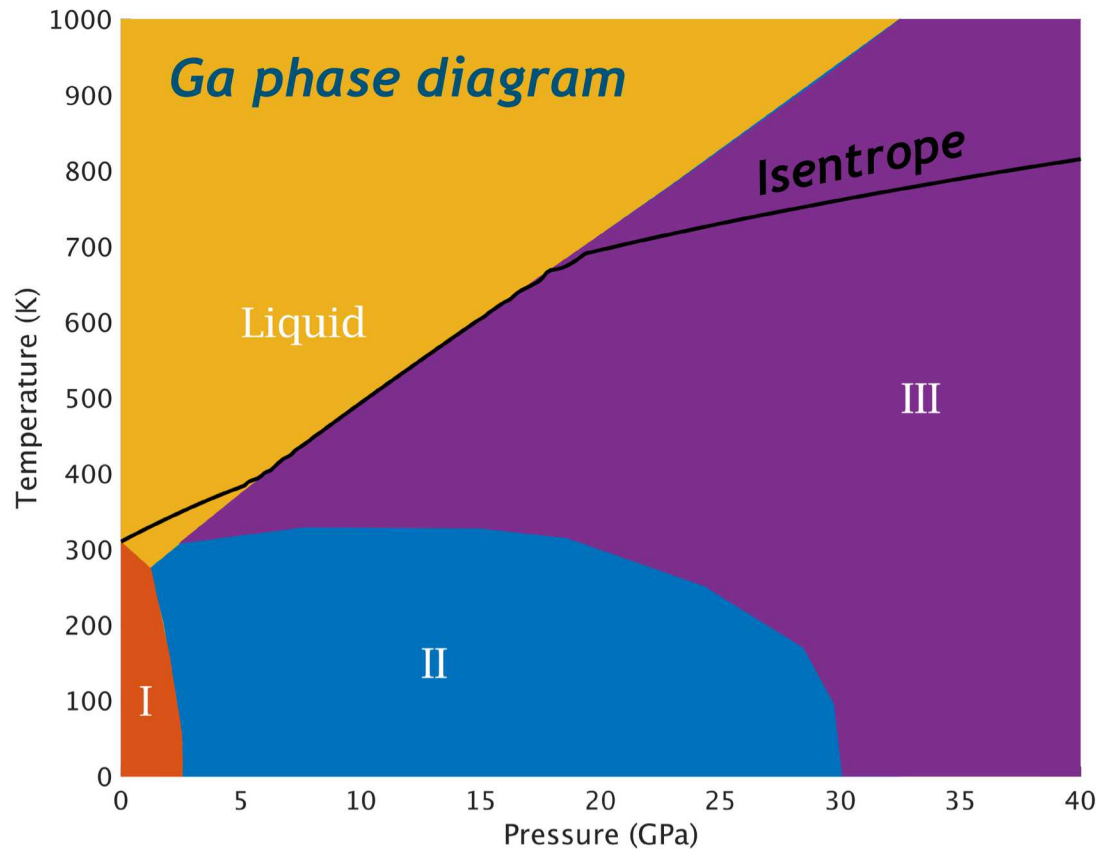
Model suggests homogeneous nucleation dominates



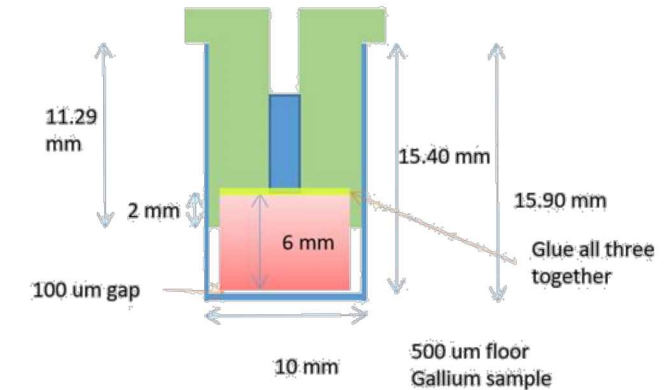
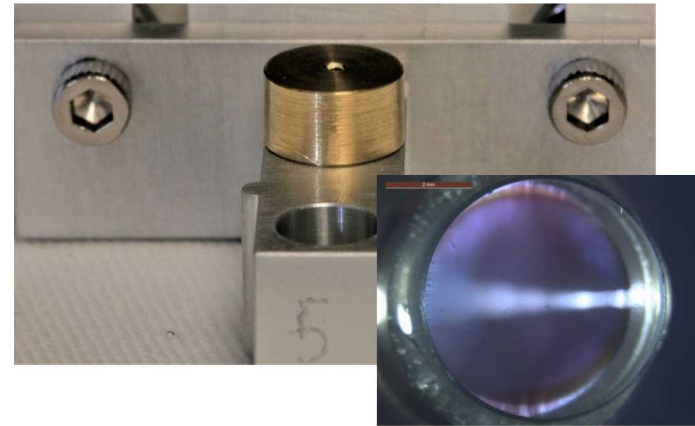
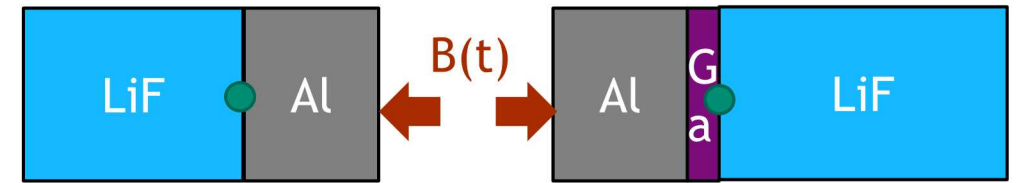
# Does a metal exhibit similar behavior?

Ga chosen as an ideal metal for Thor experiments

- Liquid near standard temperature and pressure
- Expected to solidify at pressures accessible to Thor (~40 GPa)



