SAND2019-6494PE

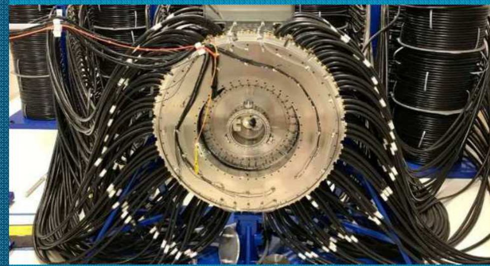
*NNSA-DP/CEA-DAM Agreement on Cooperation in Fundamental Science Supporting Stockpile Stewardship*

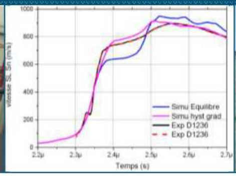
Sandia National Laboratories

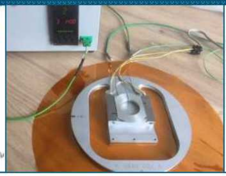
DE LA RECHERCHE À L'INDUSTRIE

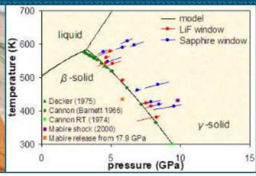
cea

# P204: Kinetics of phase transformations in metals under dynamic compression

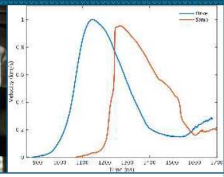










*PRESENTED BY*

Jean-Paul Davis (SNL), Camille Chauvin (Gramat)

*2019 General Meeting & Postdoctoral Exchange Workshop*
*5-7 June 2019 in Le Barp, FRANCE*

# OUTLINE

- Introduction/Objectives
- Brief look at relevant experimental work being done at each lab
  - NNSA/SNL
  - CEA-Gramat
- Some details on near-term collaborative efforts under way
- Conclusions/Perspectives

# Introduction to P204, a collaboration in experimental material dynamics

## History

Initial discussions in 2011, but no new collaboration at that time (for several reasons)

In June 2017, Camille suggested to SNL & LANL a collaboration on pyrometry

Discussion held at APS conference in July 2017 between Camille and several SNL staff
- Decided a broader collaboration would be appropriate in experimental work on phase transitions

In April 2018, Jean-Paul hastily wrote a proposal with help from Camille
- Proposal accepted at May 2018 Steering Committee meeting, assigned P204 in September 2018

P204 held a fruitful "kick-off" meeting in November 2018 at SNL

## Phase transformation kinetics in dynamic compression of metals

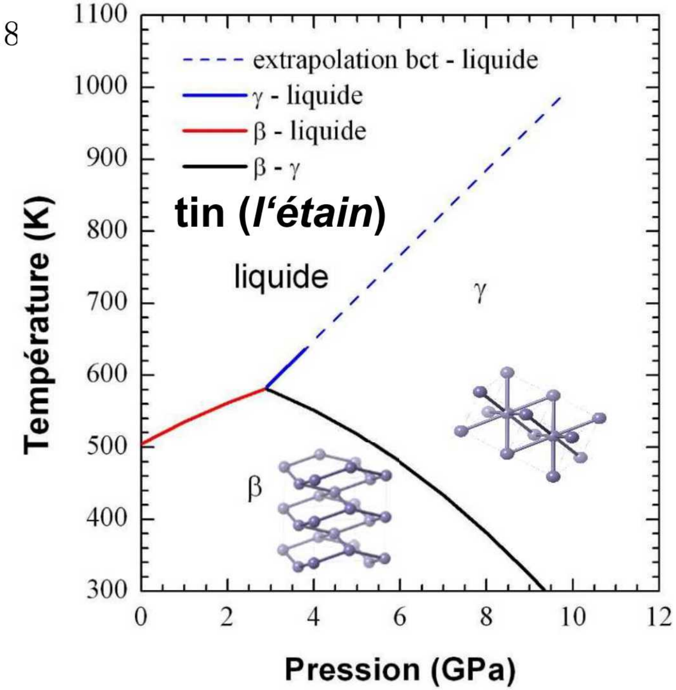
An area of fundamental research that is important to stockpile stewardship

NNSA and CEA both have programs in this area at multiple laboratories
- Existing work includes both experimental and computational/theoretical approaches

**P204 is focusing initially on pure tin (Sn) metal**
- Has previously been studied extensively by NNSA, CEA, and others
- Solid-solid and liquid-solid phase transitions below 40 GPa at easily accessible temperatures
- Need a lot of high-quality data to improve and validate multi-phase EOS for Sn

**Present Participants**

| NNSA (SNL): | CEA (Gramat): |
|---|---|
| *Jean-Paul Davis* | *Camille Chauvin* |
| *Dan Dolan* | *Thierry d'Almeida* |
| *Tom Hartsfield ** | *Fréderic Zucchini* |
| *Tom Ao* | *David Palma de Barros* |
| *Patricia Kalita* | *Jérémy Vich* |
| *Justin Brown* | |
| *Brian Stoltzfus* | ***LANL** |



# Objectives of collaboration P204

**Overarching goal** is to share knowledge and experience in all areas relevant to experimental work on phase transformation kinetics in metals under dynamic compression, including:

- design of experiments for both pulsed-power and gun drivers
- temperature, X-ray diffraction (XRD), and other diagnostics
- pre-heating and pre-cooling of samples
- analysis of experimental data
- materials modeling of phase transformations with kinetics


**Specific short-term and long-term objectives include:**

- compare/contrast 1-D simulations of each other's ramp experiments
- compare/contrast small-pulser load designs (ICE-16 vs Thor)
- share design/data/analysis information for any experiment on Sn
  (each lab has experiments on Sn planned as part of their own programs)
- collect and synthesize data on Sn against which to test models
  (investigate influence of crystal orientation and grain size)
- collaborate on a proposal for dynamic XRD experiments at DCS
- compare dynamic XRD results (Gramat X-pinch vs SNL flash-diode)
- collaborate on investigating interface coatings for pre-heat, pyrometry
- collaborate on development and implementation of new models/EOS
- jointly publish journal articles
- …

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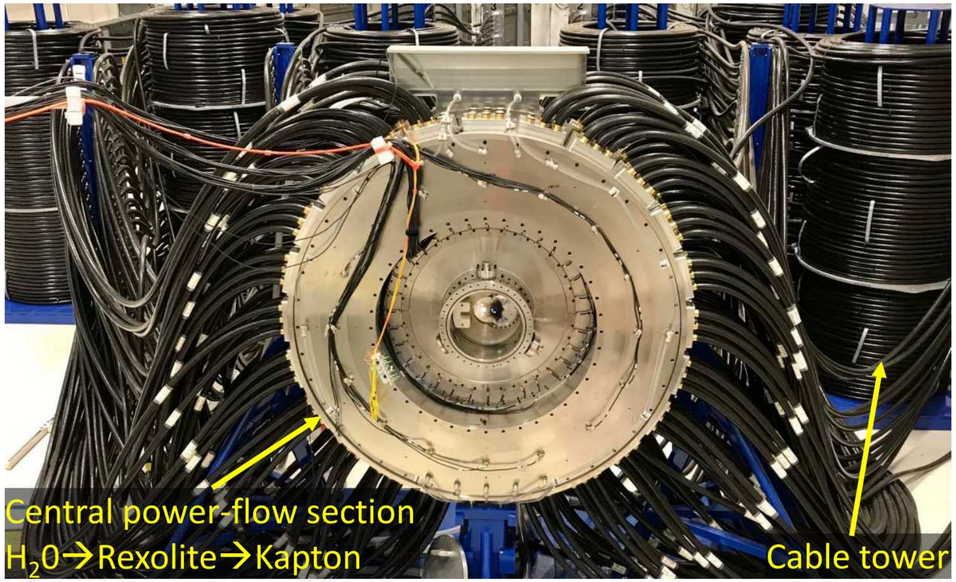
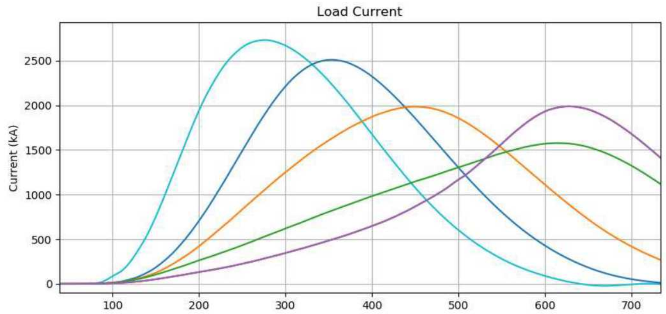
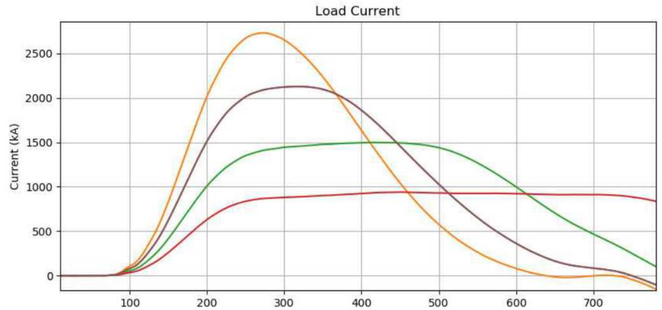
# The Thor-64 driver at SNL provides highly controllable pulse shaping




