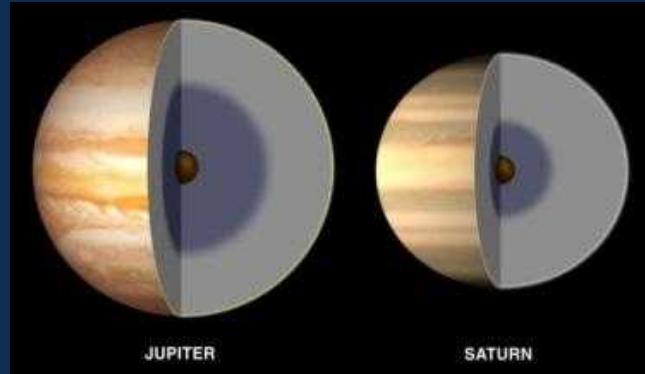
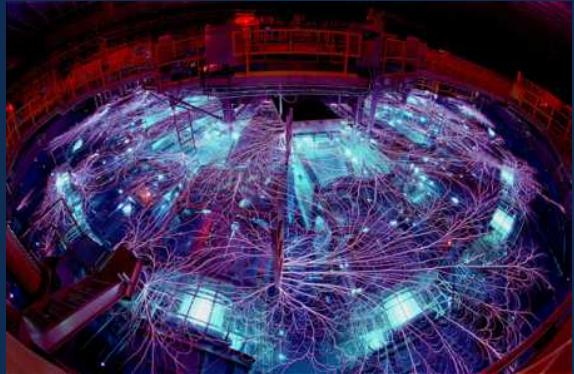


*Exceptional service in the national interest*



# Dynamic compression experiments on liquid deuterium above the melt boundary

**Marcus D. Knudson**

**Sandia National Laboratories  
Albuquerque, NM**



Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

## Experiment Design/Analysis

Marcus Knudson

Ray Lemke

Kyle Cochrane

Devon Dalton

Dustin Romero

## Diagnostics

Charlie Meyer

Jeff Gluth

Devon Dalton

Anthony Romero

Dave Bliss

Alan Carlson

# Acknowledgements

## QMD Calculations

Mike Desjarlais

Andreas Becker

Winfried Lorenzen

Ronald Redmer

## Planetary Modeling

Nadine Nettelmann

Andreas Becker

Ronald Redmer



## Pulse Shaping

Ray Lemke

Jean-Paul Davis

Mark Savage

Ken Struve

Keith LeChien

Brian Stoltzfus

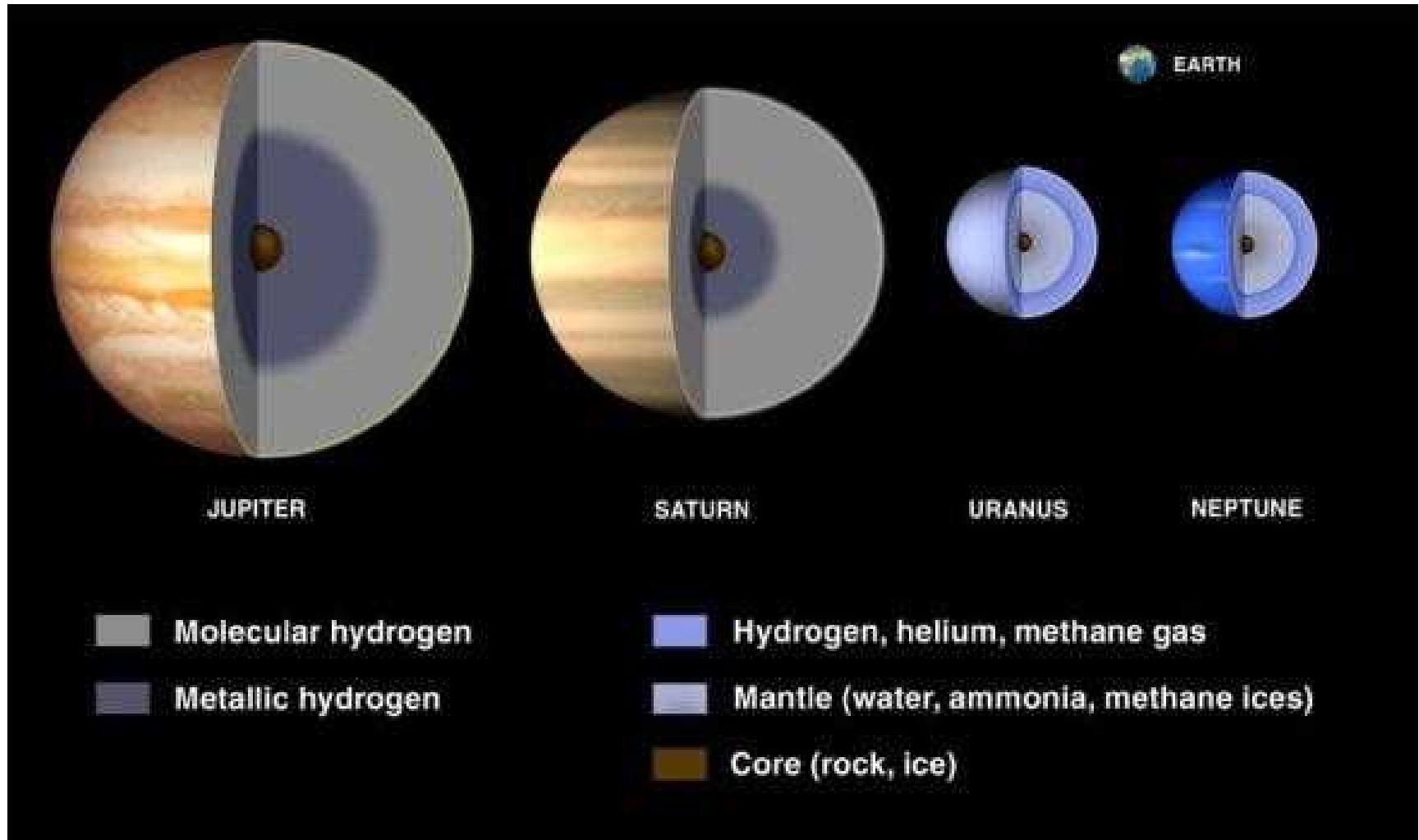
Dave Hinshelwood

Entire Z crew

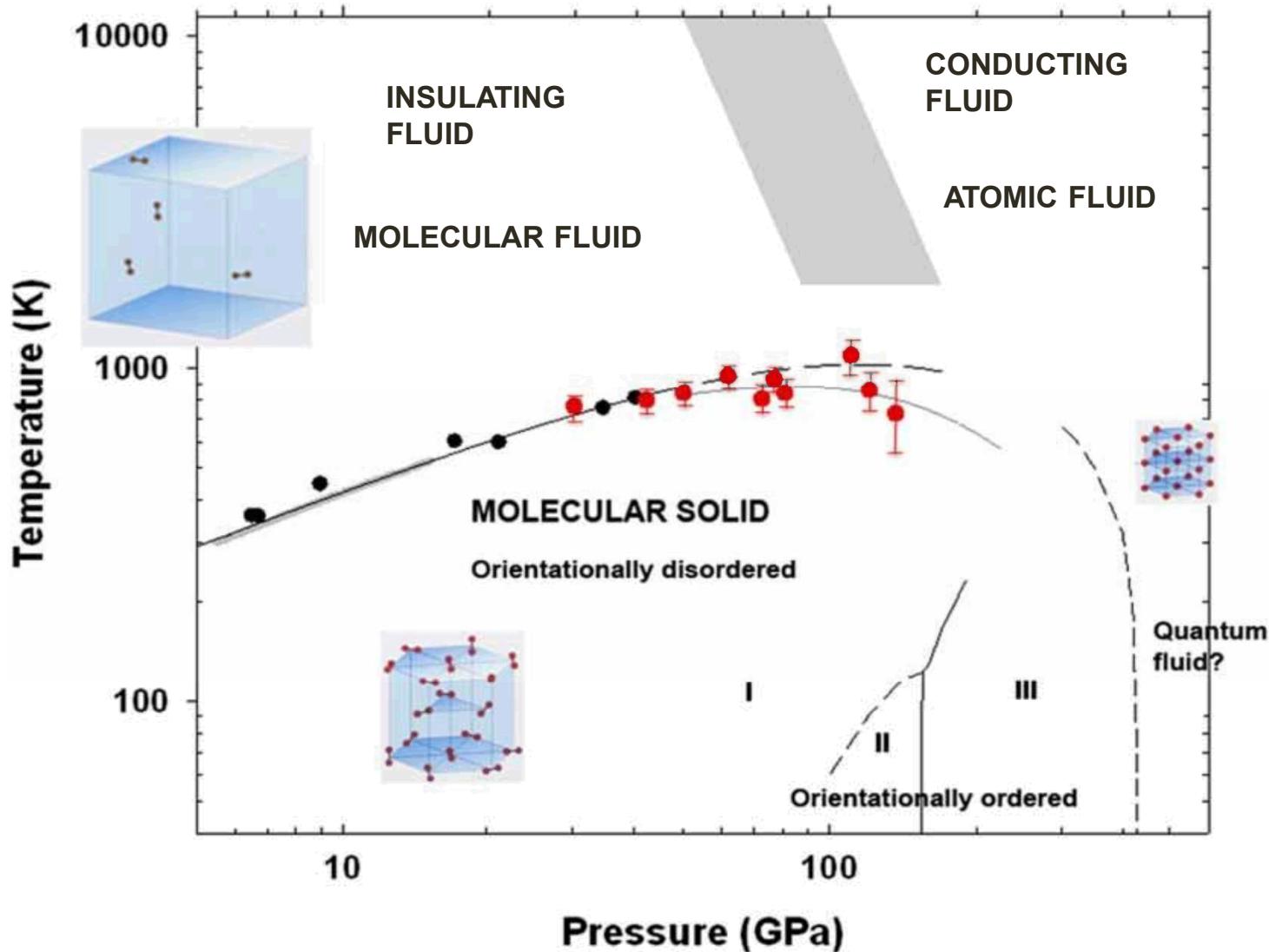
University of Rostock

# Giant planets in the Solar system

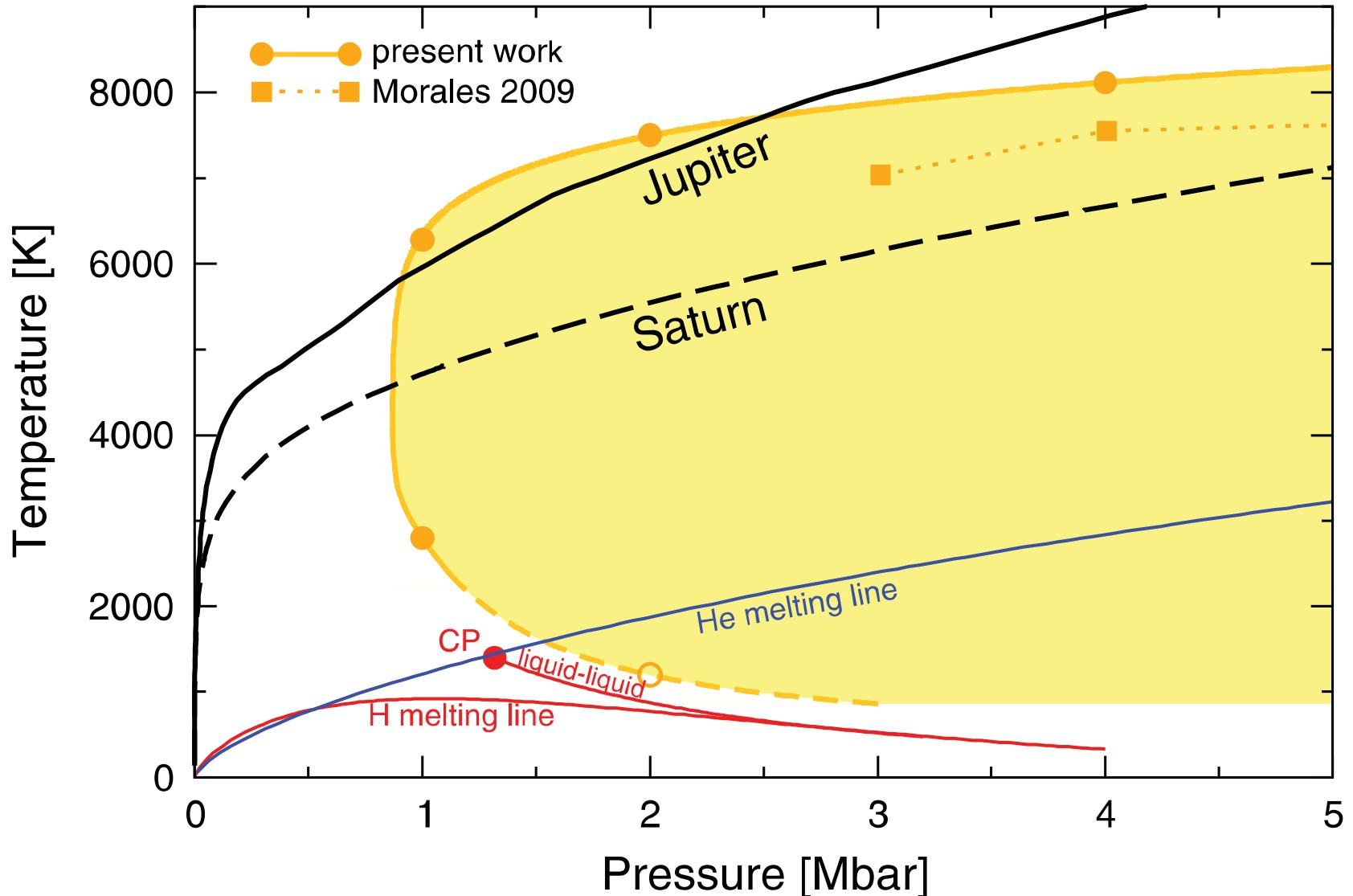
Interior composed of the lightest elements H & He, hydrides NH<sub>3</sub>, OH<sub>2</sub>, CH<sub>4</sub> (ices) and small amounts of heavier elements (cores)