*Crockett and Greeff, SCCM 1195(1), 2009*



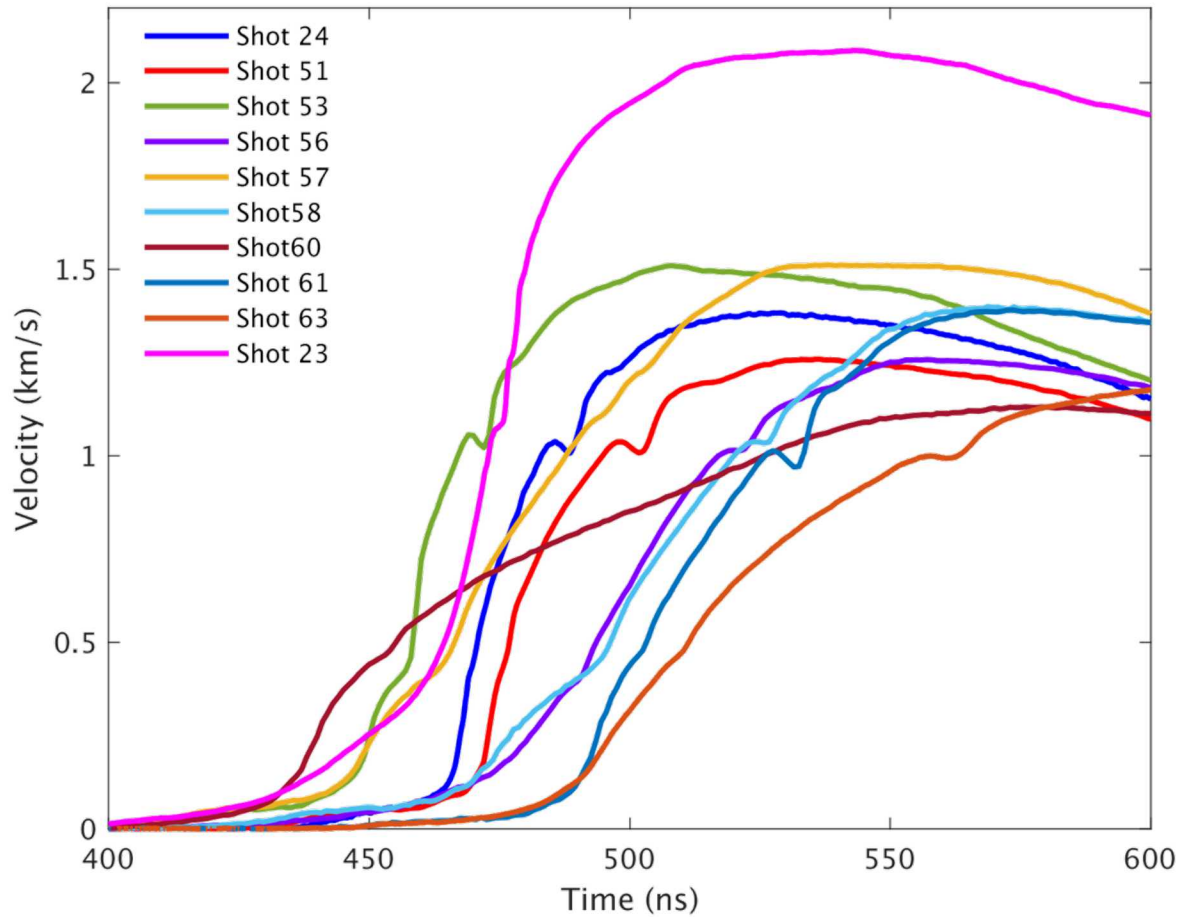
Experiments contain Ga sandwiched between Al and LiF

- Entire central portion of machine is heated to ~34C
- Cell is assembled with liquid Ga and immediately loaded into Thor
- Ga is 50-250  $\mu\text{m}$  thick
- Significant pressure gradient at bigger thicknesses
- Ga interacts with Al
  - In initial attempts, the Al panels fell apart
  - The panels were anodized to prevent this interaction
- Simultaneous VISAR and PDV from a single probe
  - Reflect directly off of the Ga/LiF interface (no spot coating)

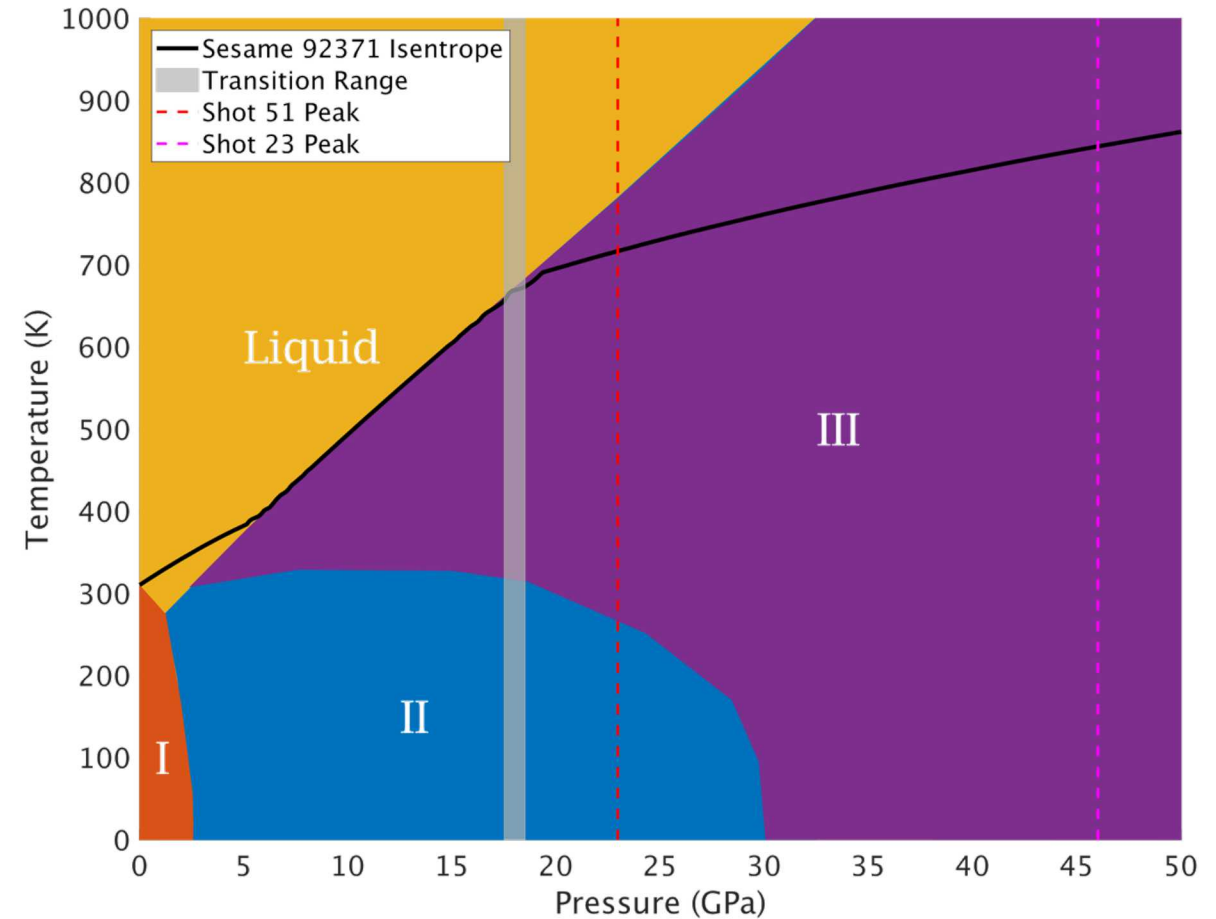
# Clear evidence of Ga solidification is observed!