Vary loading rate by a factor of ~10

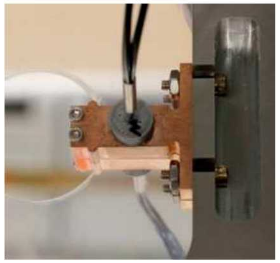
Flat-top loading to study phase-transition kinetics



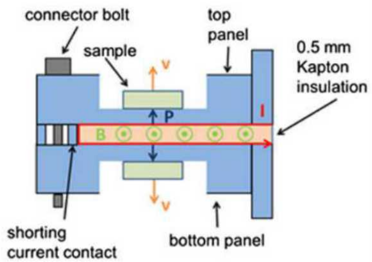

64 independently switched "bricks" arranged in 8 towers

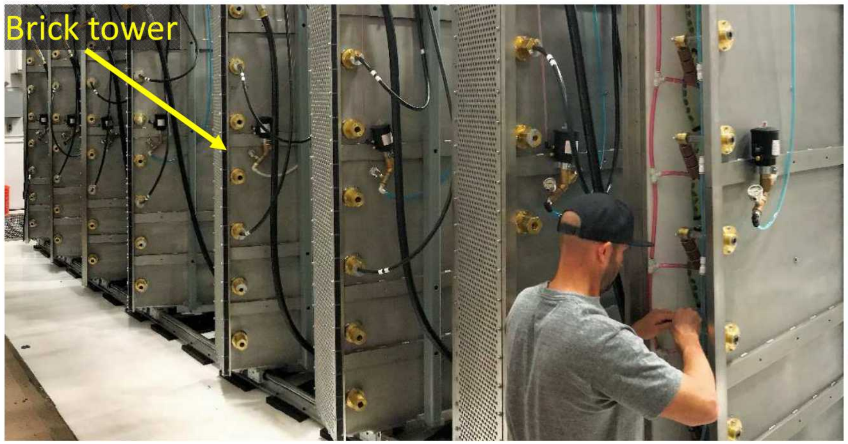
Transmission cables 250 ns long for time isolation of switches

Up to 2.5 MA, pulse shaping to 500-ns trigger spread (cable round-trip)



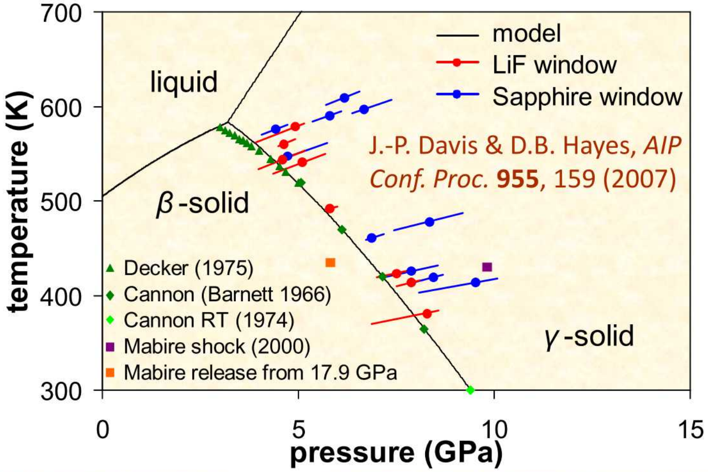
10-mm wide panel
→ ~20 GPa peak

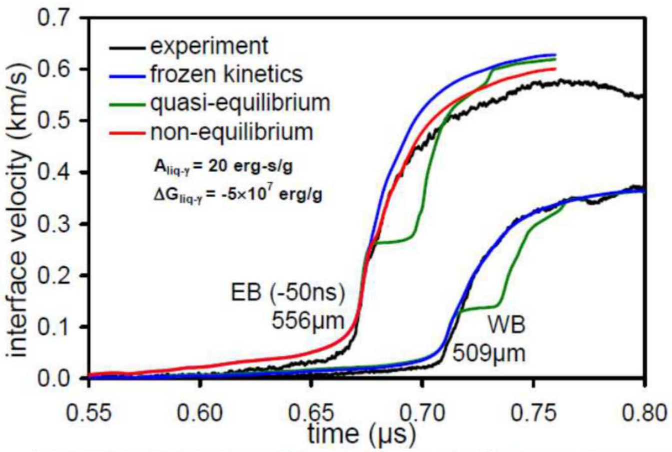


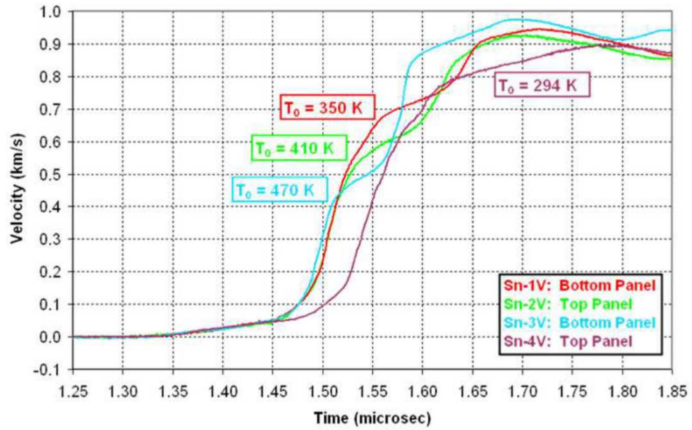



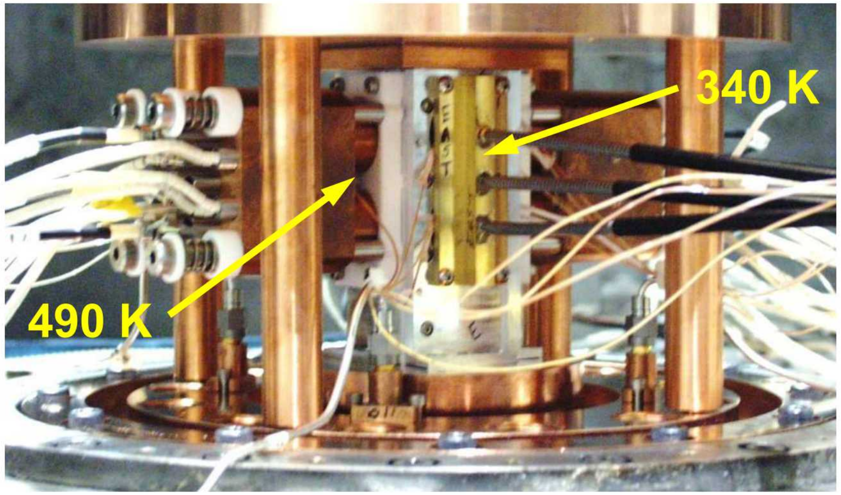
# Pre-2010 work on pre-heated tin at SNL could bear re-investigation

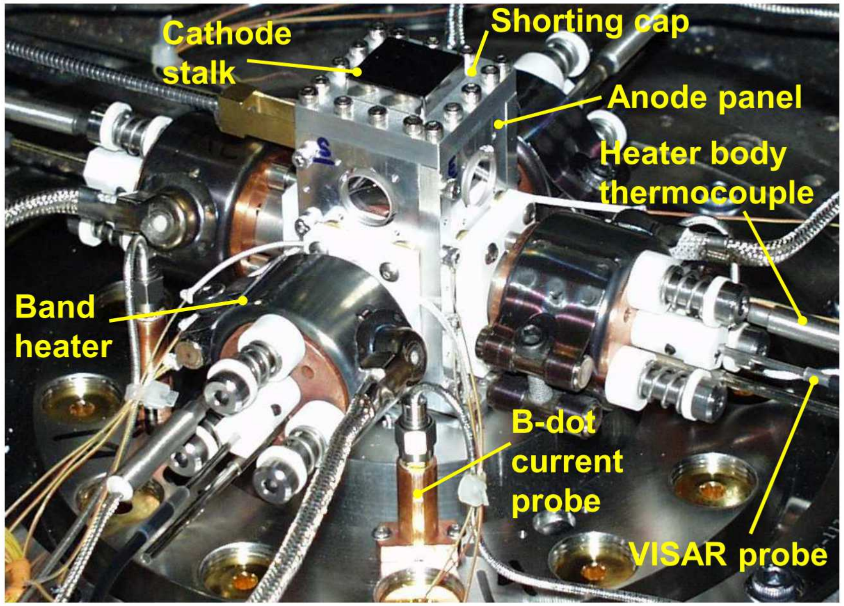
Ramp compression of pre-heated solid and liquid tin on the Z machine