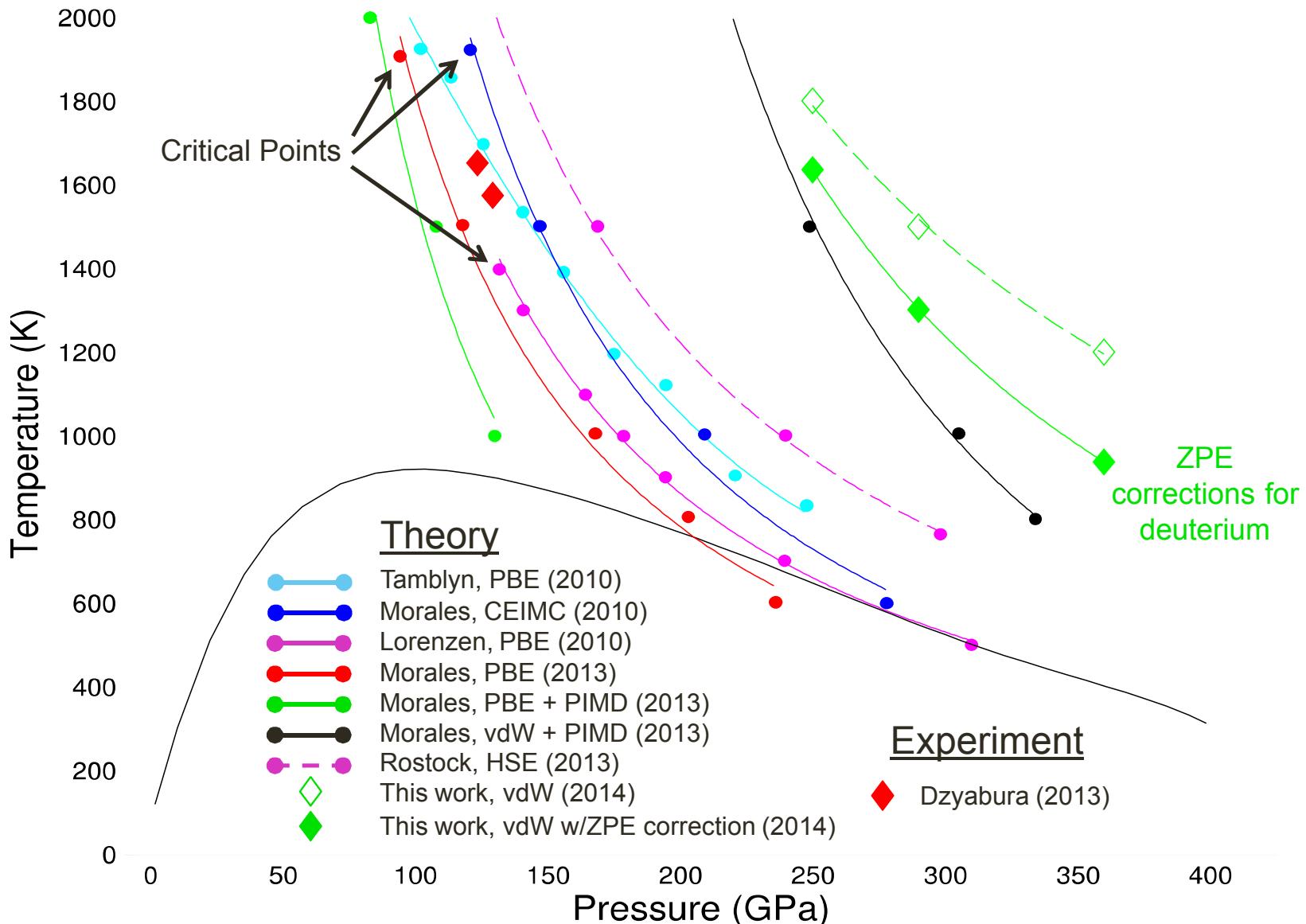
# Hydrogen at high pressures – the known phase diagram so far



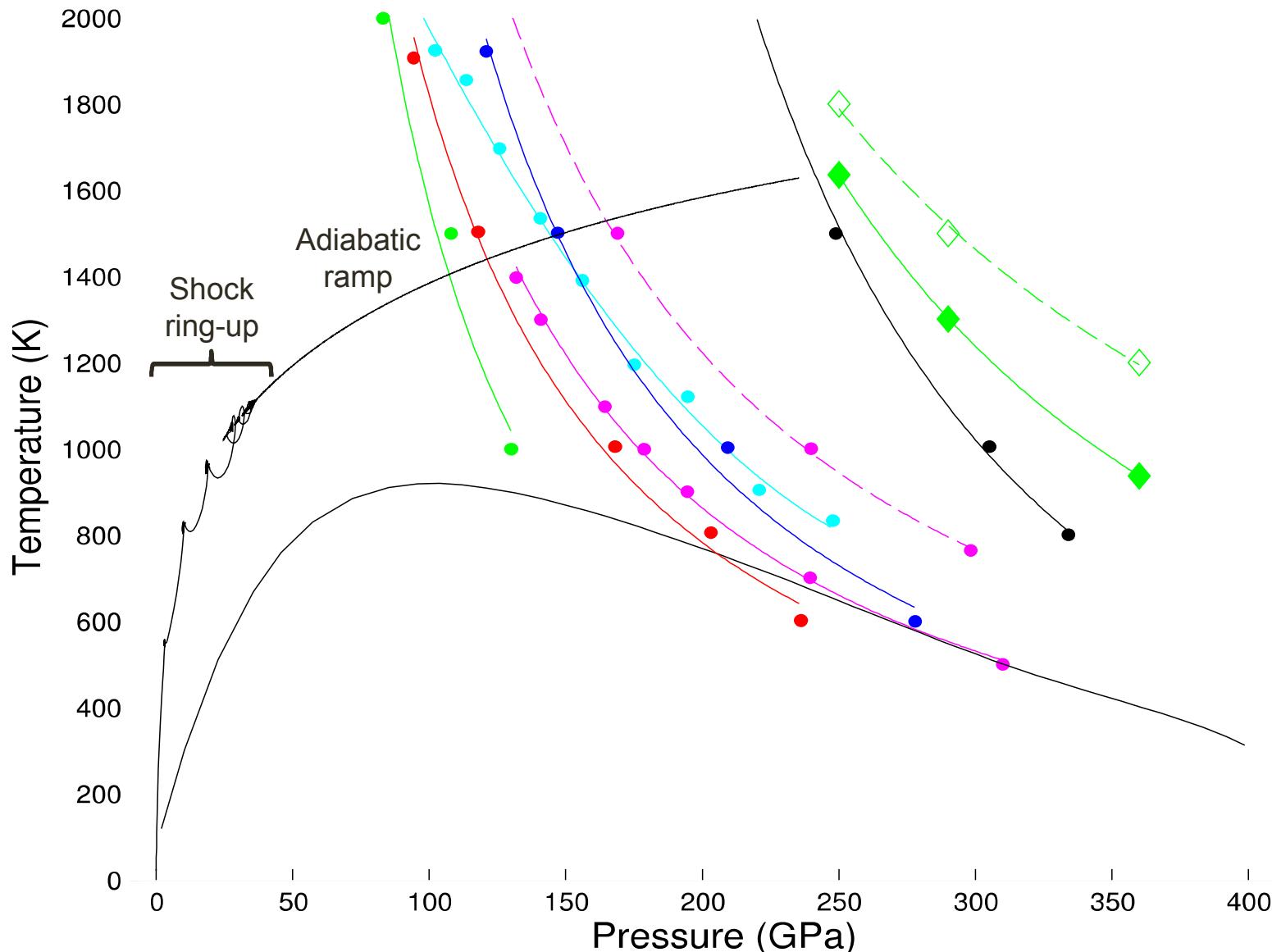
# H-He de-mixing appears to be precipitated at low T and P by metallization in hydrogen