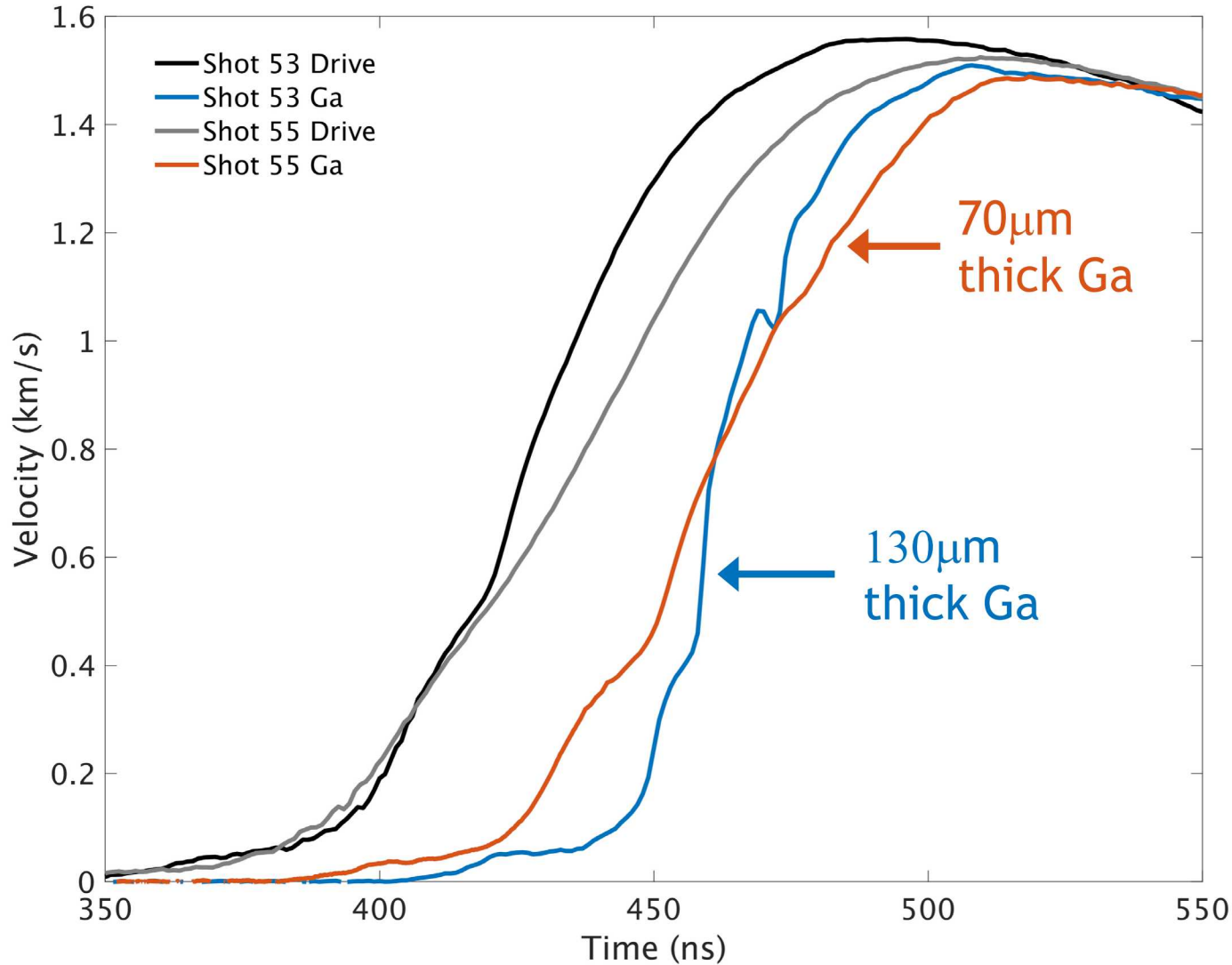
Signatures are qualitatively similar to what was observed in water.



Solidification is consistent with our baseline EOS

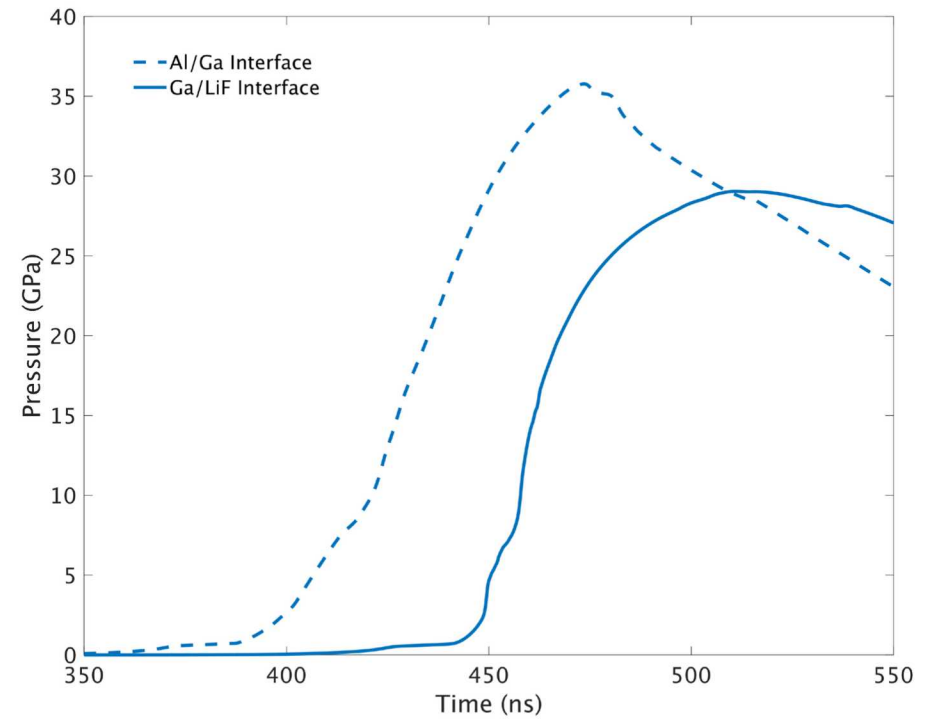


# We are still trying to understand how to interpret the data



The solidification signature depends on the pulsheshape and Ga thickness

- For a given pulsheshape there is a critical thickness where the signature will not be observed
- Thicker samples induce a pressure gradient across the sample
  - Is the higher pressure driving solidification?





Observe clear evidence of solidification in the velocity signatures

The nature of the signature seems to be a complicated function of pulshape and Ga thickness

Analysis is ongoing

- Can replicate the data with the LLNL kinetic model by tuning the single free parameter

*Appl. Statist.* (2018)

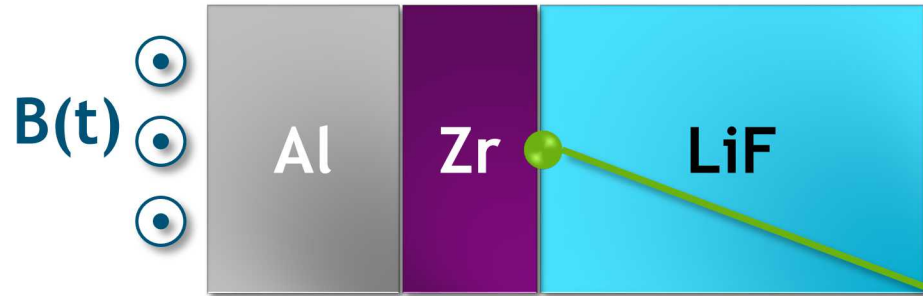
**Estimating material properties under extreme conditions by using Bayesian model calibration with functional outputs**