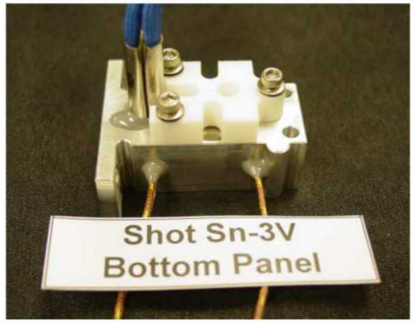




Pre-heated solid tin on the Veloce small pulser

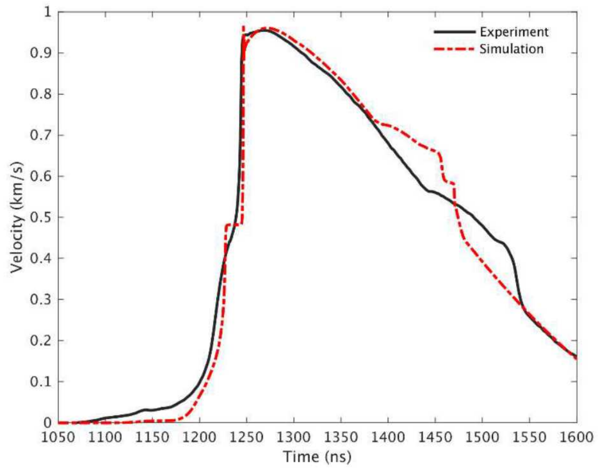



Experiment design & analysis has since improved dramatically

# Recent work at SNL has focused on shock-ramp loading & strength

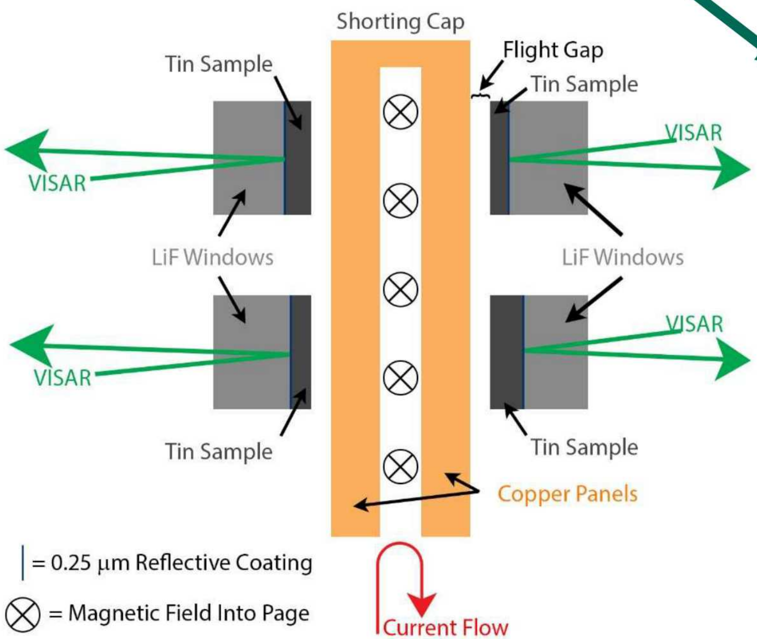
Experiment on Thor-64 (Justin Brown)

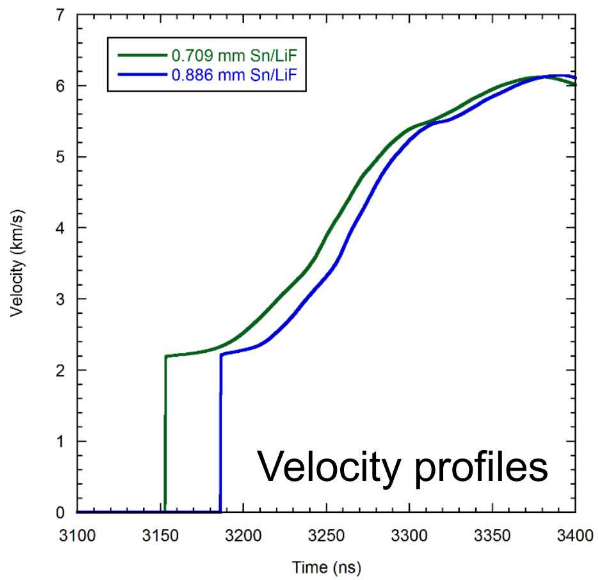
- ramp to 22 GPa, measure release through elastic-bulk transition in γ phase
- simulations to match data suggest little to no strength after transition

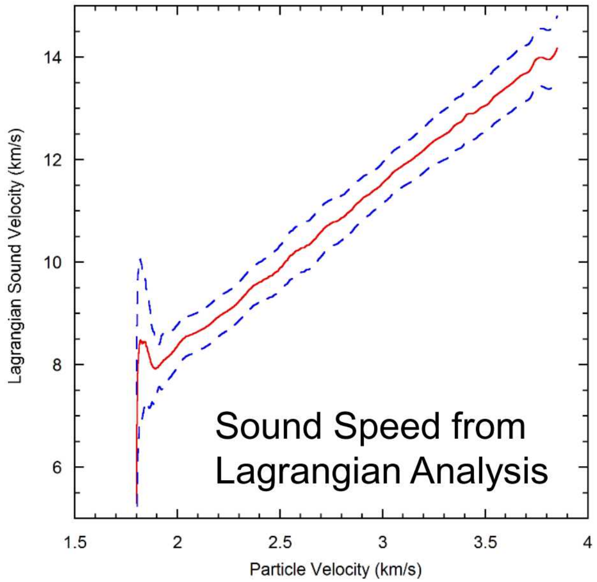



Experiment on Z (Chris Seagle)

- shock to 70 GPa, followed by ramp to 230 GPa
- Ramp initially elastic, shock state in mixed phase?