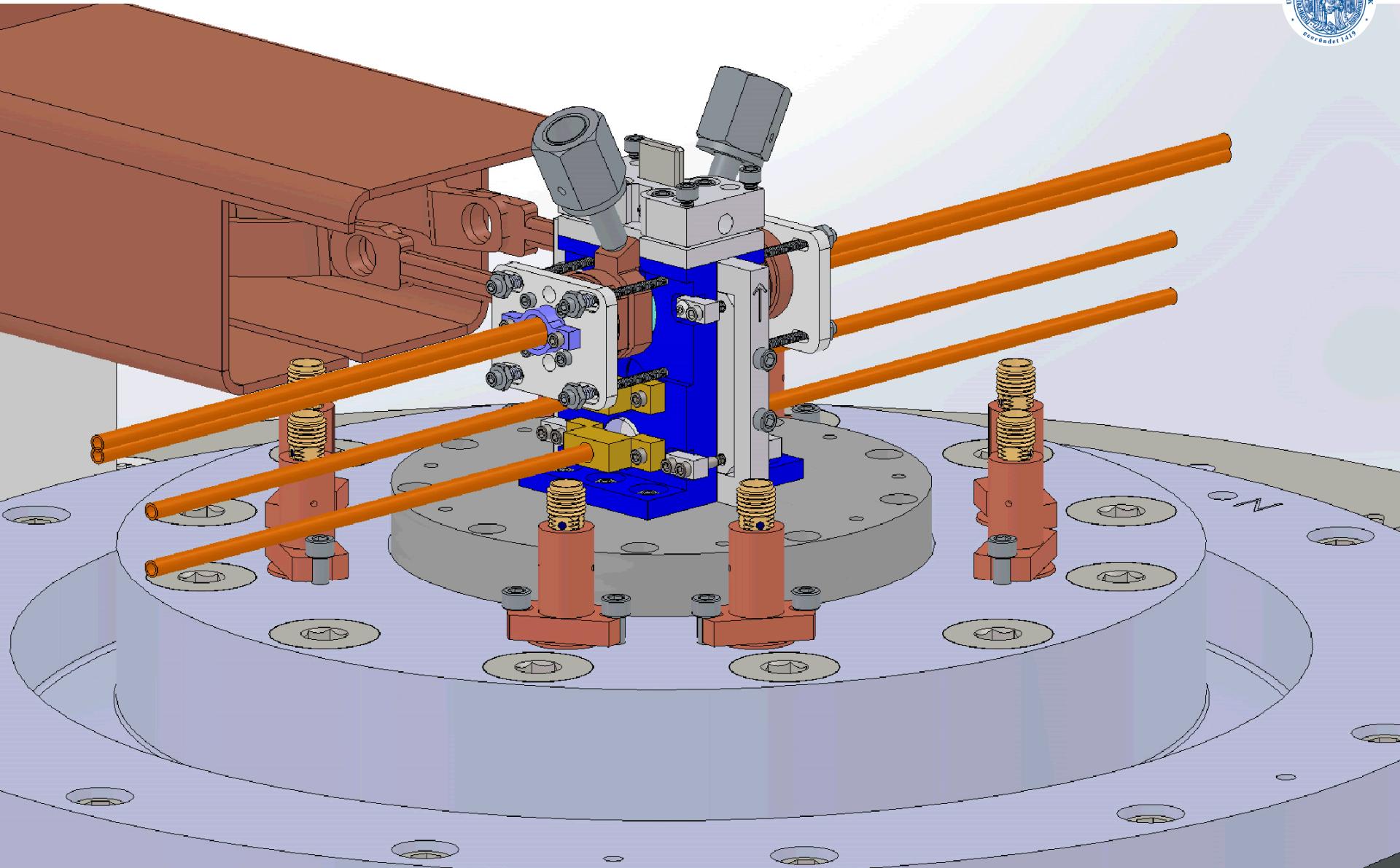
# Recent predictions for LL-IMT in H



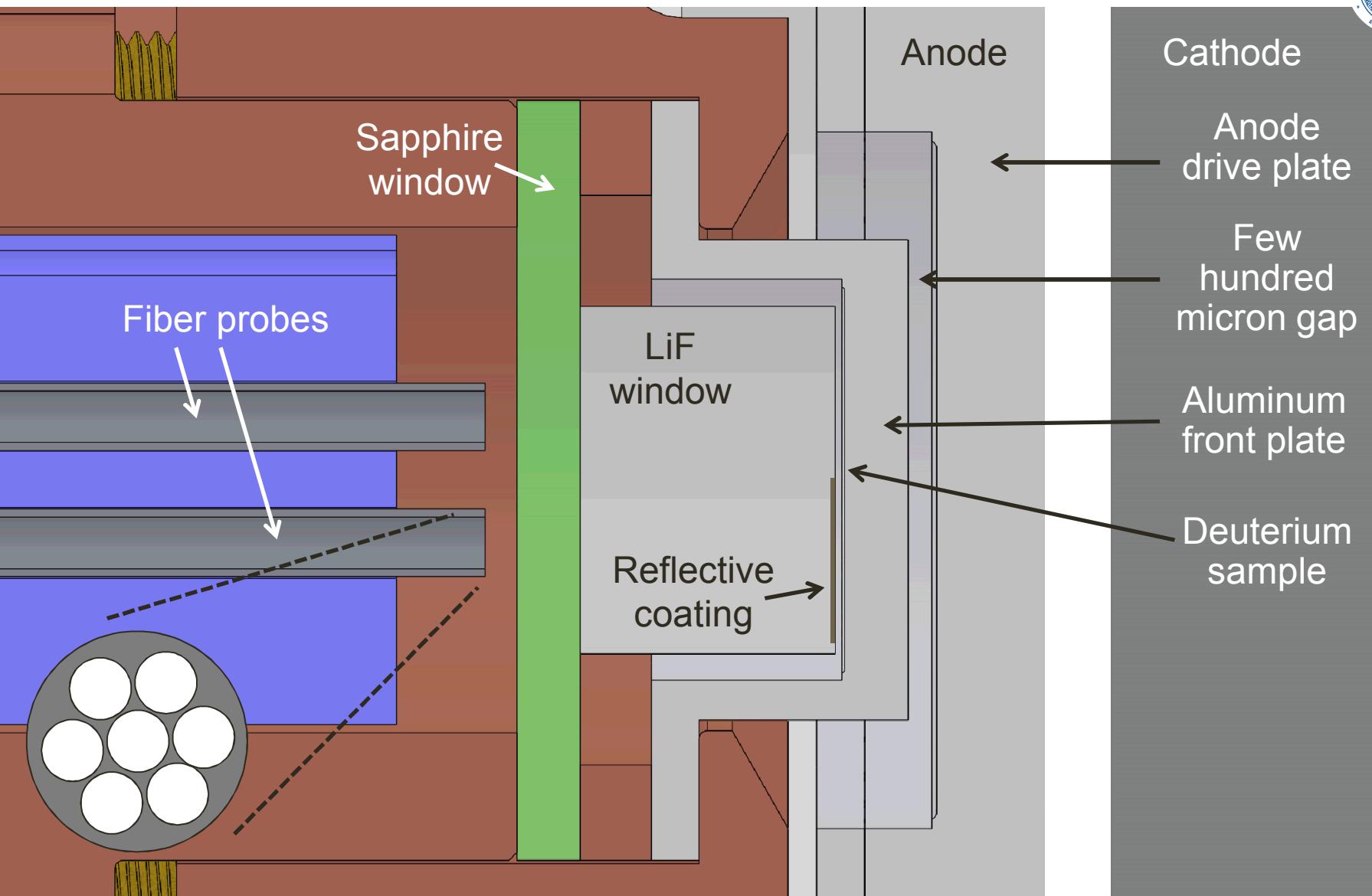
# Proposed Experiment



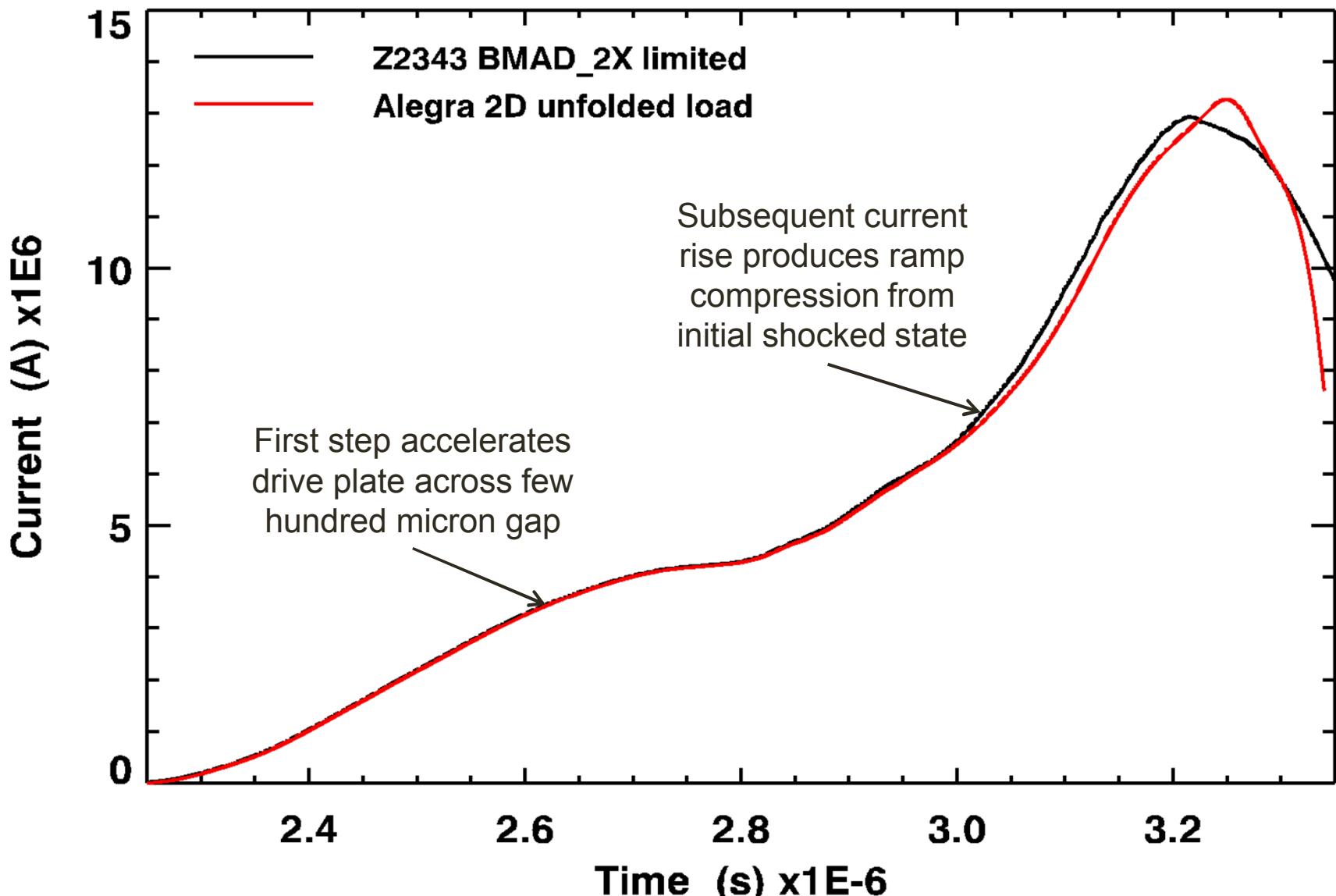
# Coaxial experimental configuration



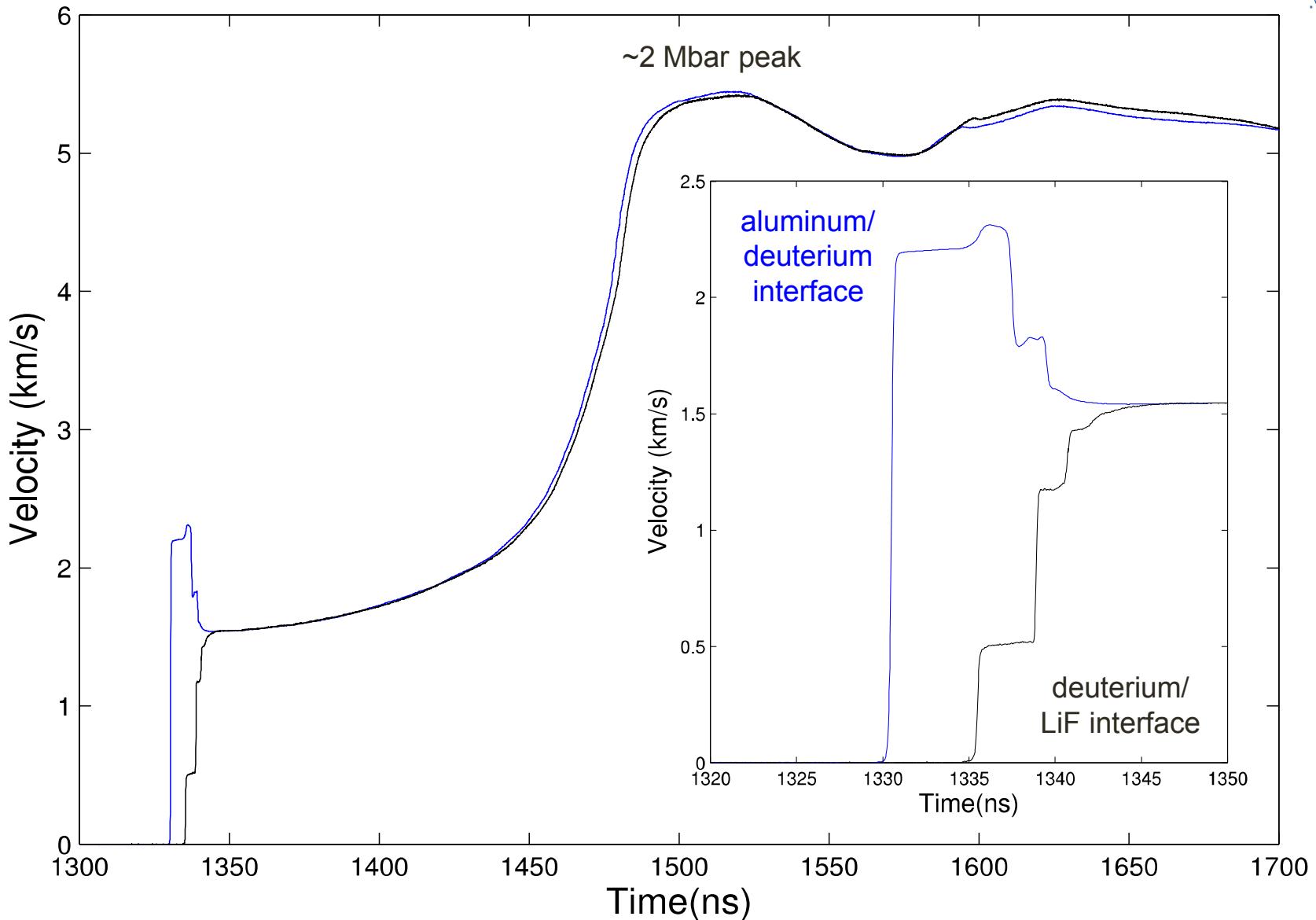
# Experimental configuration



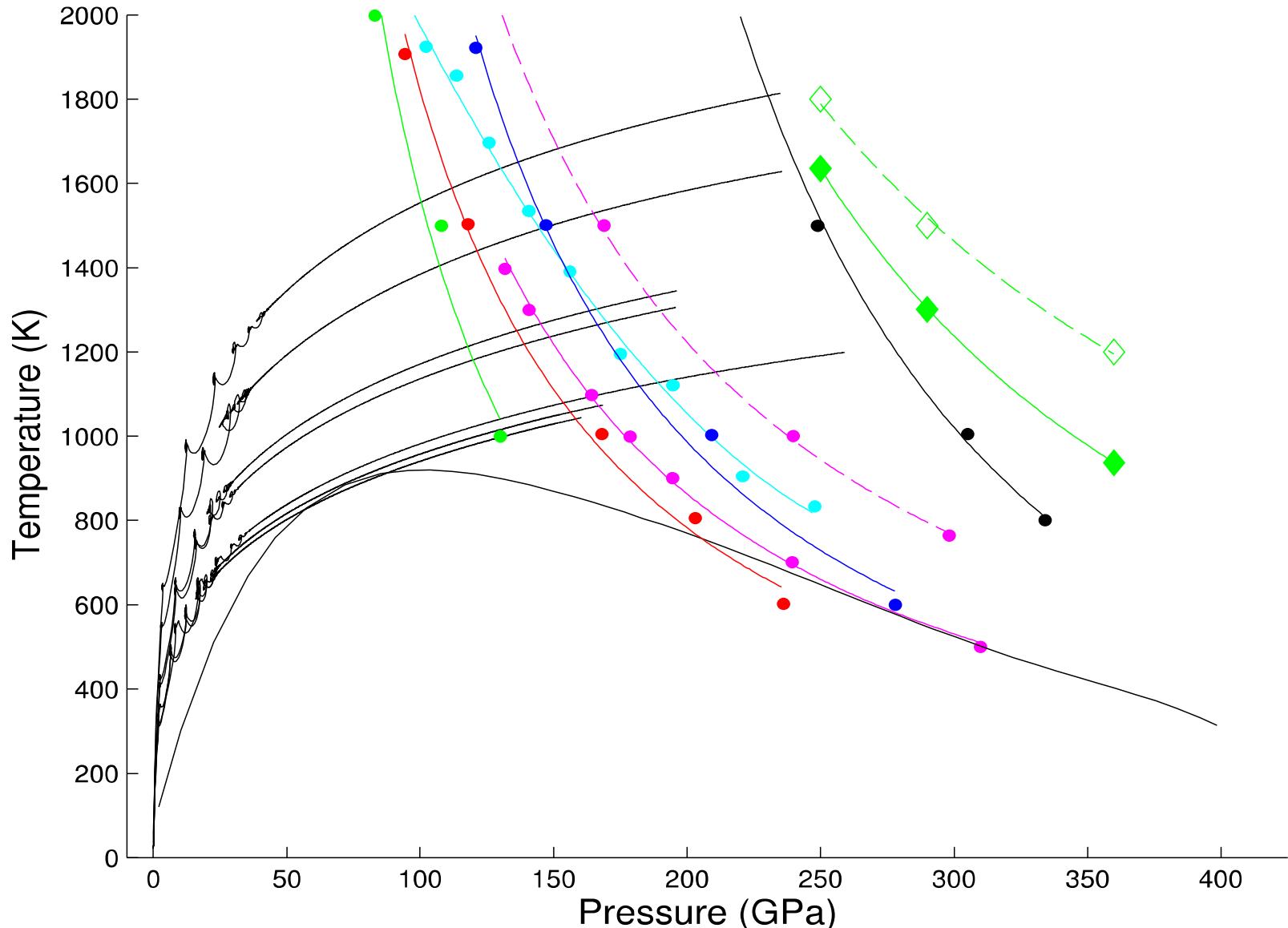
# Two-step pulse shape provides shock-ramp profile