# Bayesian calibration of models against multiple data sets

Justin Brown, Lauren Hund

Kinetics of phase transformations in metals under dynamic compression kickoff meeting, Nov. 26-28, 2018

# Inverse Problem Definition



## Typical Experimental Uncertainties

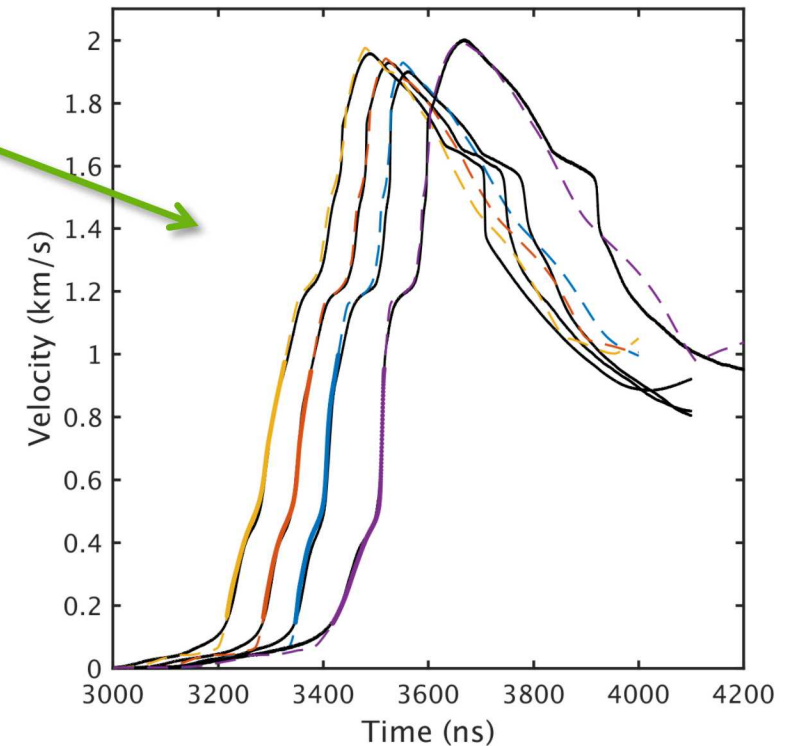
Uncertainty	Standard Error
Al Thickness	3 $\mu\text{m}$
Zr Thickness	3 $\mu\text{m}$
Relative Timing	200 ps
B-Field Scaling	0.5%

Assuming we treat Al and LiF as standards, can we calibrate material model parameters based on comparisons between measured and simulated velocities?

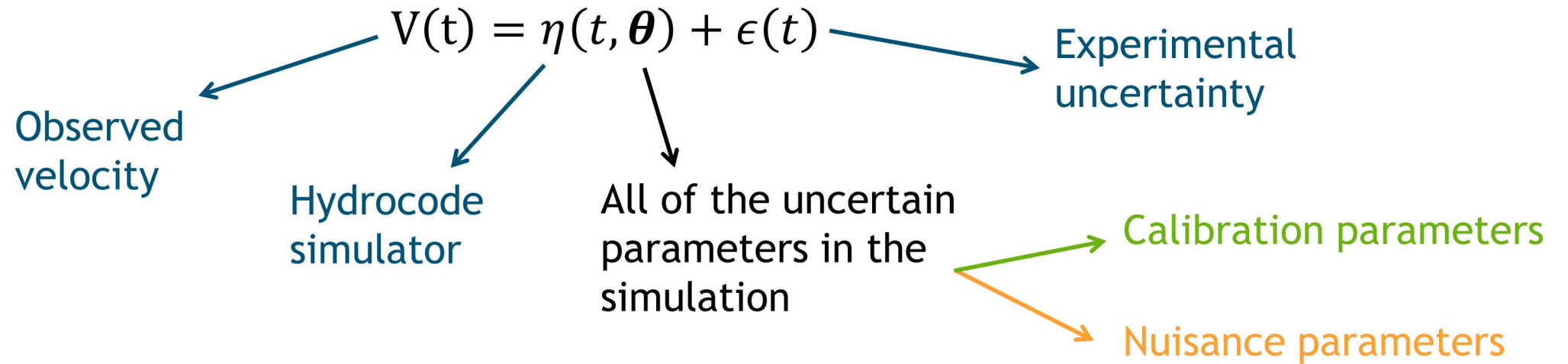
Can we quantify uncertainties?

Can we incorporate multiple experiments within a single calibration?

**Bayesian Calibration**



A standard Bayesian model calibration framework is used



Likelihood reflects difference between simulation and experiment:

$$l(V|\theta) = \prod_{i=1}^n \frac{1}{\sqrt{(2\pi)^n |\Sigma_d|}} \exp\{-\mathbf{r}^T \Sigma_d^{-1} \mathbf{r}\}$$

Likelihood

Covariance matrix of Gaussian data uncertainties

Vector of residuals (difference between VISAR and simulation at each time)

Sample from posterior of  $\theta$  using MCMC

# There are several aspects of this calibration which are unique to our application



## 1. Functional data

- We are interested in calibrating against the entire velocity-time history, not distinct features