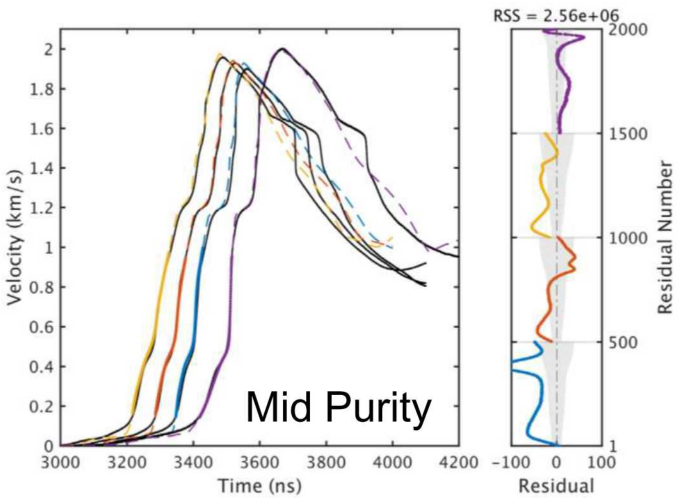



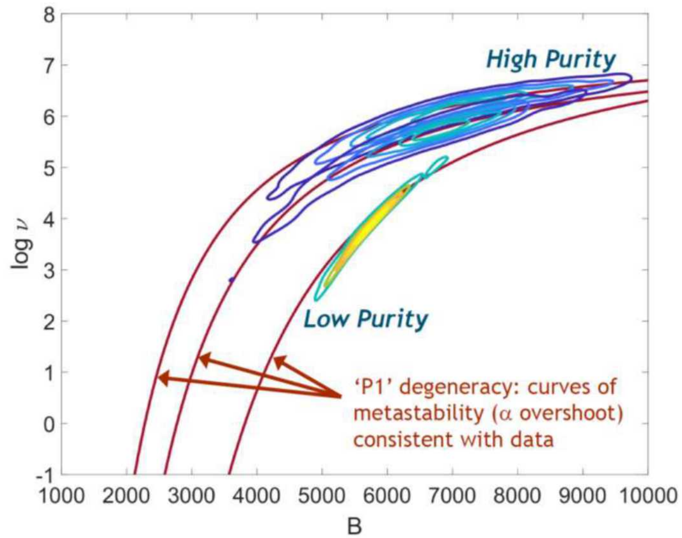



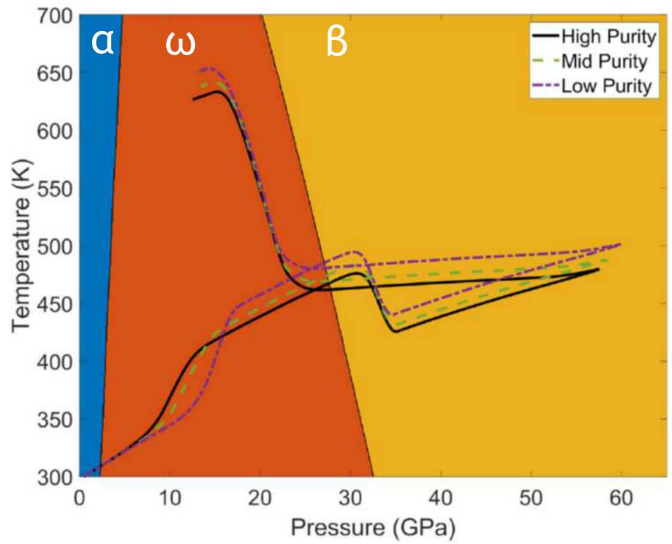
# SNL has been developing more advanced methods for data analysis

Bayesian calibration of EOS and/or kinetics parameters against set of multiple velocity profiles

- Example: room-temperature data on ramp compression of Zr (three different purity levels)
- Calibrate 2 parameters of Greef kinetics model, holding EOS fixed
- Uses Laslo 1-D Lagrangian code, Dakota framework for statistics, optimization, calibration



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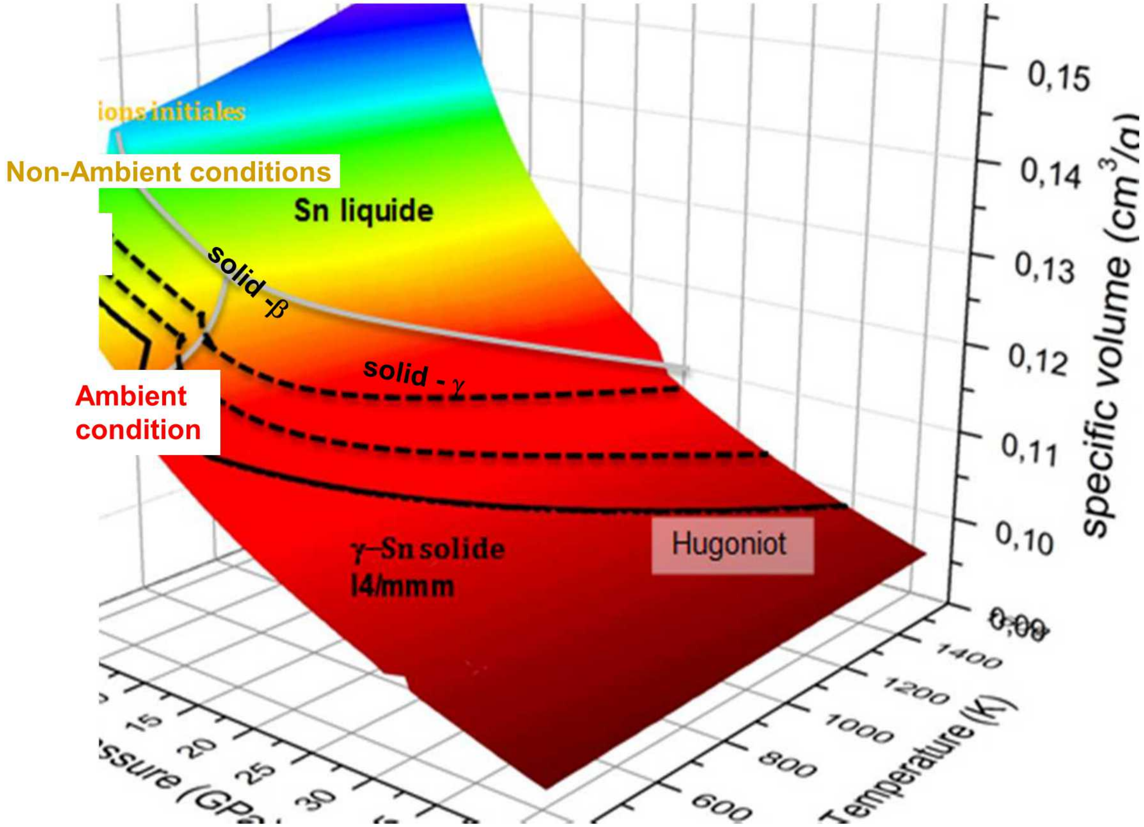
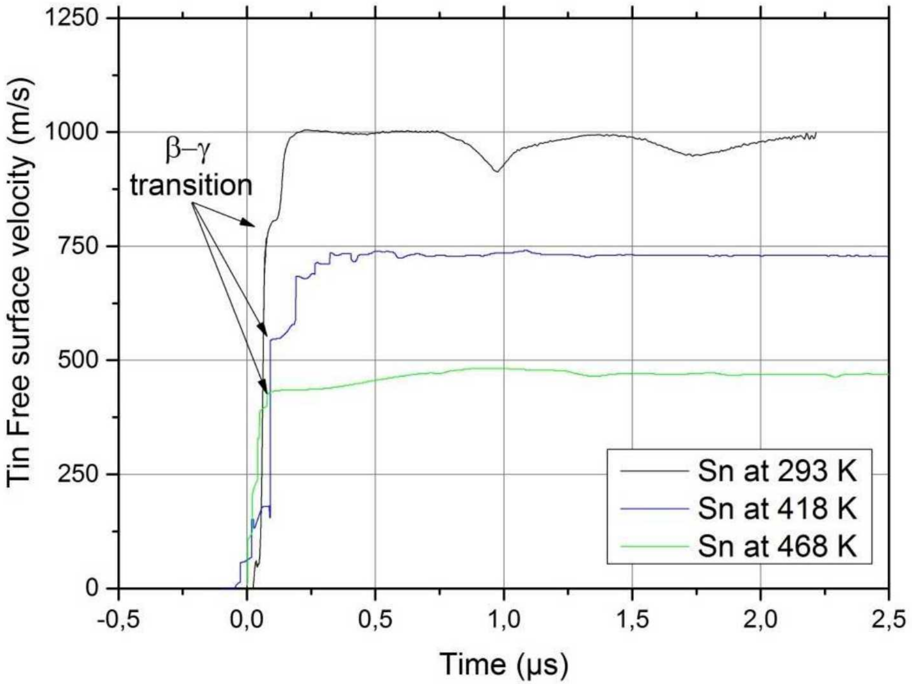
# Investigation of the β–γ boundary under shock: pre-heated tin

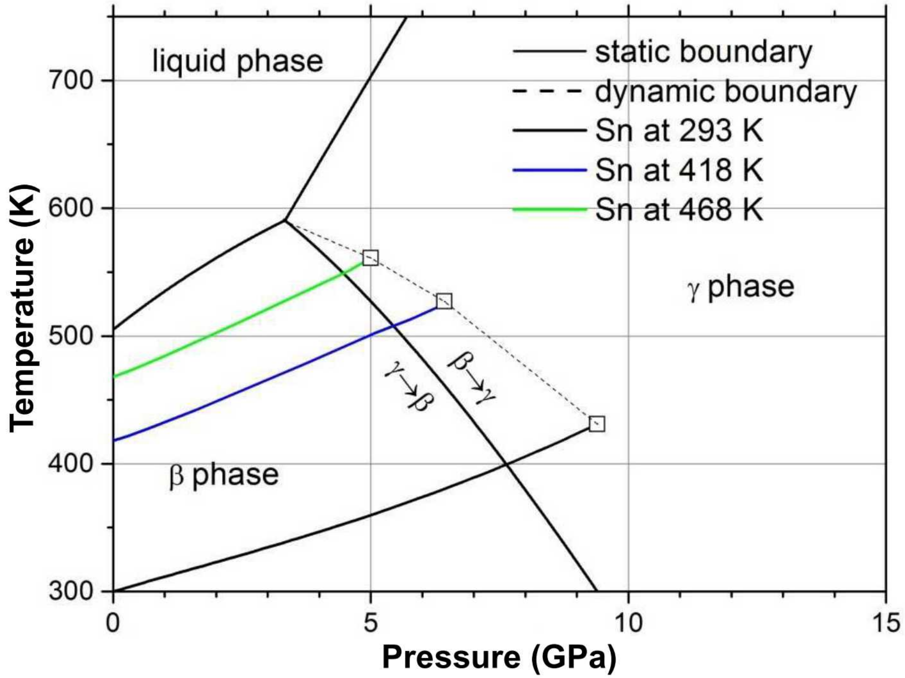
- Pre-heated sample




Loading samples from various non-ambient initial temperatures expands the region where the phase transition can be examined.