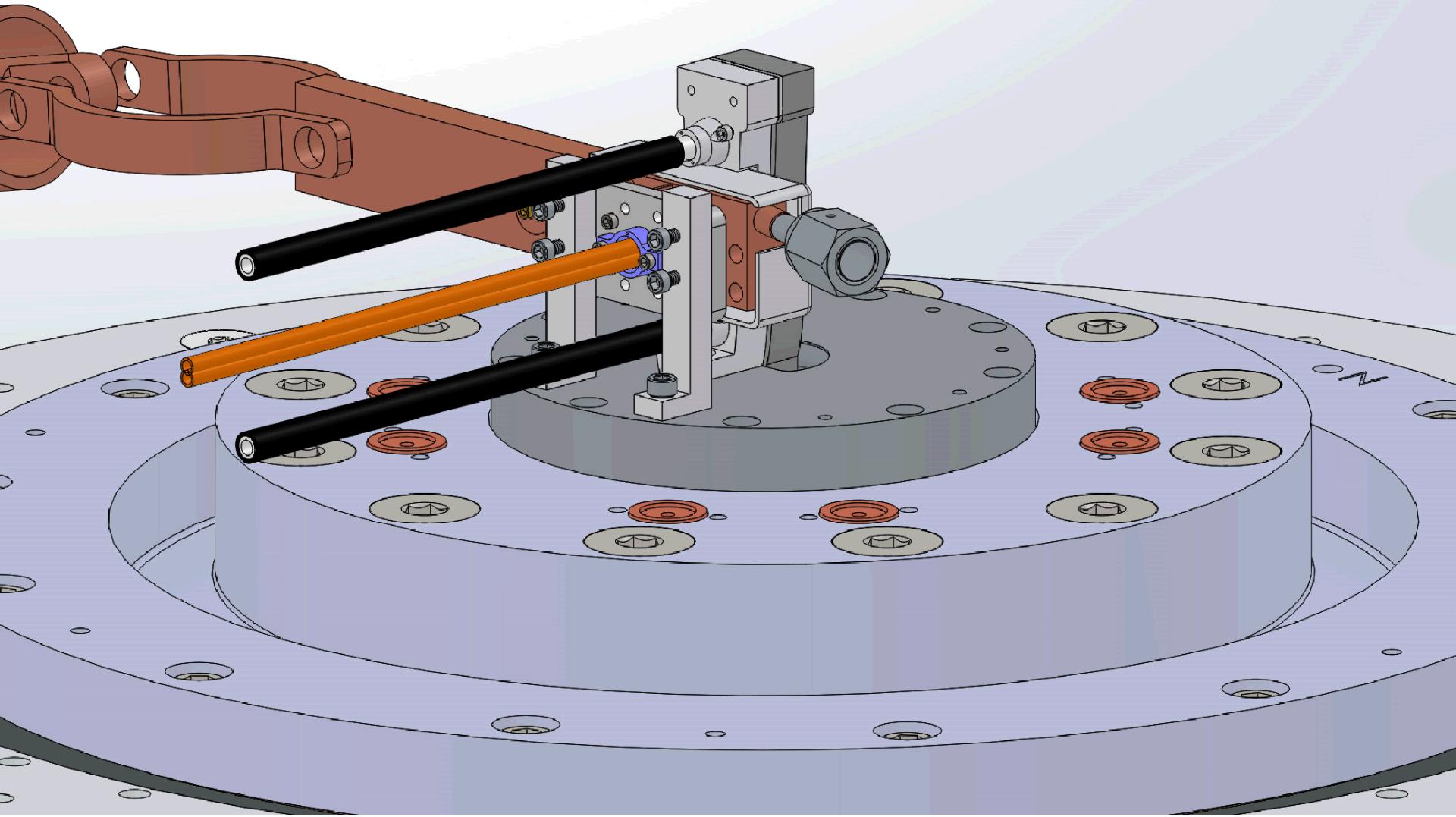
# Coaxial experimental profiles



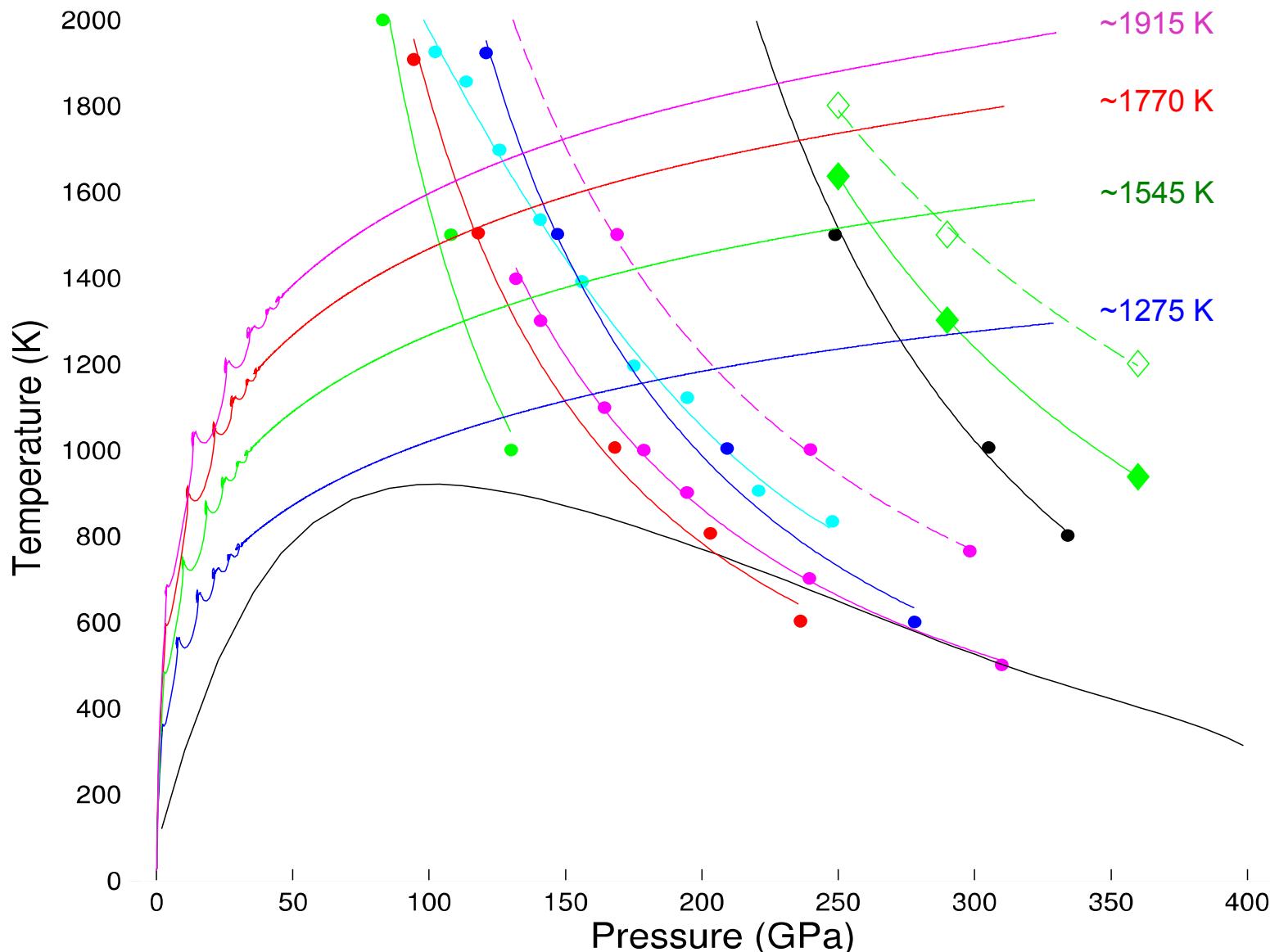
# Coaxial experiment PT paths



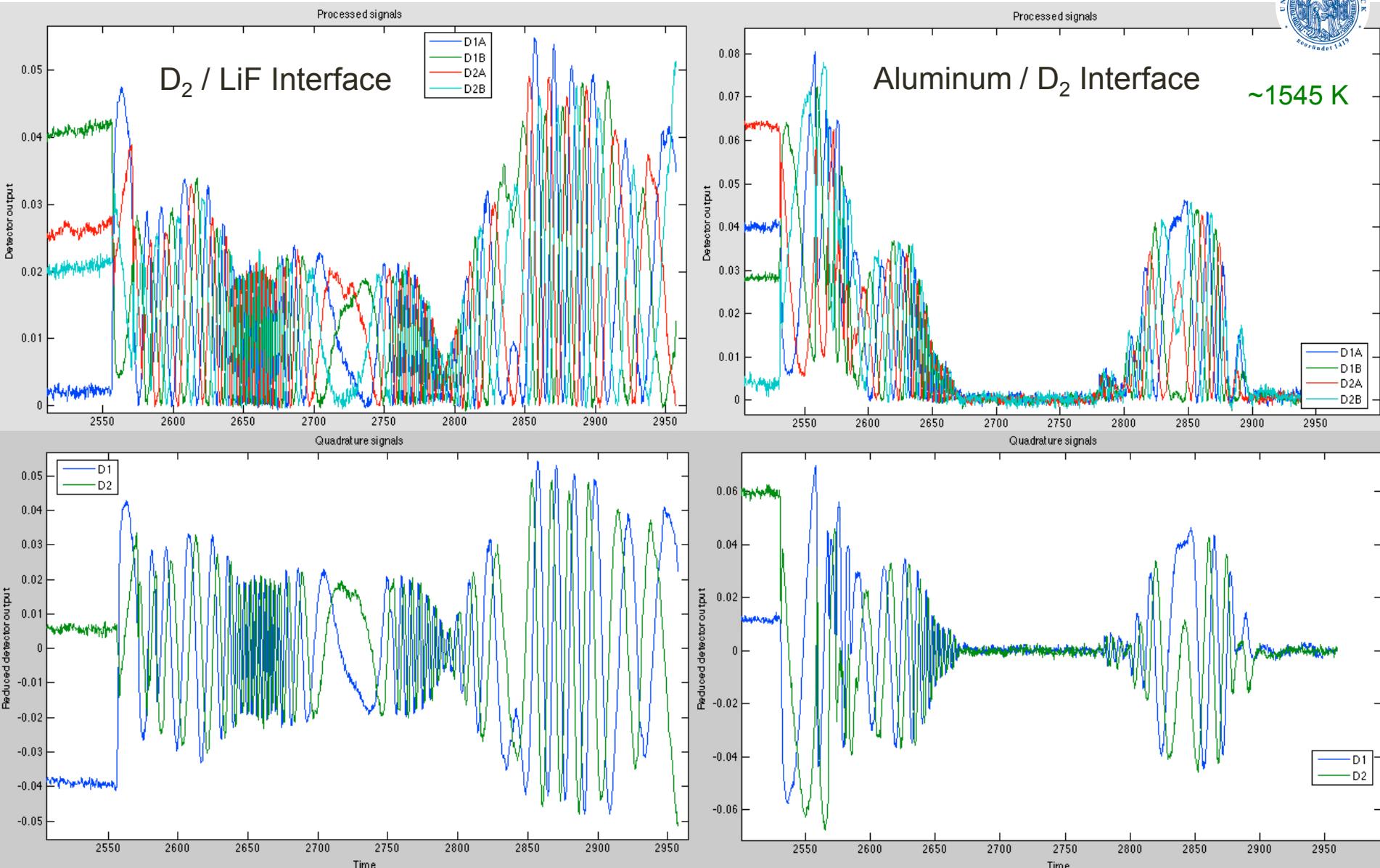
# Stripline experimental configuration



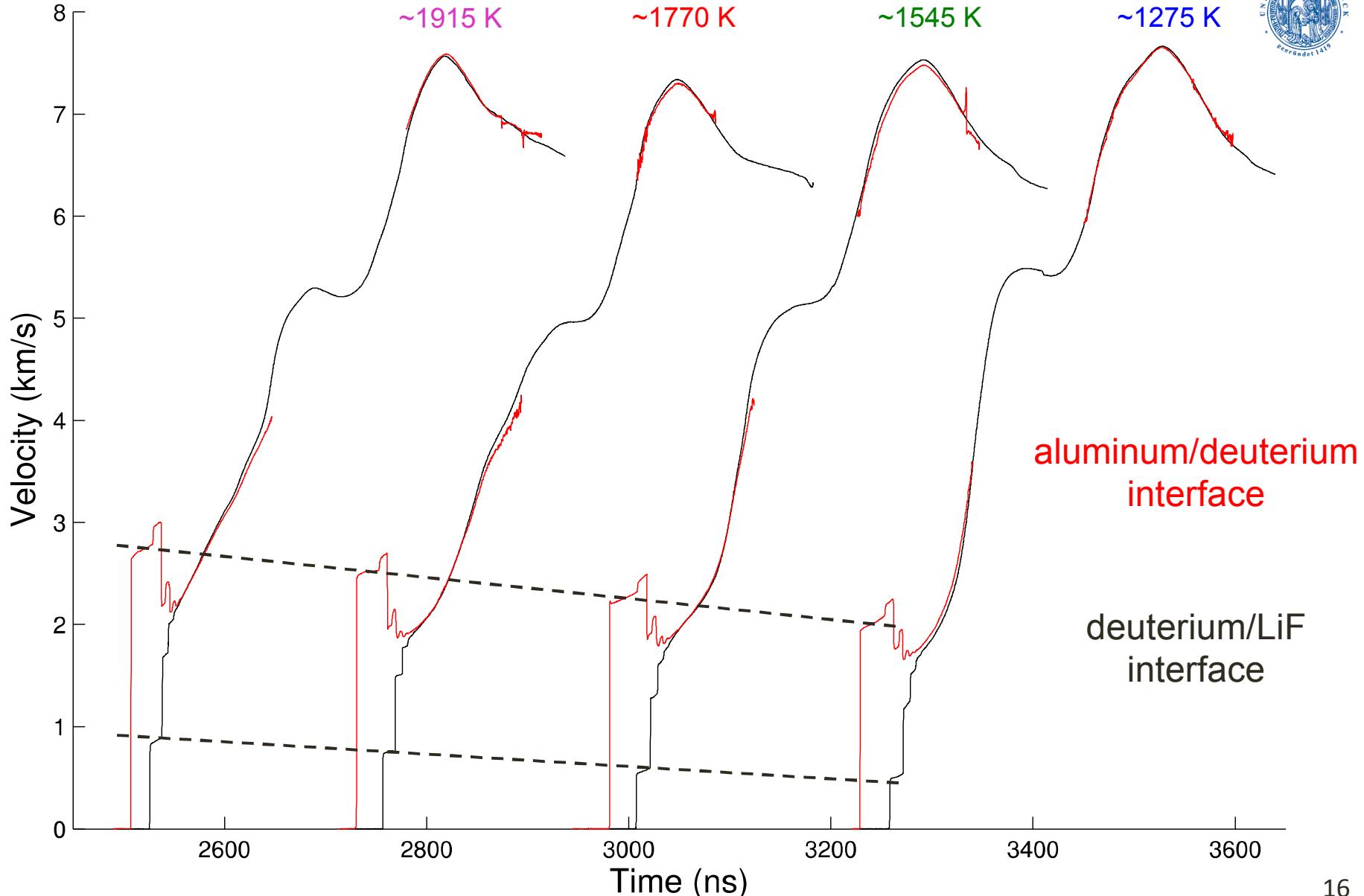