## 2. Expense of hydrocode simulations

- Even 1D simulations take a prohibitive amount of time to run for MCMC sampling

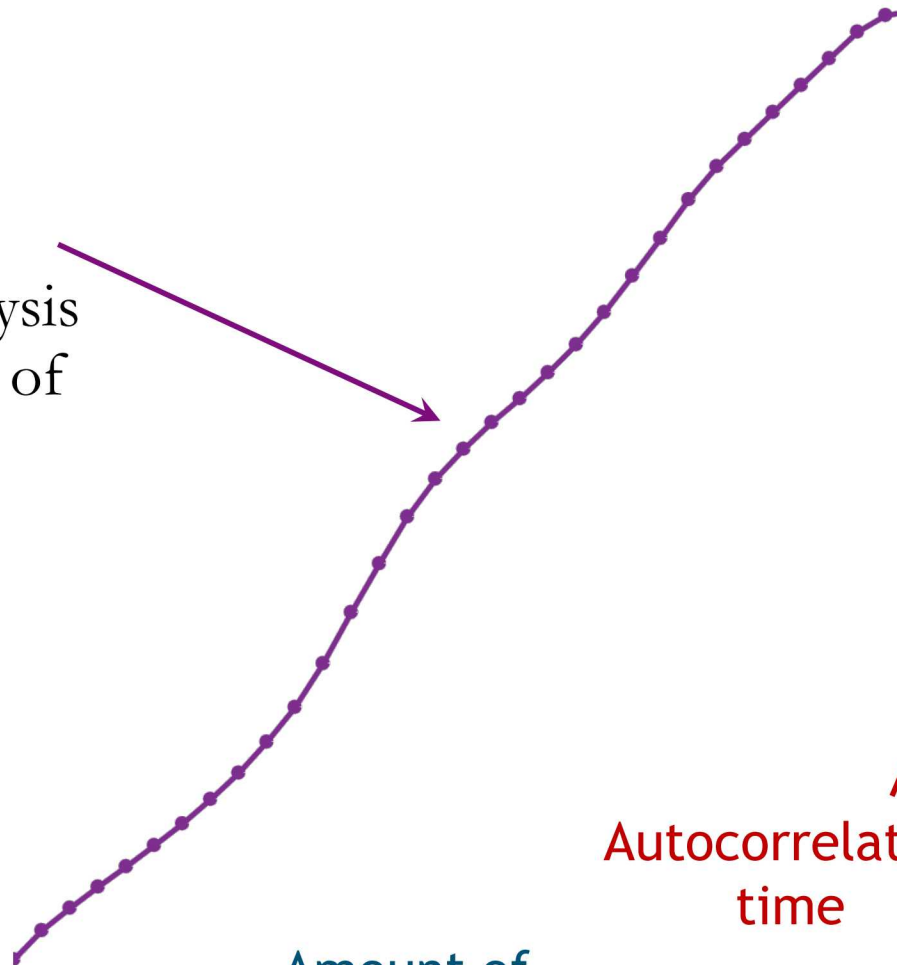
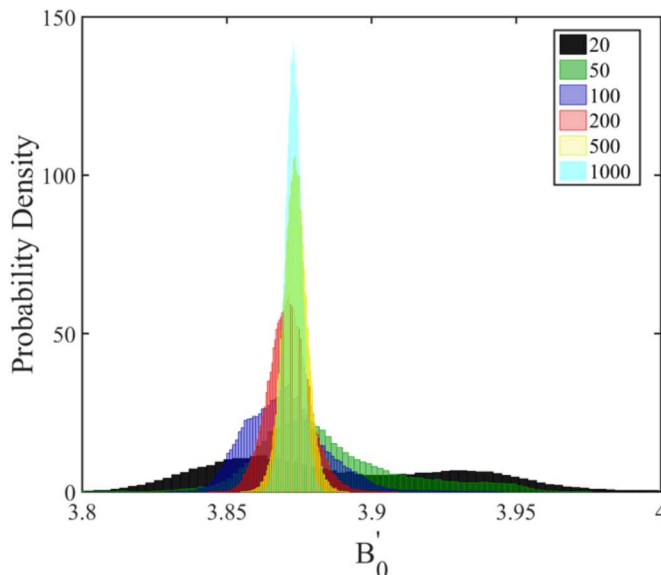
## 3. Dealing with the nuisance parameters

- For low numbers of experiments there is not enough information to constrain inference of both the calibration and nuisance parameters

A VISAR profile can be discretized into an arbitrary number of points,  $n$

In a standard statistical analysis this is  $n$  independent pieces of information

- Variance scales as  $1/n!$



The typical approach is to estimate the autocorrelation function within the calibration

We propose scaling the likelihood by the effective sample size (ESS):

$$\tau = 1 + 2 \sum_{k=1}^{\infty} \nu(k)$$

Autocorrelation time

Autocorrelation in the residuals at lag  $k$

Amount of information contained in a given profile



$$ESS = \frac{n}{\tau}$$

## Challenge #2: hydrocode emulation



Markov Chain Monte Carlo (MCMC) used to sample Bayesian posteriors is a serial process

- Even 1D simulations ( $\sim 1$  minute run times) are prohibitively expensive

### Solution: use an emulator

- Sample the parameter space using random sampling
- Can perform a massive number of simulations in parallel
- Construct emulator for each time point based on this set of training data
- Can now use MCMC to sample from the emulator very quickly

### We use Gaussian Process (GP) emulators

- Exactly reproduces training data
- Smooth interpolation for values not sampled in training data

$$\text{Corr}(\boldsymbol{\theta}, \boldsymbol{\theta}') = \exp \left\{ \sum_{k=1}^m -\omega_k (\theta_k - \theta_{k'})^2 \right\}$$

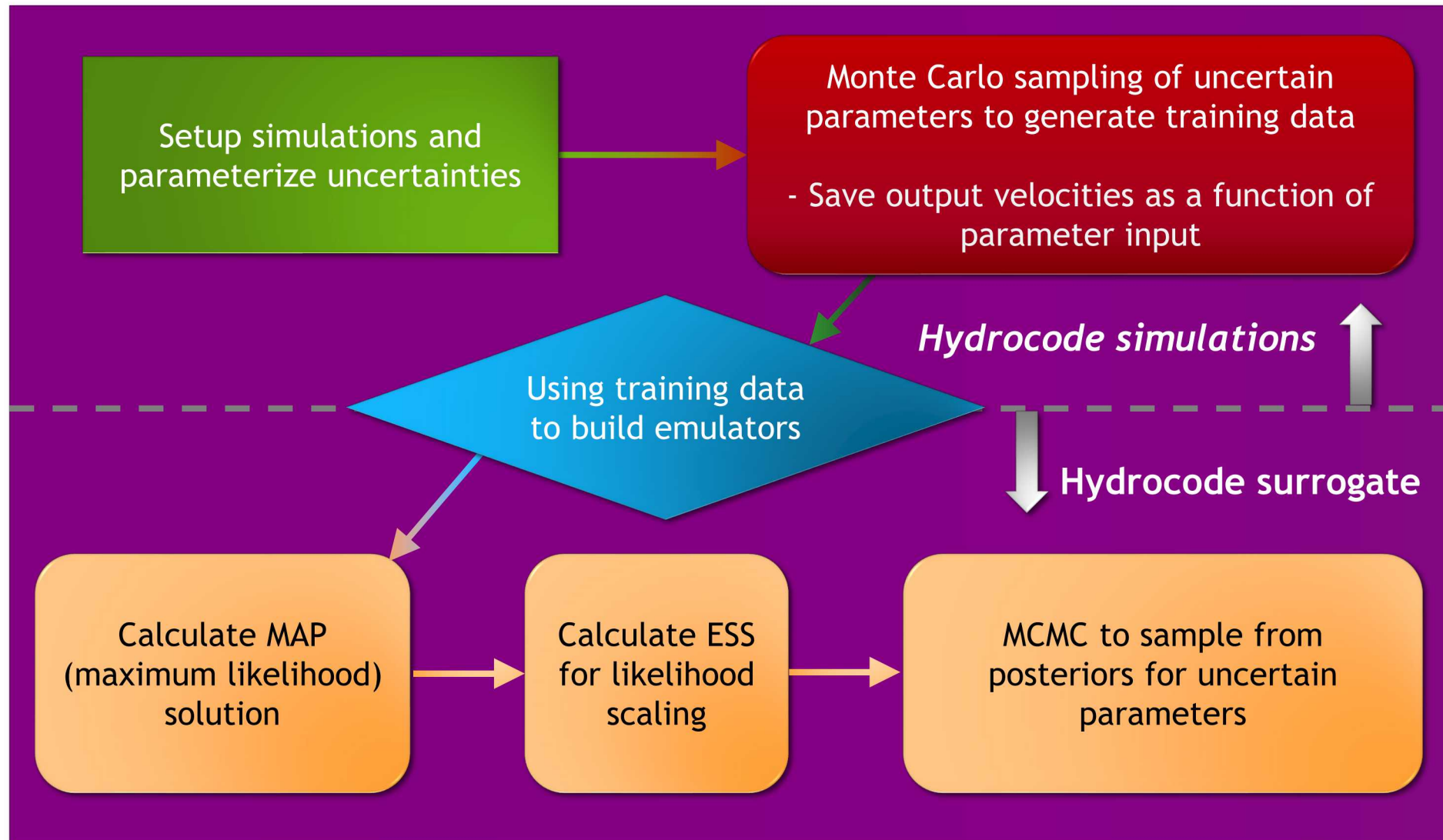


Nuisance parameters are all of the extra uncertain parameters in the simulation which affect the simulated velocity