# Investigation of the β–γ boundary under shock: pre-heated tin



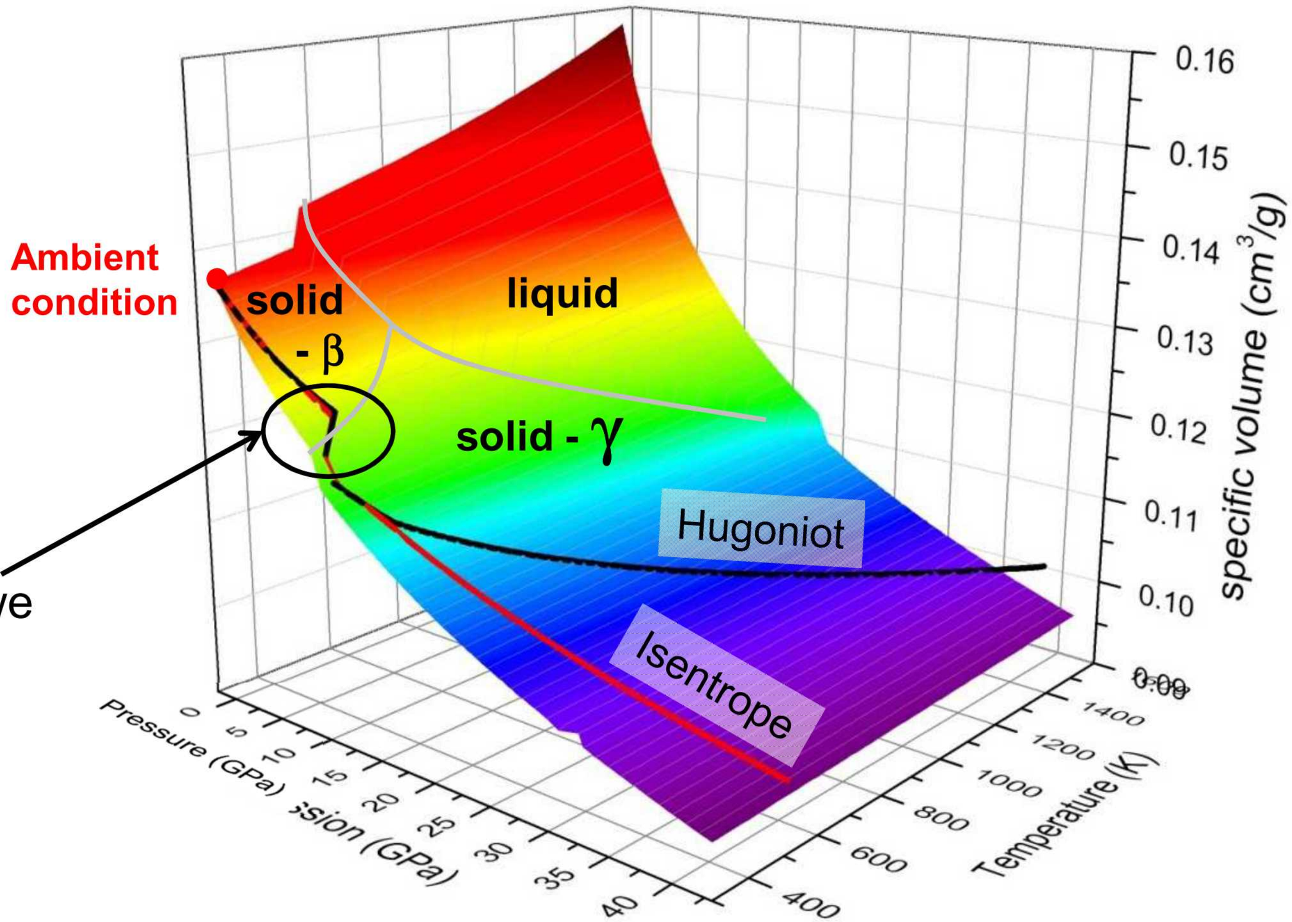




- The Hugoniot elastic limit (HEL) grows with increasing initial temperature
- These data indicate a hysteretic overshoot of the phase transition under shock loading
  
  the overshoot gets closer to the static boundary as the initial temperature increases
- Spall occurs, as indicated by a plateau on the free surface velocity
- Gas gun experiments can include a three-channel mid-infrared (IR) pyrometer.

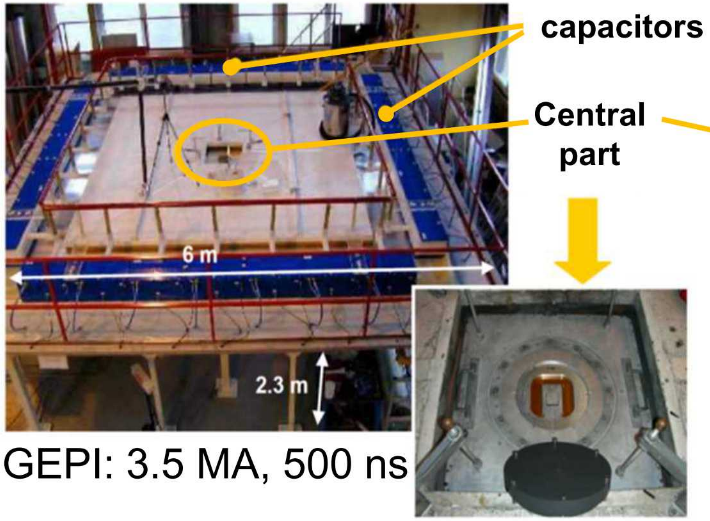
# Investigation of the β–γ boundary under quasi-isentropic compression

**Shockless compression experiments allow to explore region of phase inaccessible to traditional shock compression experiments.**

From these kind of experiments, we can examine the kinetics of phase transitions and material's phase behavior.



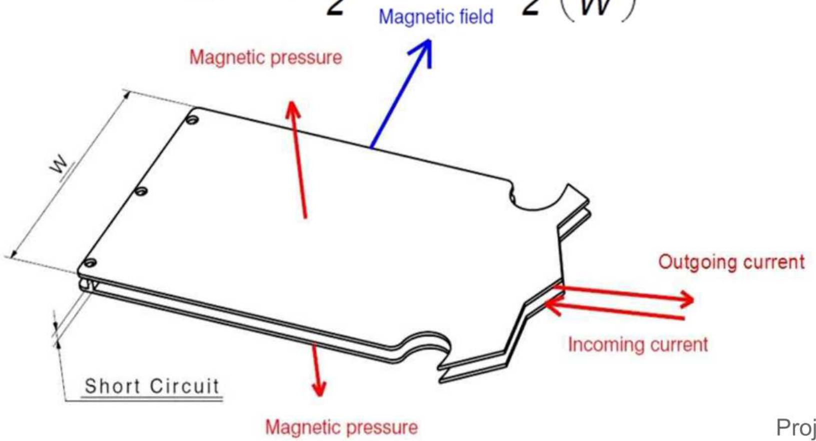
# ICE drivers at CEA: GEPI and ICE 16

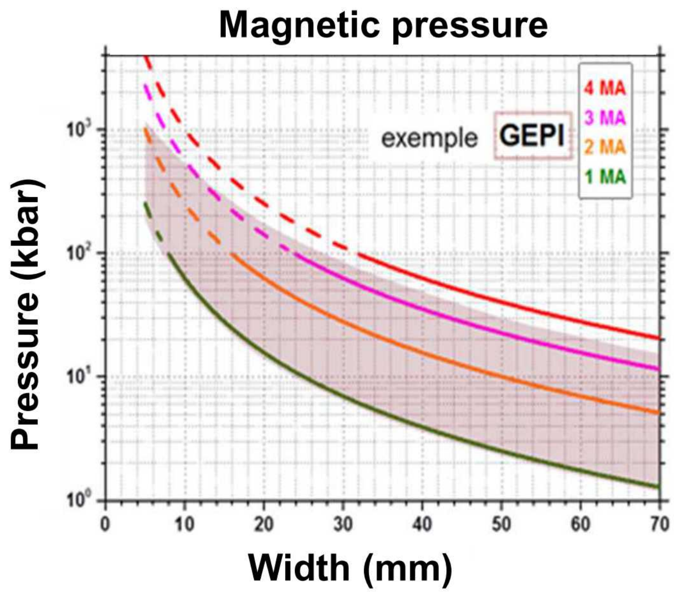



GEPI: 3.5 MA, 500 ns

ICE 16: 6 MA, 1 µs

$$p_{mag} = k_P \frac{\mu_0}{2} H_{th}^{\ 2} = k_P \frac{\mu_0}{2} \left( \frac{I}{W} \right)^2$$