# Stripline experiment PT paths



# Processed VISAR signals

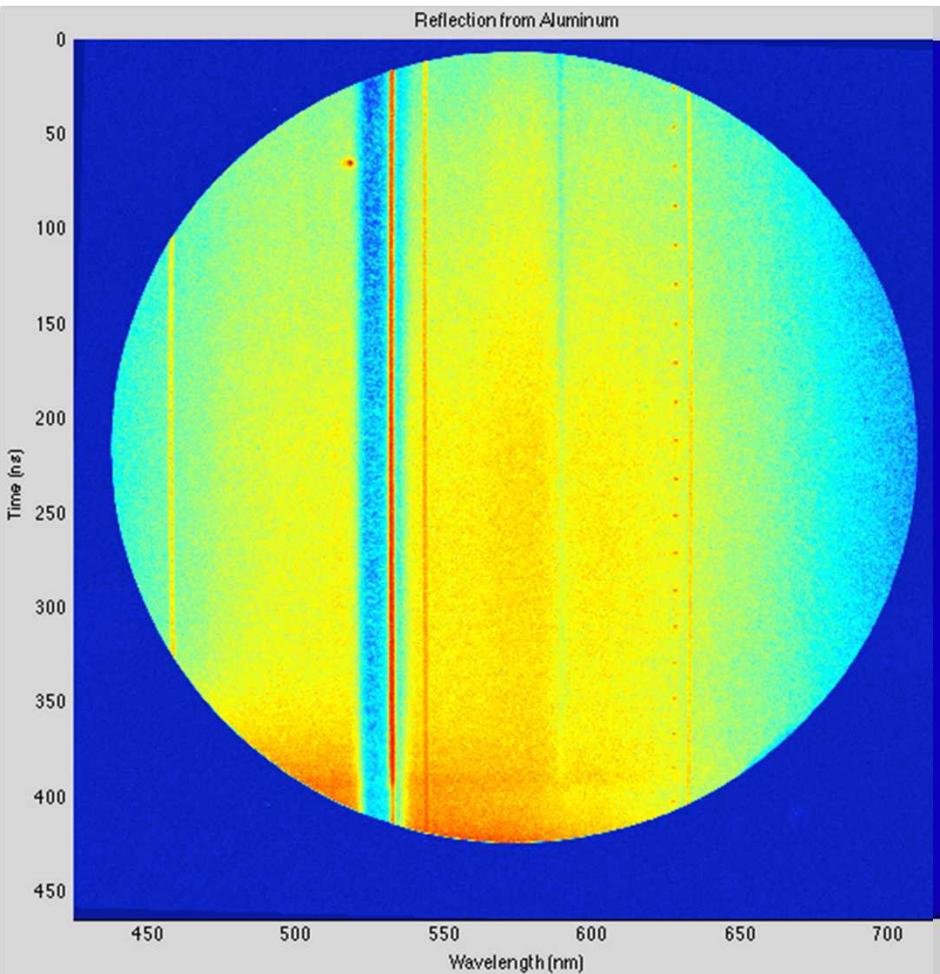


# Stripline experimental profiles



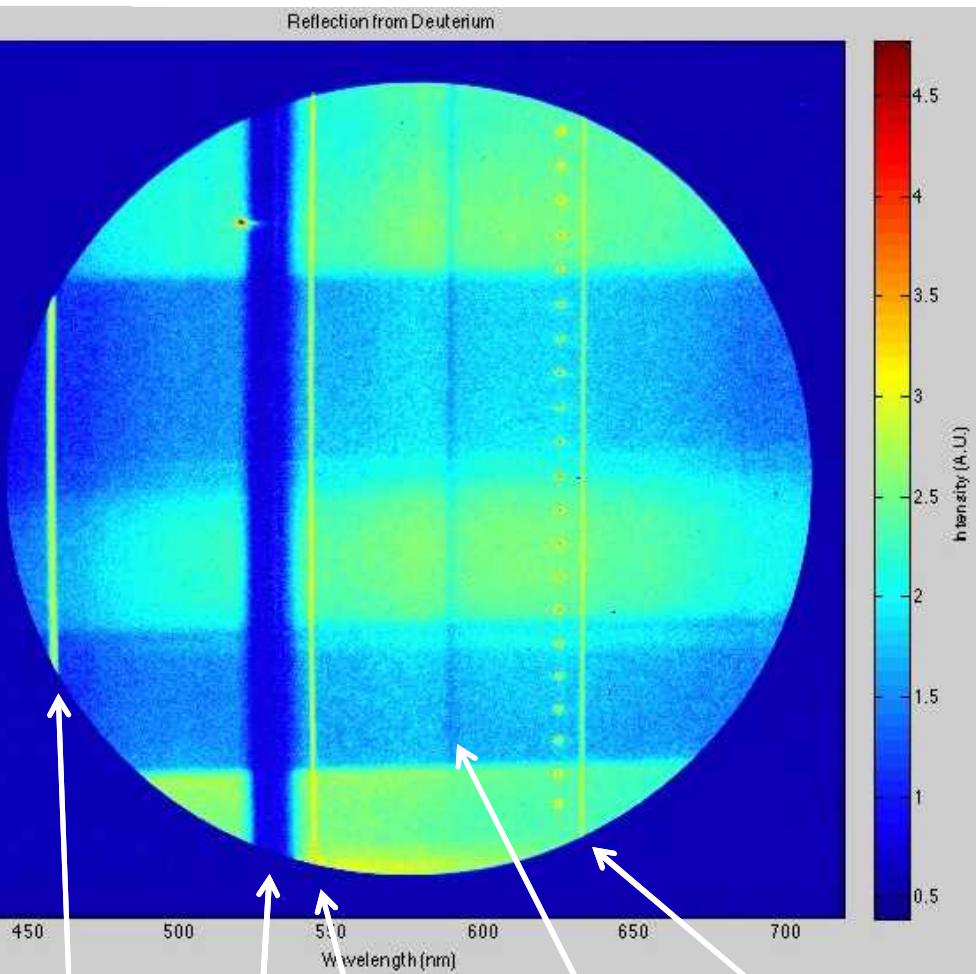
# SVS system provides data to infer reflectivity