- Examples: thicknesses, magnetic field, standard model parameters (electrode and window), artificial viscosity, mesh size

Our approach:

- Use “modularization” as a sensitivity analysis
  - Modularization: sample the nuisance parameters priors at each step in the MCMC without updating them
    - Posterior = prior
    - This is a way to incorporate nuisance parameter uncertainty without biasing the calibration parameters
    - **Con: not full Bayesian inference, the estimated posterior distributions do not converge to true posteriors**
- Compare full Bayesian calibration with modularized calibration and use best judgment
  - Is there enough data to identify the nuisance parameters?
  - Modularization is generally a more robust (unbiased) and conservative method

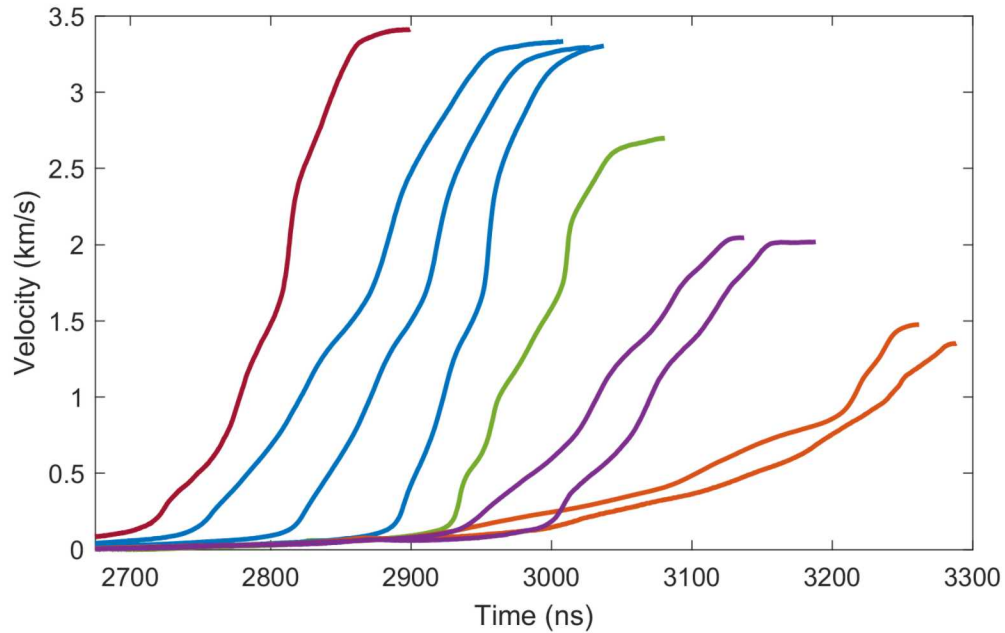


# Example from the paper: Ta cold curve calibration

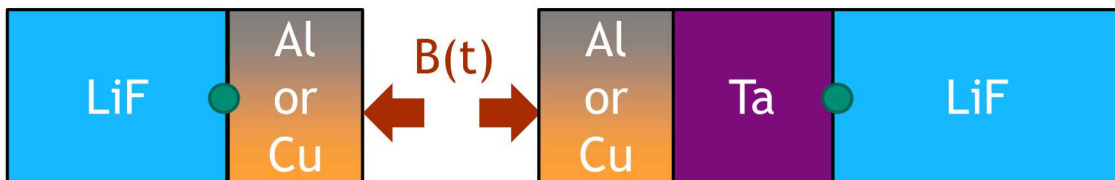
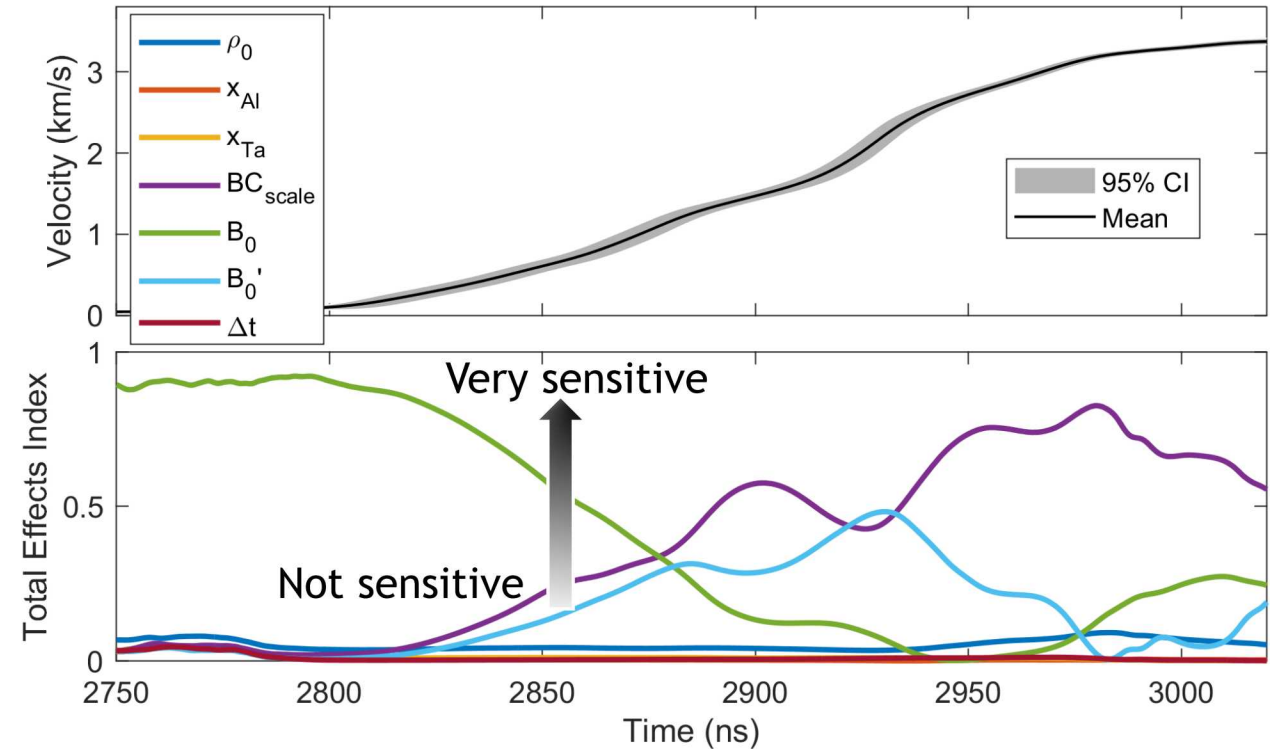