Features (GEPI/ICE16)

- 28 / 16 capacitors with switch
- 85 / 80 kV max charging voltage
- 3.5 / 6 MA Peak current
- 70 mm / 140 mm maximum width
- Planar electrodes

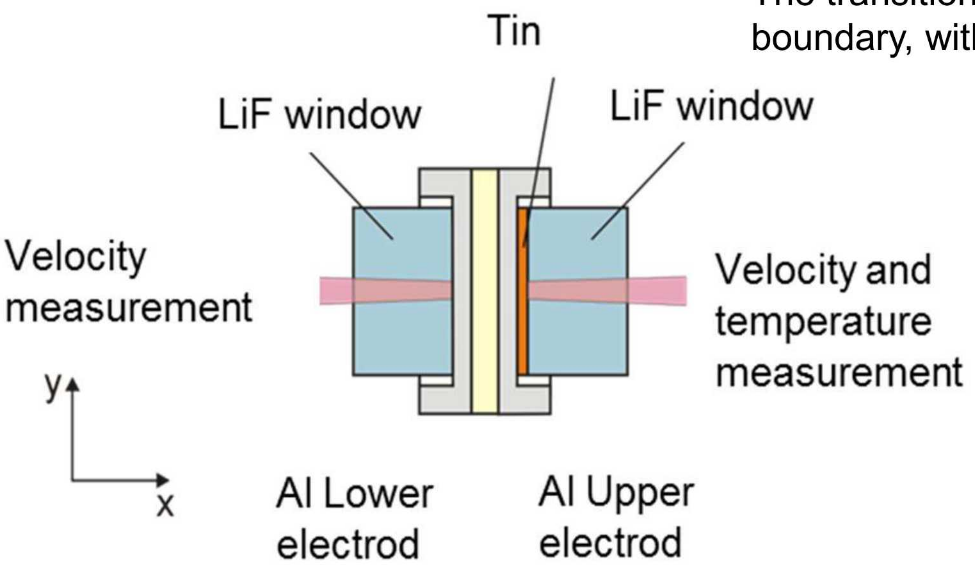
Use

- Materials dynamics
- Damaging and spallation
- EOS and phase diagrams
- Flyer plates

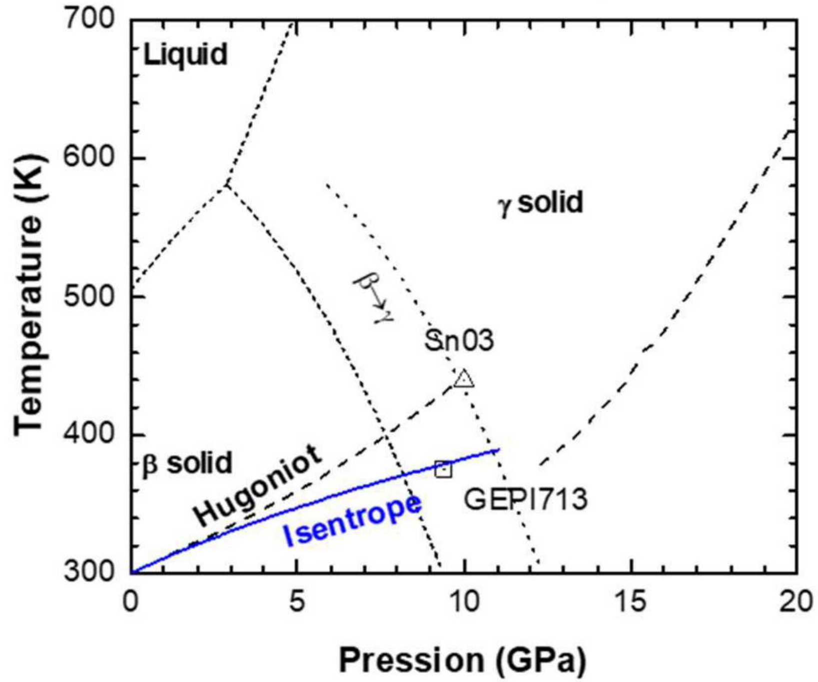
# Comparison between quasi-isentropic and shock loading

## GEPI ICE experiment to study β–γ phase transition.

The transition under quasi-isentropic loading appears closer to the equilibrium phase boundary, with less hysteretic overshoot, than under shock wave compression.



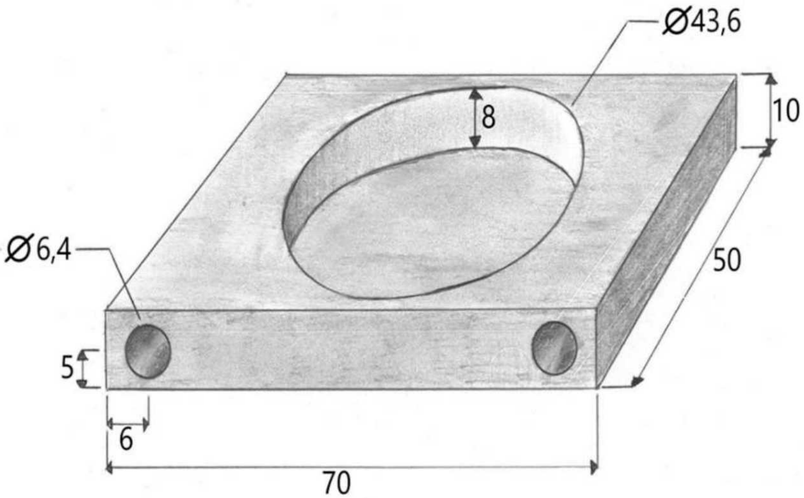

ramped loading = quasi-isentropic compression

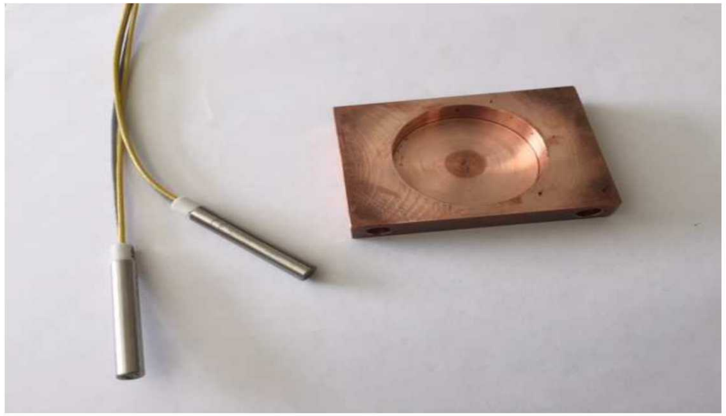



Loading samples from various non-ambient initial temperatures can significantly extend the range of our studies into previously unexplored thermodynamic paths and help constrain Equation Of State (EOS) models incorporated in numerical codes with **velocity and temperature measurements.**

# Investigation of the β–γ diagram under quasi-isentropic compression: pre-heating device on GEPI

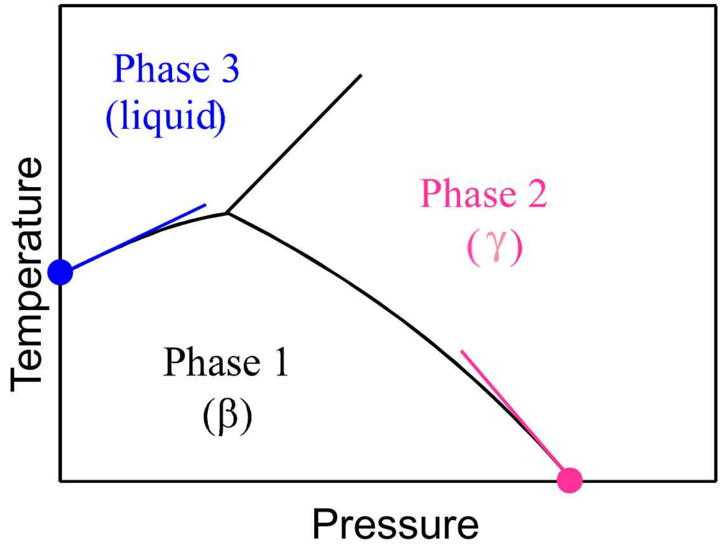
- **Selected components**
  - These heating devices are being integrated to ICE-16 and GEPI
  - Their performance and versatility are potentially valuable for extending  the range of thermodynamic paths achievable under ramp loading using high pulsed power drivers.