Reflection from aluminum coating



Wavelength range ~450-700 nm

Reflection from deuterium



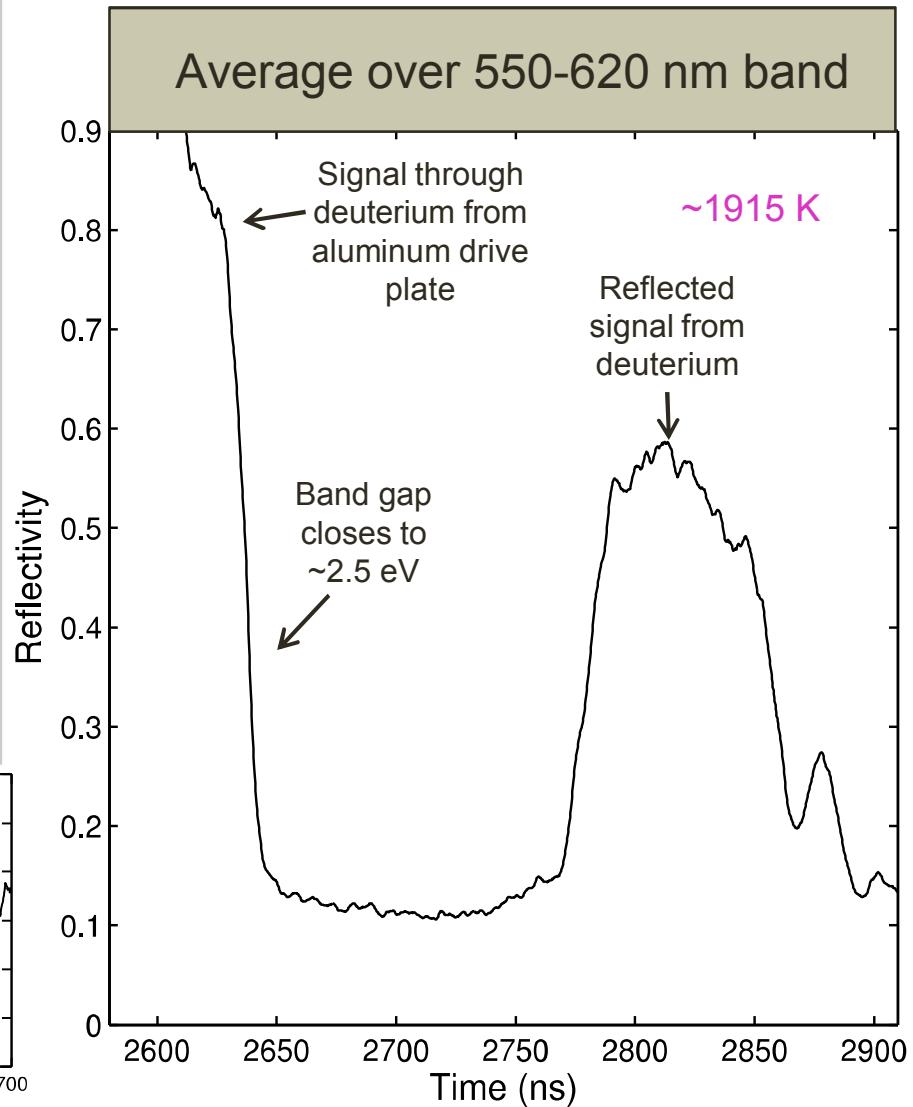
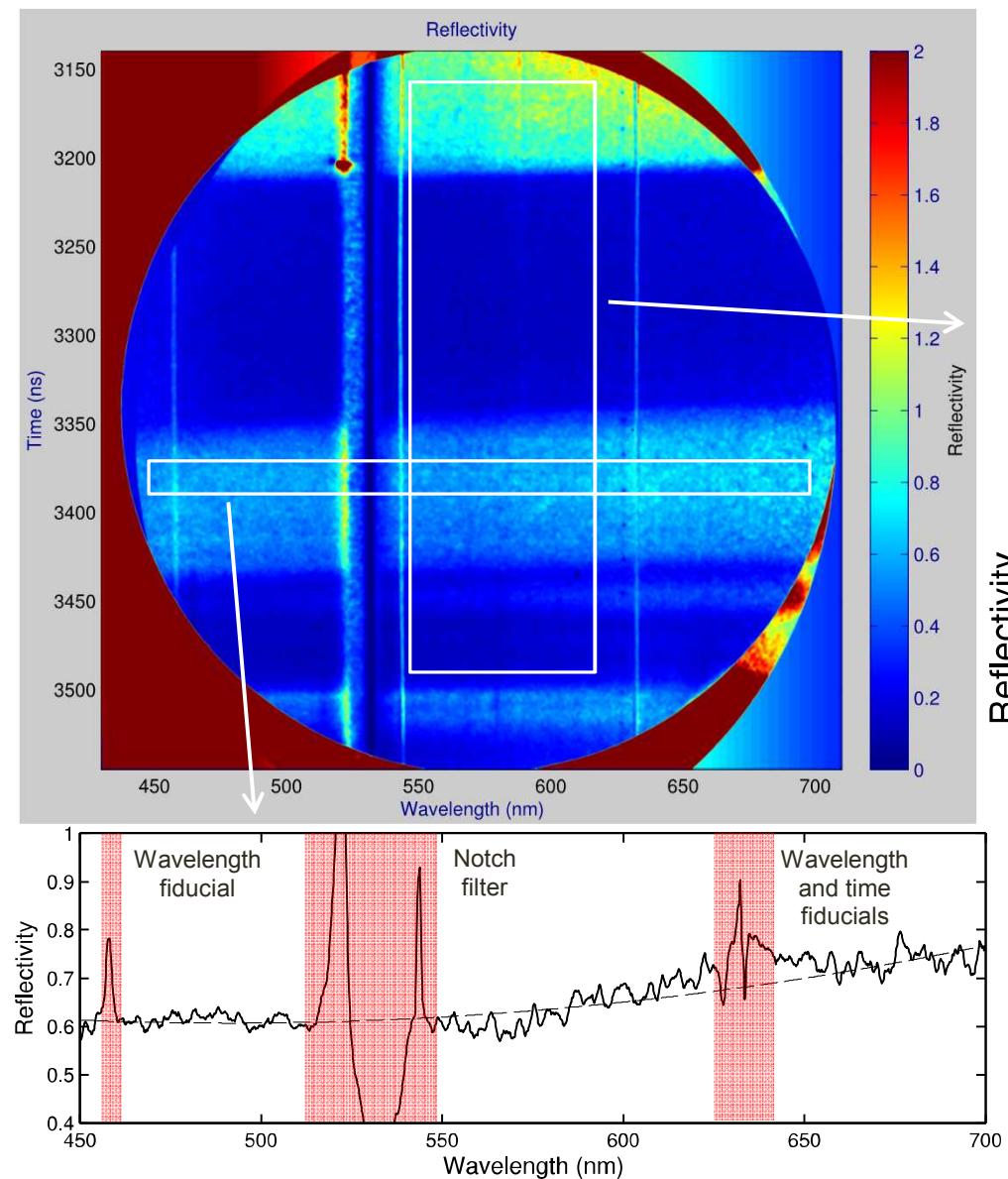
457.9 nm

532 / 543.5 nm

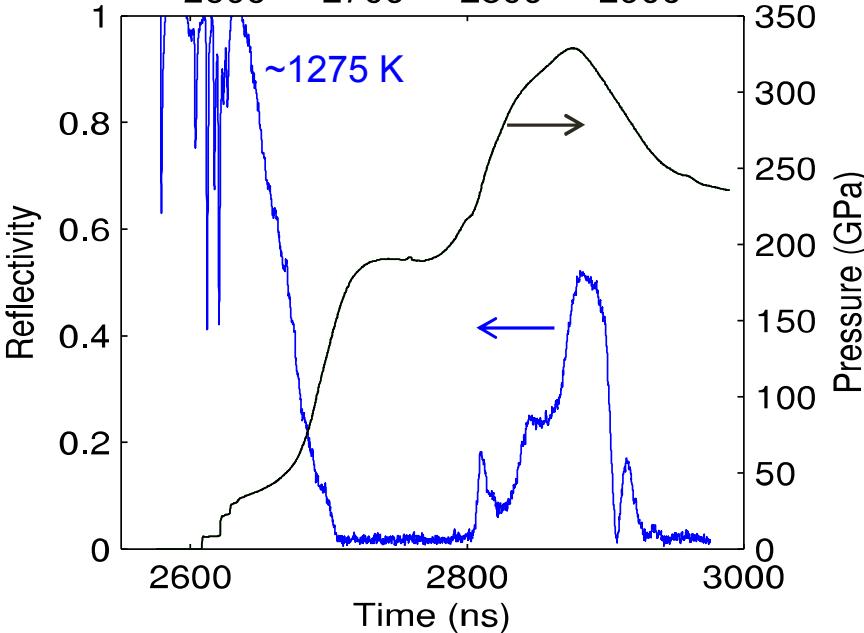
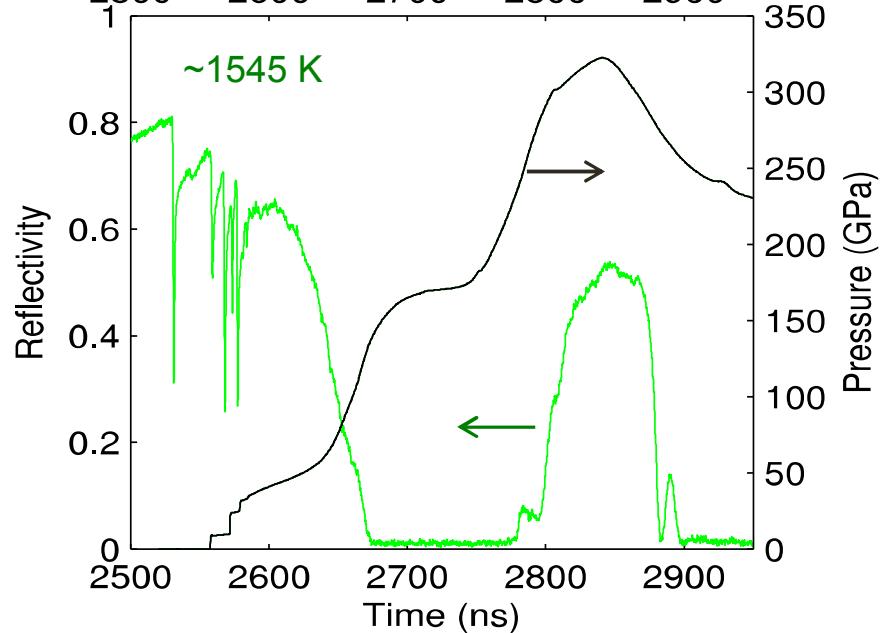
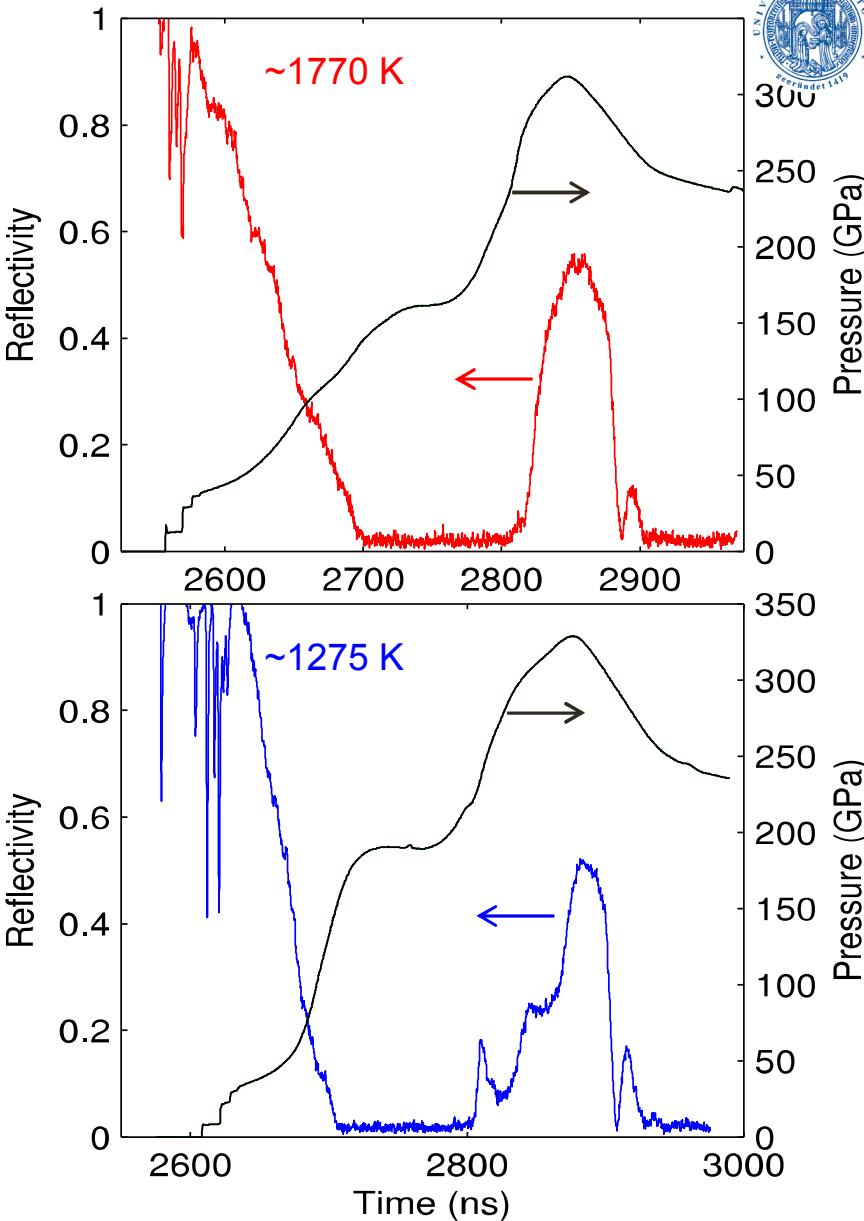
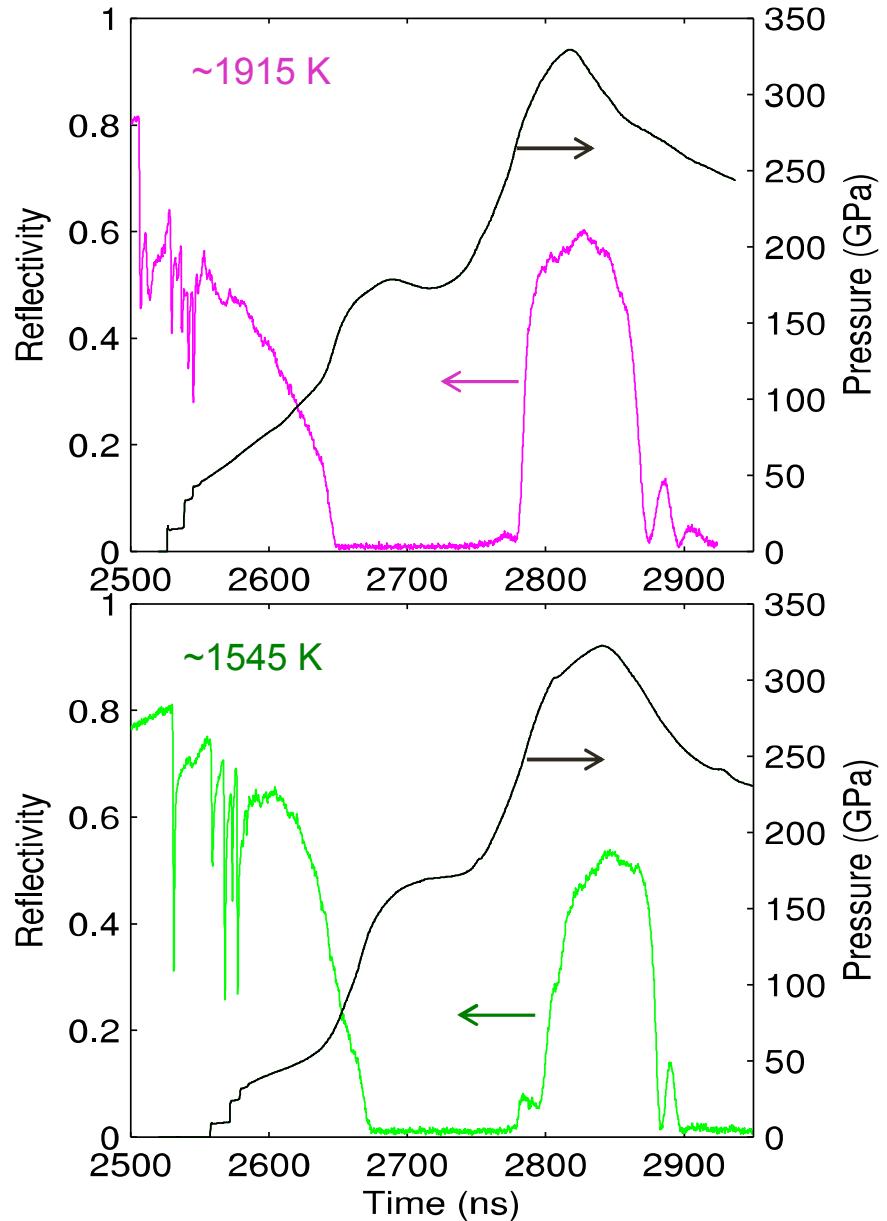
589.3 nm