Ta ramp compression data to 2.5 Mbar

- 5 experiments, 8 velocity profiles

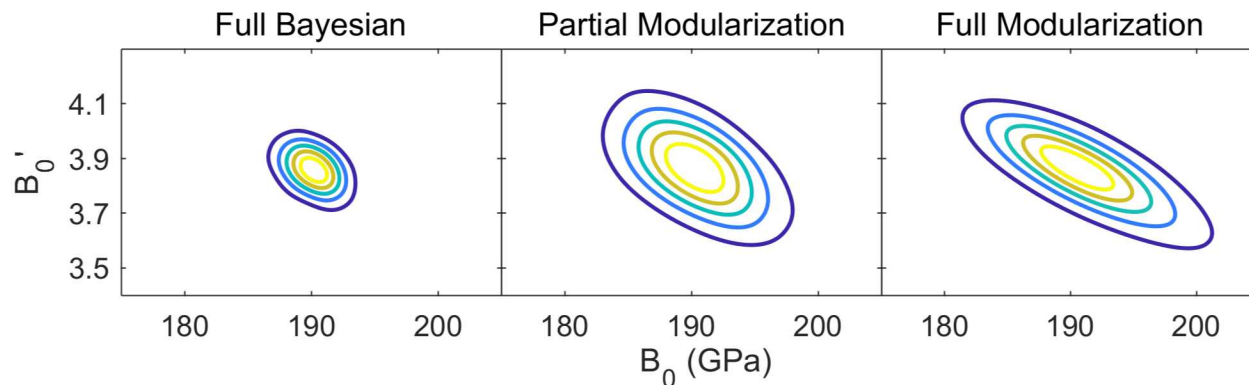
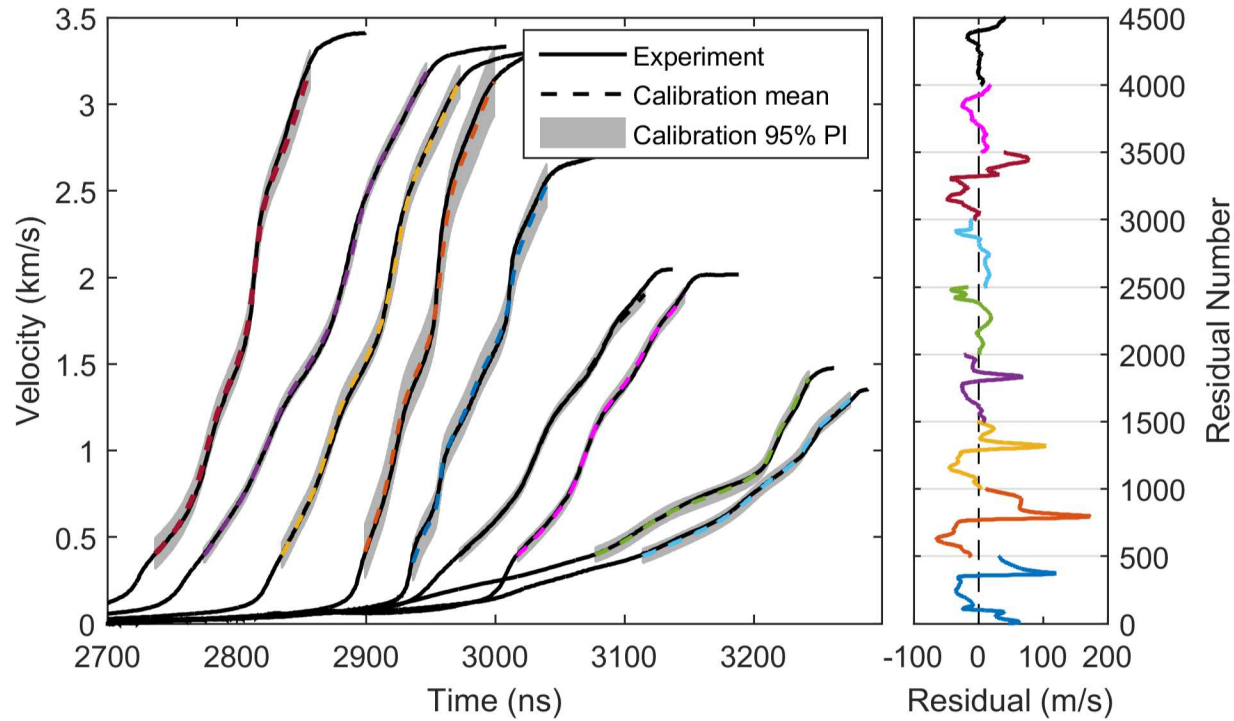


Global variance based sensitivity analysis (Sobol)



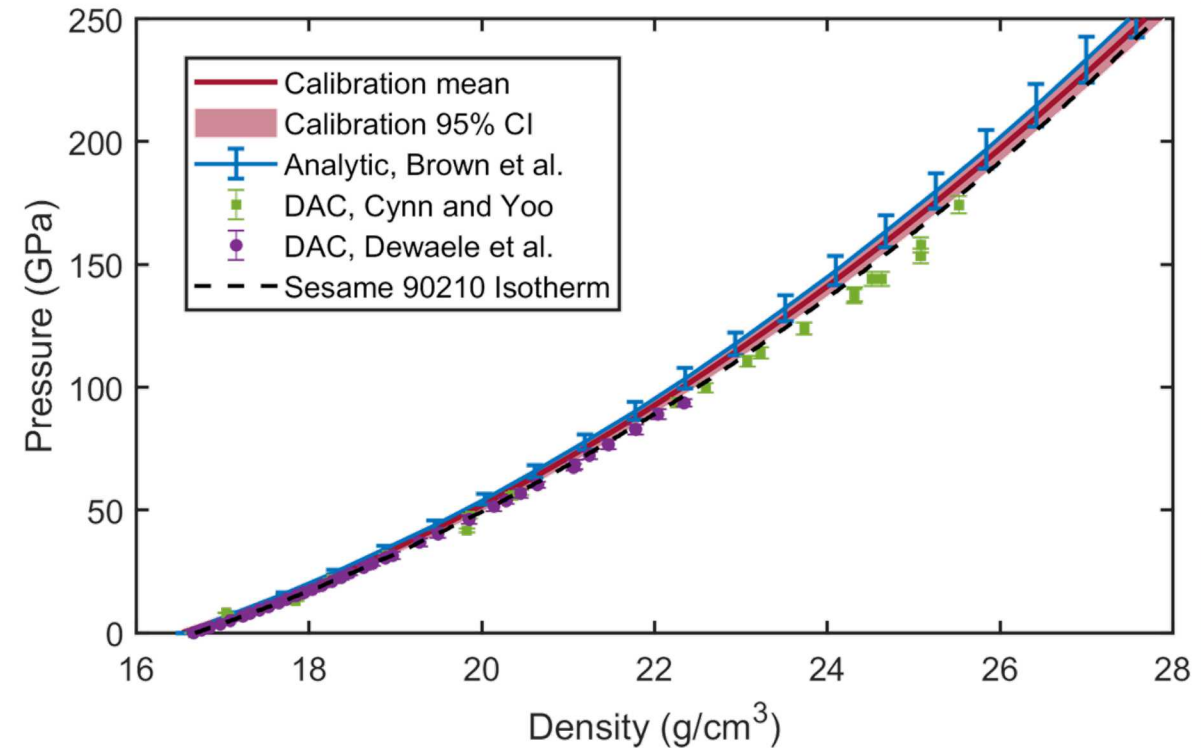
Sensitivity analysis based on prior distributions gives an indication for which parameters are identifiable within the calibration