# Multiphase EOS at CEA Gramat

- Multiphase EOS is integrated in a 1-D Lagrangian code Unidim that includes MHD and thermal conduction.
- The phase boundaries are known from DAC, dP/dT & Δvij are determined.
- For each phase, we chose a Mie-Grüneisen EOS with the isotherm as reference.
- To reproduce the phase transition between two phases, we used kinetic models from the literature.




Kinetic model (Greeff) $$\dot{\varphi} = \upsilon(1-\varphi)\frac{\Delta G}{B} e^{\left(\frac{\Delta G}{B}\right)^2}$$

Kinetic model (Mabire) $$\dot{\varphi} = \frac{1-e^{\vartheta \Delta G^*} - \varphi}{\tau} = \frac{1-e^{\vartheta(\Delta G + A_r)} - \varphi}{\tau}$$

The parameters were fit to reproduce the velocity profile around the polymorphic transition.

# Comparison between empirical models under shock compression

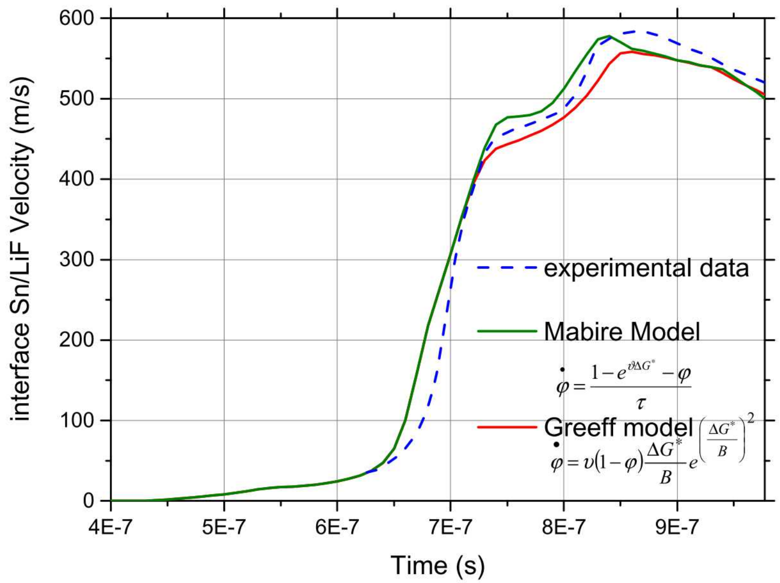
→ Mabire Kinetic model

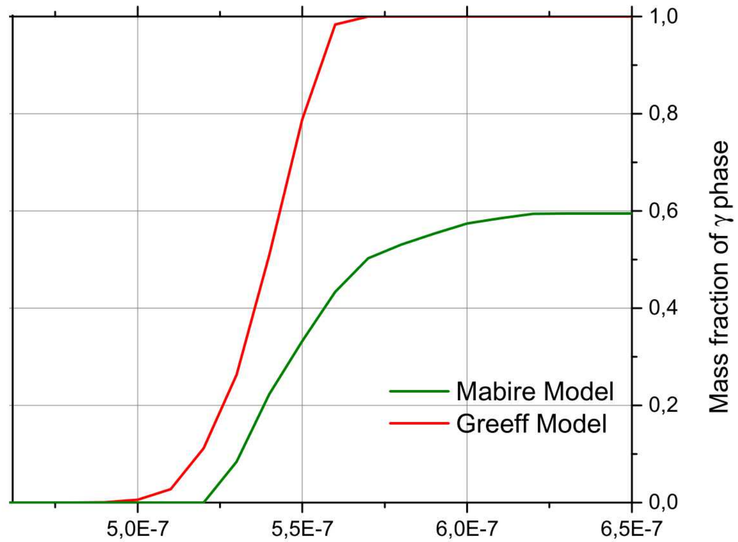
$$\dot{\varphi} = \frac{1 - e^{\vartheta \Delta G^*} - \varphi}{\tau}$$

→ Greeff Kinetic model

$$\dot{\varphi} = \upsilon(1-\varphi)\frac{\Delta G^*}{B} e^{\left(\frac{\Delta G^*}{B}\right)^2}$$

**Velocity at Sn/LiF interface and $\lambda_2$, the mass fraction of $\gamma$ phase in the bulk Sn**




This underlines the limitations of empirical kinetic models:

→ **Need for X-ray diffraction measurements to provide more accurate kinetic model in the multiphase EOS**

# Experimental and modeling work

- In both labs, a large body of experimental data and modeling, but still there are many questions.

- An extensive interaction within the framework of the fundamental-science agreement can help us to better understand our data.

- Future collaborative work investigating phase transitions under dynamic compression will include complementary experiments:
  - different loading rate,
  - different microstructure sample,
  - shock vs ramp,
  - …

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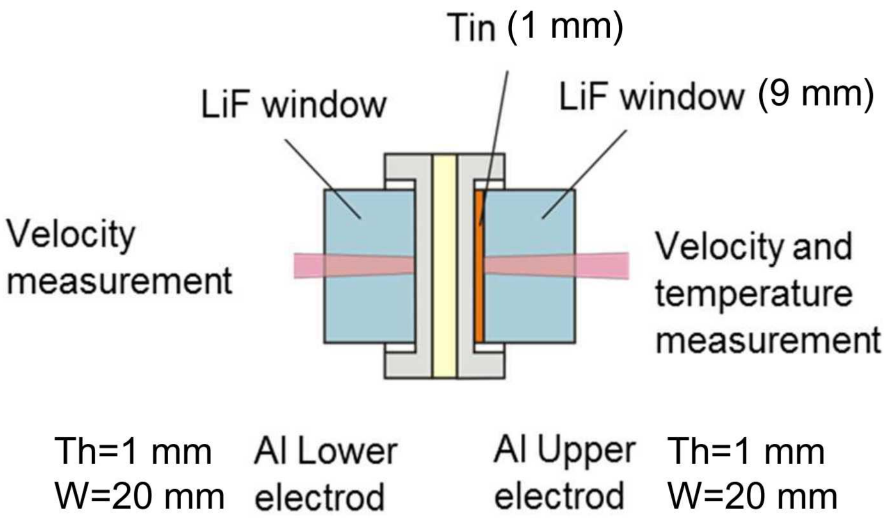
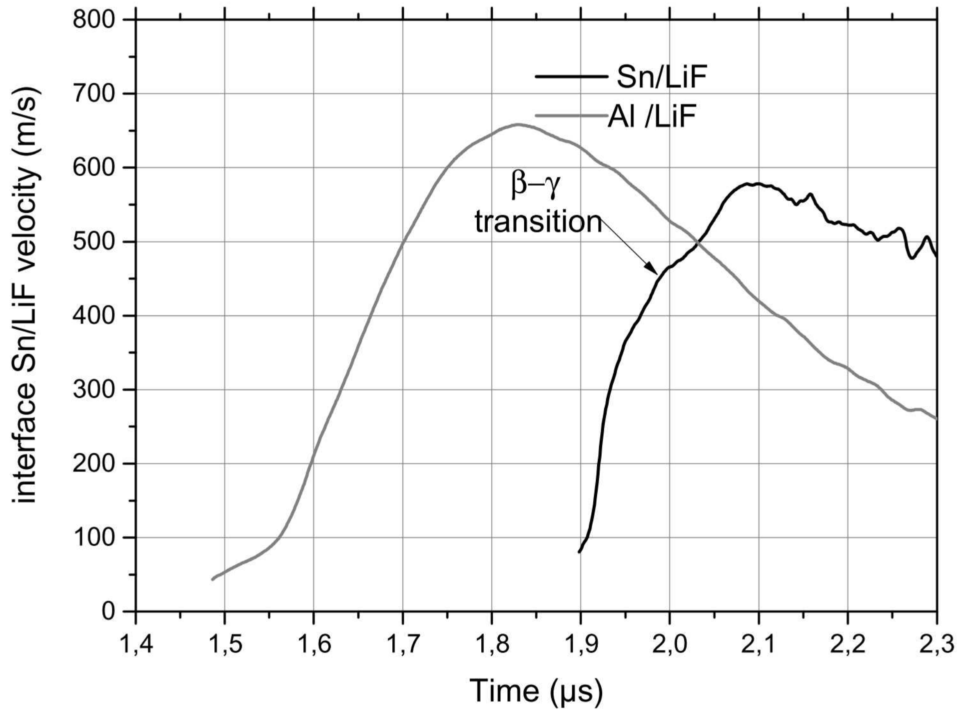
# 1-D simulations of quasi-isentropic compression experiments