633 nm

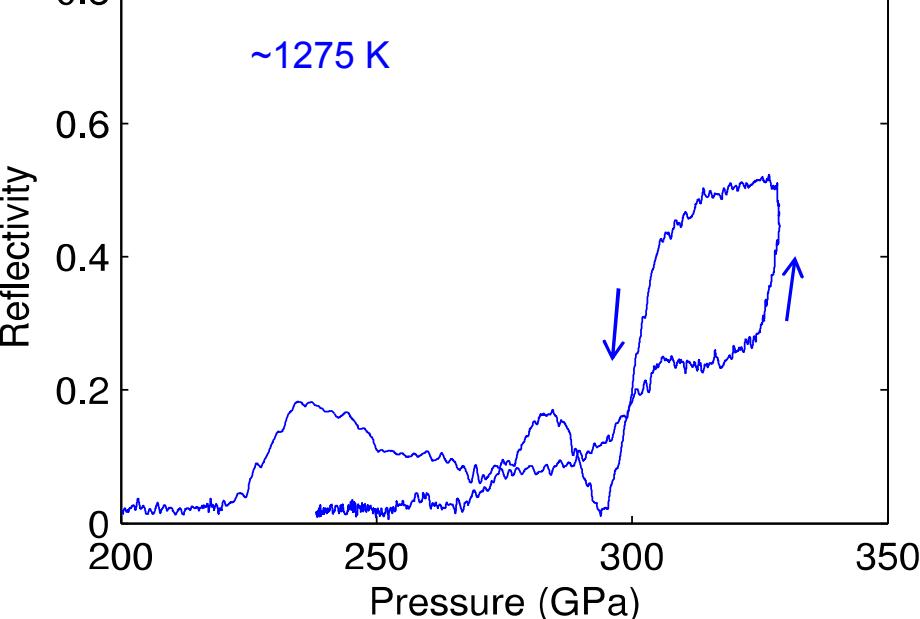
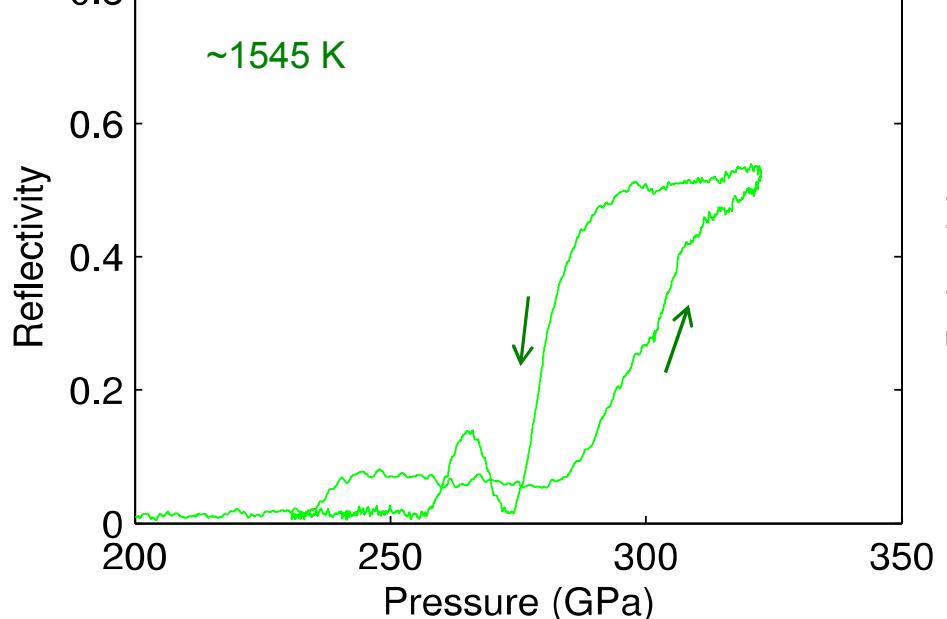
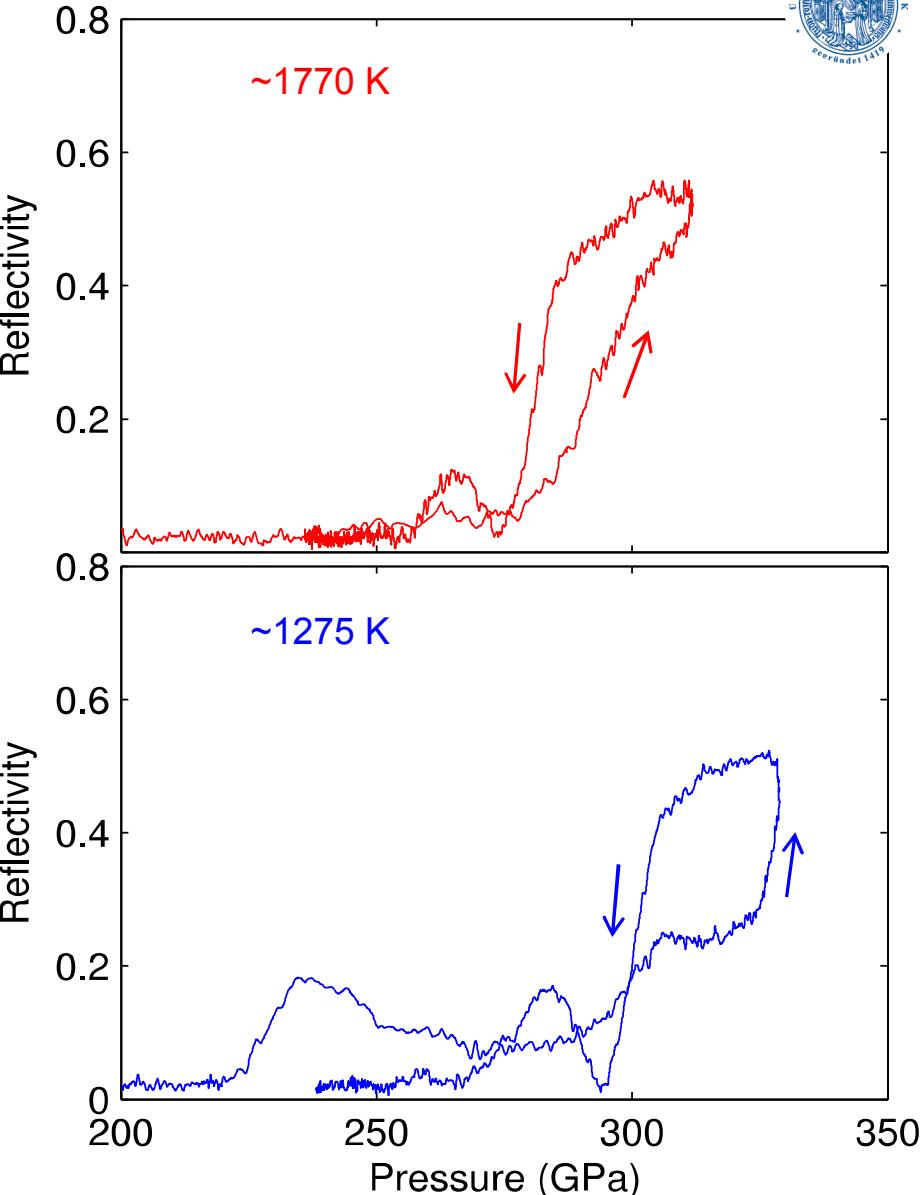
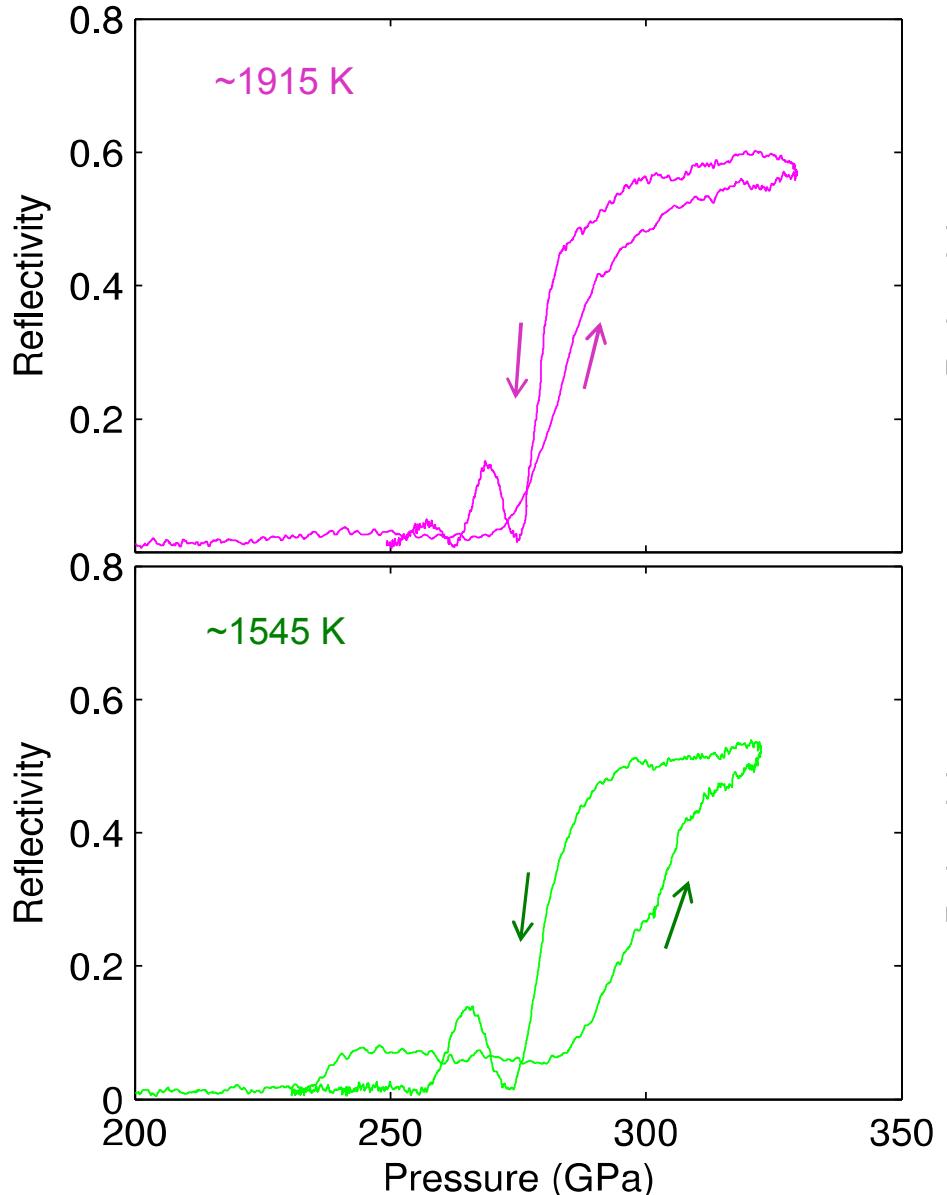
# SVS system provides data to infer reflectivity