## Ta calibration is consistent with expectations



Vinet model for cold curve  $\eta = \left(\frac{\rho_0}{\rho}\right)^{1/3}$

$$P(\rho) = 3B_0 \left(\frac{1-\eta}{\eta^2}\right) \exp\left\{\frac{3}{2}(B_0' - 1)(1-\eta)\right\}$$





Believe we have a robust method for performing calibrations to estimate material model parameters

- Obtained reasonable results for several problems of interest

Bayes methodology allows for incorporation of multiple uncertainties and data sets

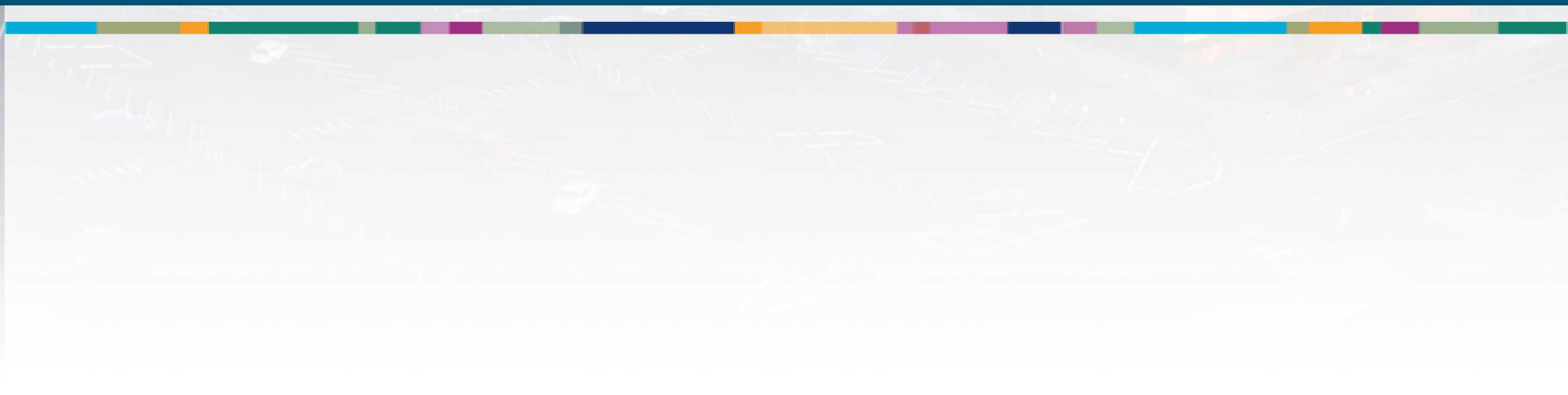
- Have focused on velocity measurements, but it is possible to incorporate other types of data

This is an active area of research

- Discrepancy modeling
  - Standard approaches (GP model) and power likelihood methods
- Incorporation of external data sets
  - Examples: DAC, strength data, etc.
  - Weight likelihood appropriately, or transfer posteriors to a new calibration of each data set?



# BACKUP SLIDES

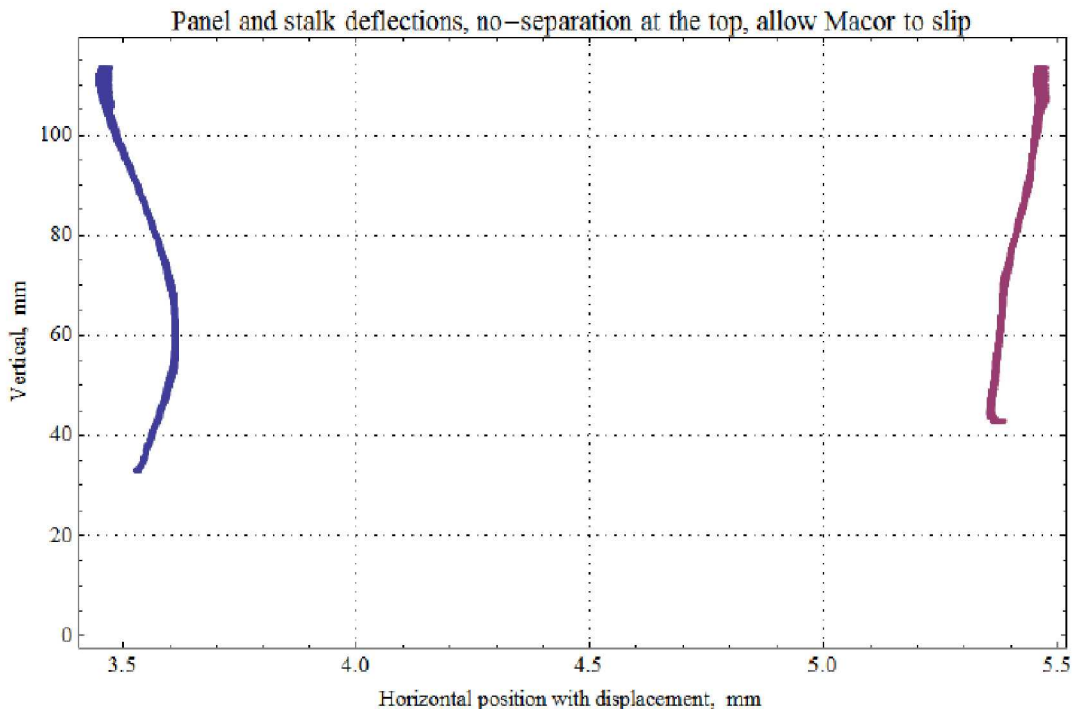


## Some interesting design features/observations



The panels do not remain parallel in the simulations

- Parallelism is  $\pm 100 \mu\text{m}$  from top to bottom
- The analysis methodology roughly accounts for this
  - The magnetic field at each position is calculated
- The drive data are inconsistent with this prediction
  - Trend is opposite: the middle position has the lowest magnetic field



There is significant magnetic field between the heater blocks

- Requires  $\sim 30\%$  more current to reach the same pressure
- These can be separated further, but it was not a concern in these experiments