- Compare/contrast 1-D simulations of GEPI/ICE-16 and Thor-64 experiments on tin

Share experiment specification, data; simulate each other's experiments

**GEPI 588**




- Goals

➔Ensure that our multi-phase Sn models are equivalent

➔Verify our codes produce the same result when using the same material models

# 1-D simulations of quasi-isentropic compression experiments

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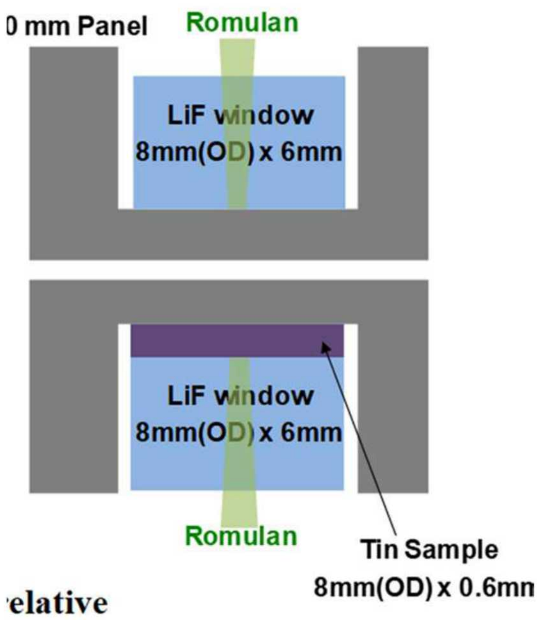
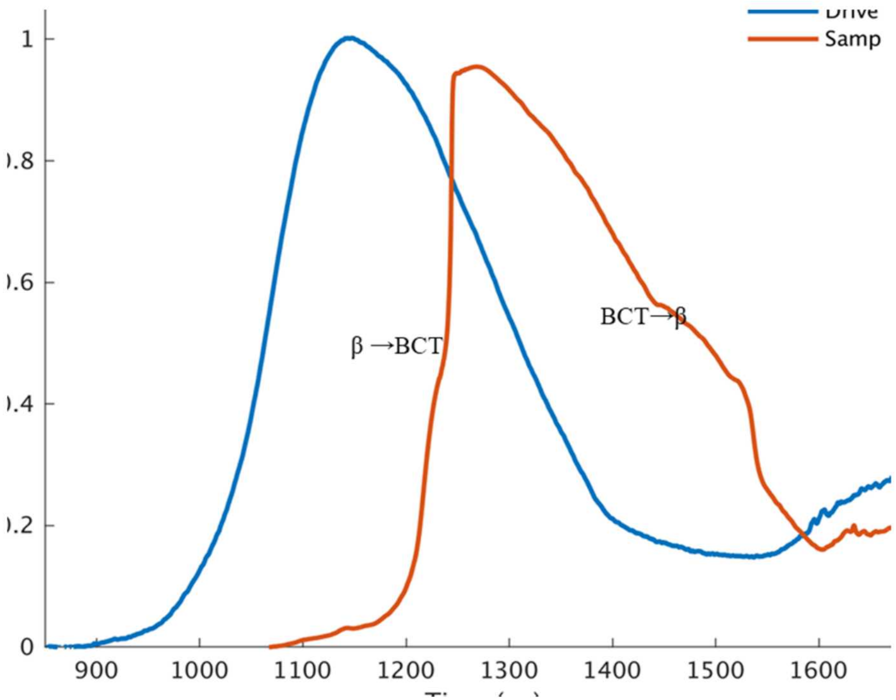
**Thor64-0030 Sn01**

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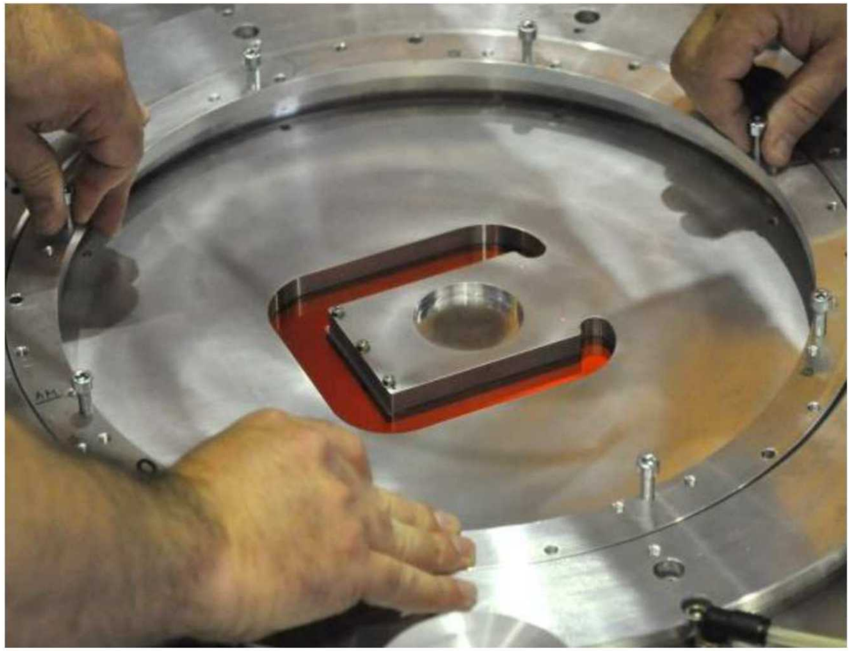
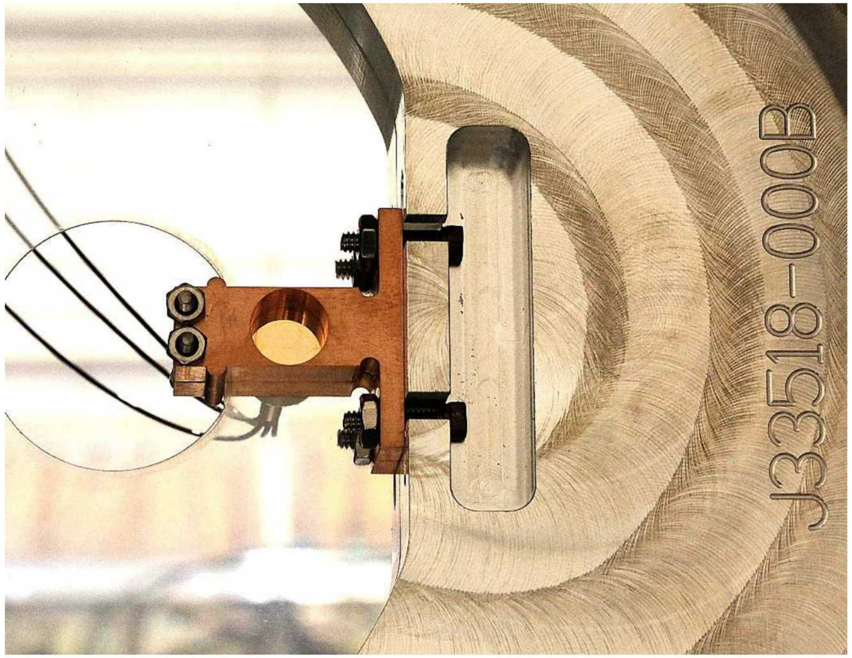
# Found unexpected differences in our approaches to experiment






- Gramat brings inner-most electrodes of machine close around panel, SNL does not
- CEA uses collimated PDV probes, SNL uses bare-fiber PDV probes

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# There is much we can work together on

Experiments under shock and ramp (and shock-ramp) loading to gain insight into mechanisms of phase transitions

- Use of pre-heating systems
- Velocimetry, pyrometry, and X-ray diffraction diagnostics
- Use of 1-D code (Unidim, Laslo) to analyze data
- Ultimately develop improved multi-phase EOS and kinetics models

# Interactions have continued and will continue frequently and regularly

Kick-off meeting 28-30 November 2018: C. Chauvin & T. d'Almeida visited SNL

Meeting out-brief document by J.-P. Davis became regularly updated "working" document

- Action items, near-term and long-term plans, planned visits and meetings

Continuing meetings every 2-3 months by video-/tele-conference (8:30 am at SNL = 4:30 pm at Gramat)

J.-P. Davis visited Gramat 3-4 June 2019

Planning face-to-face meeting in Portland (Oregon) during APS shock compression conference

Planning to submit proposal for experiments at DCS in early 2020