# Reflectivity and pressure vs. time from VISAR

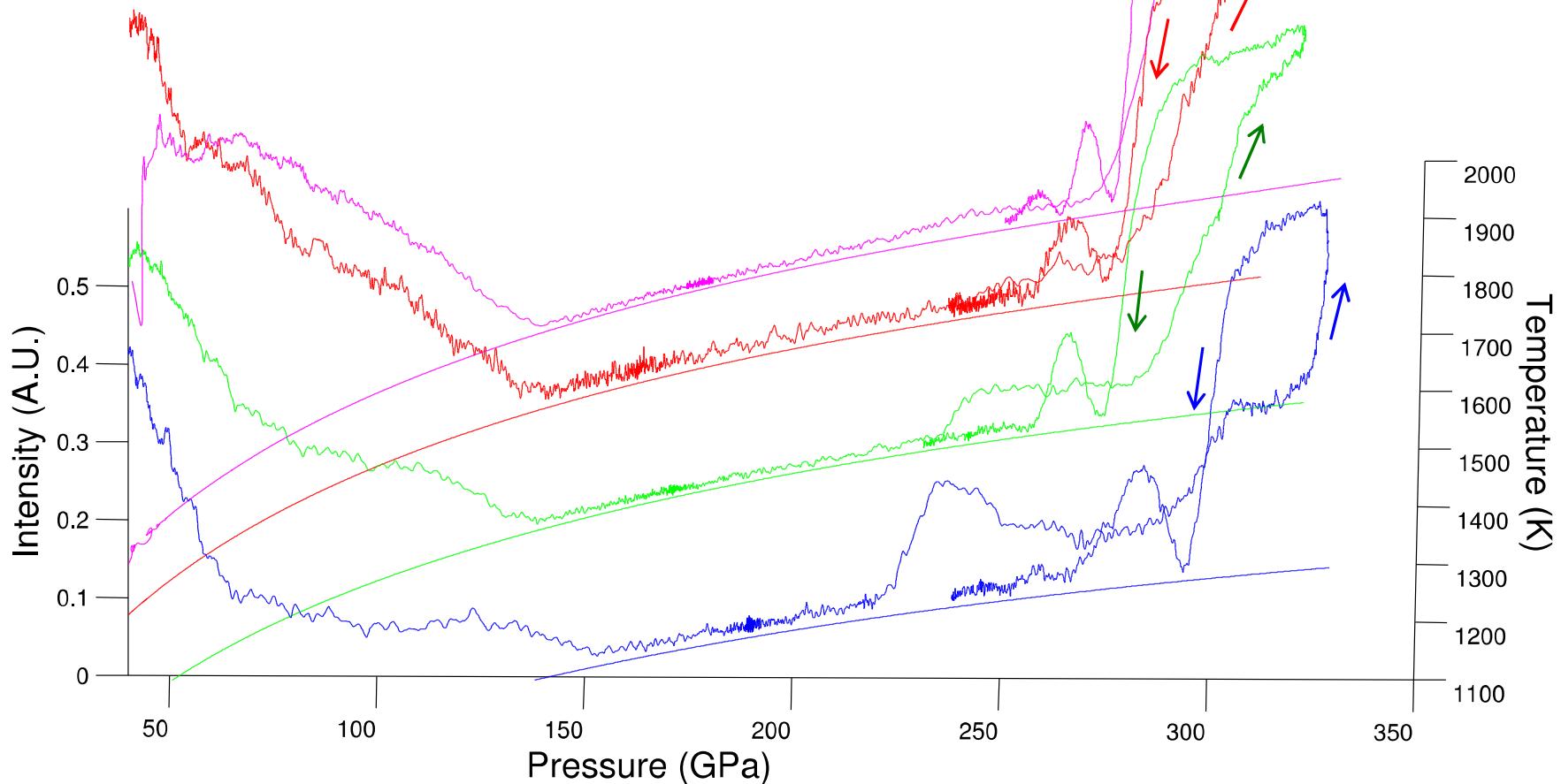


# Reflectivity signals mapped to pressure

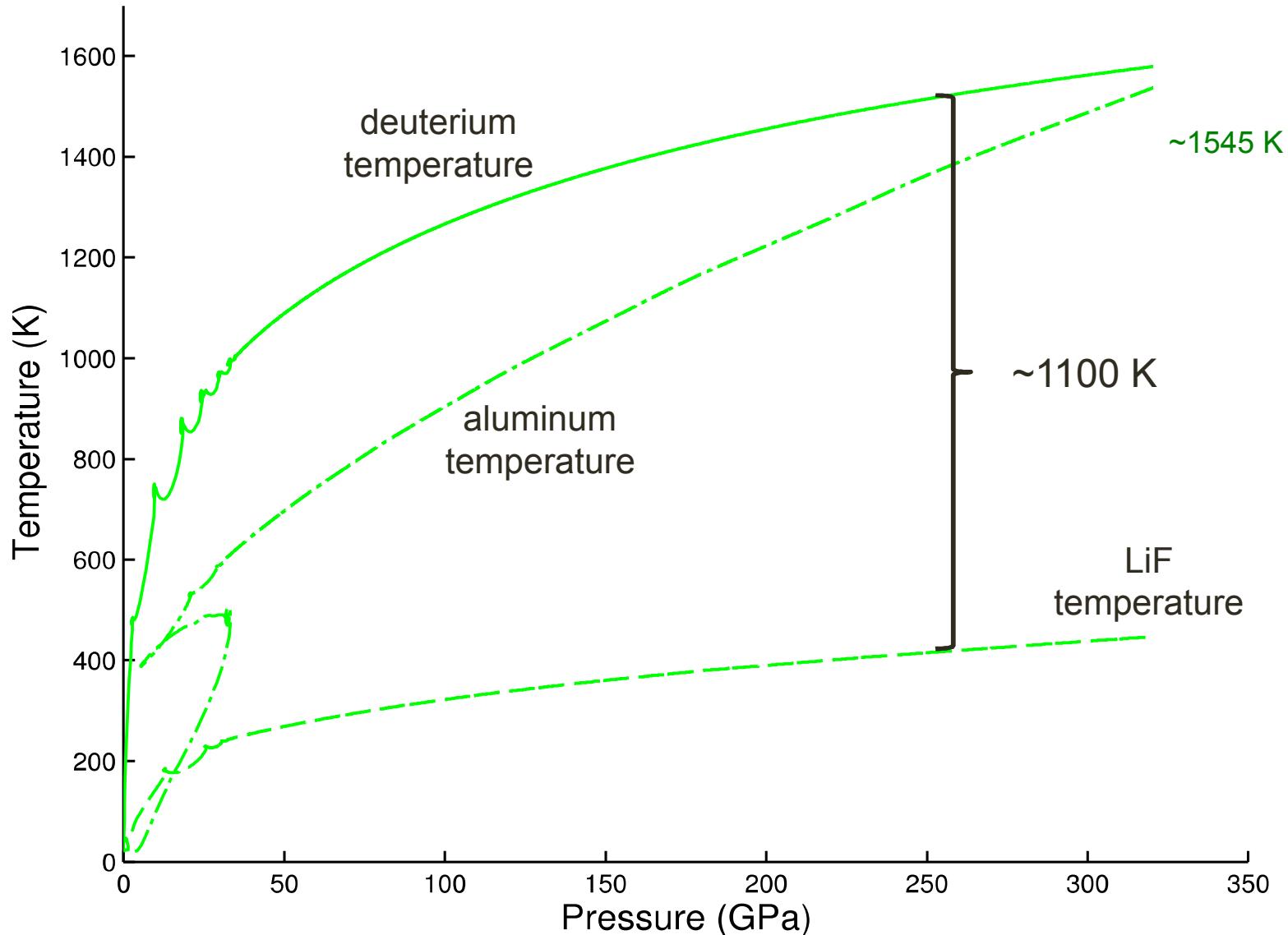


# Deuterium reflectivity mapped to both pressure and temperature

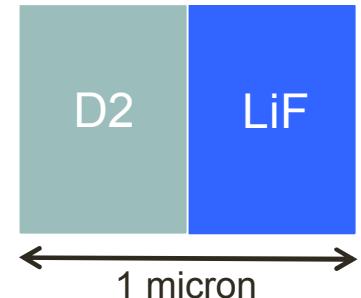
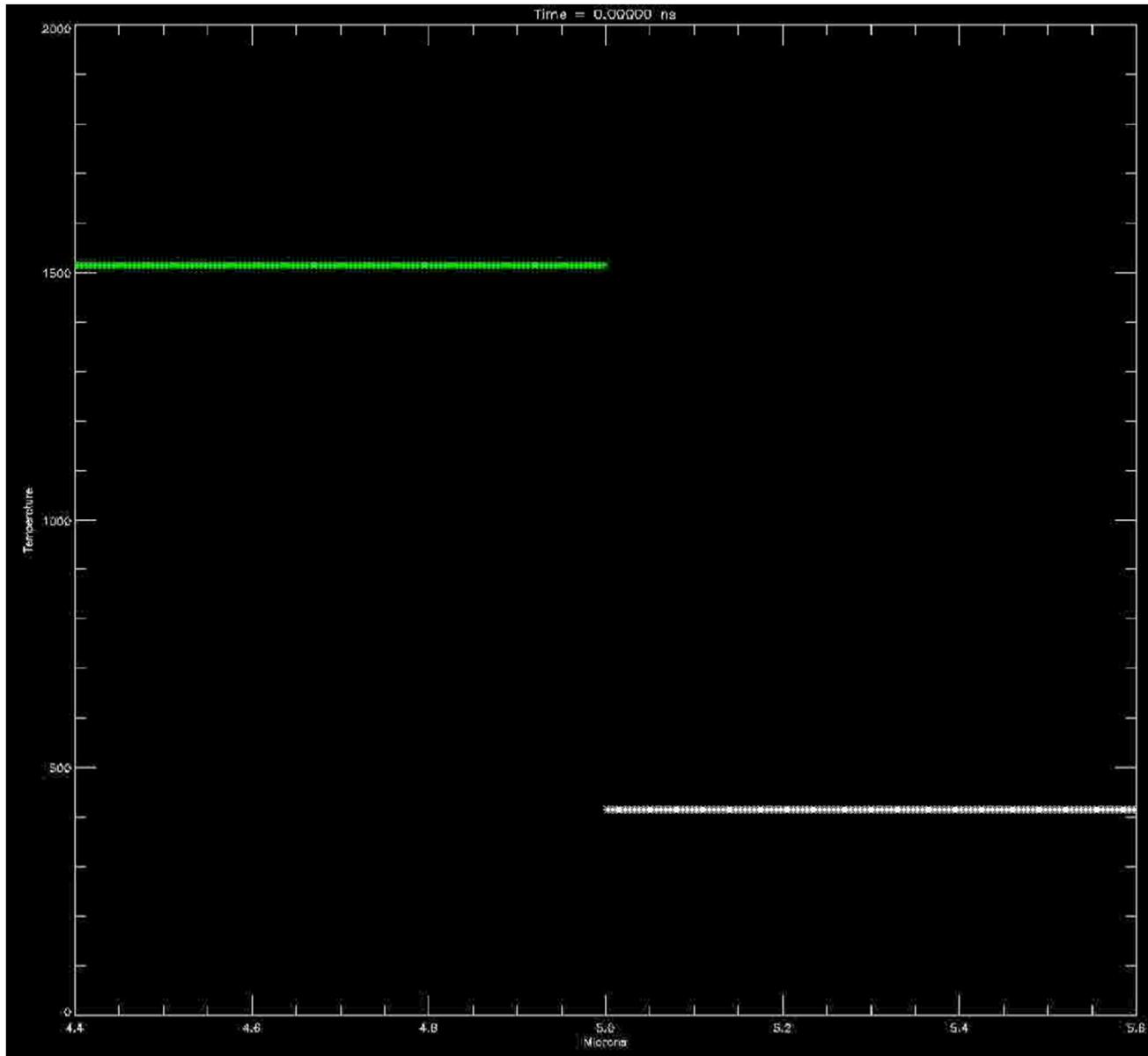
Asymmetry observed in the reflectivity is likely caused by time evolution of thermal gradients at the deuterium/LiF interface



# There is a significant temperature difference at the deuterium/LiF interface



# Thermal conduction at D2/LiF interface



deuterium

$$P_1 = 250 \text{ GPa}$$

$$\rho_1 = 1.923 \text{ g/cc}$$

$$T_{b1} = 1515 \text{ K}$$

$$\kappa_1 = 0.36 \text{ W/mK}$$

LiF

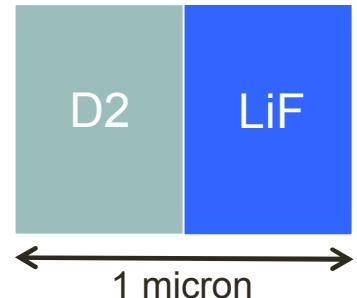
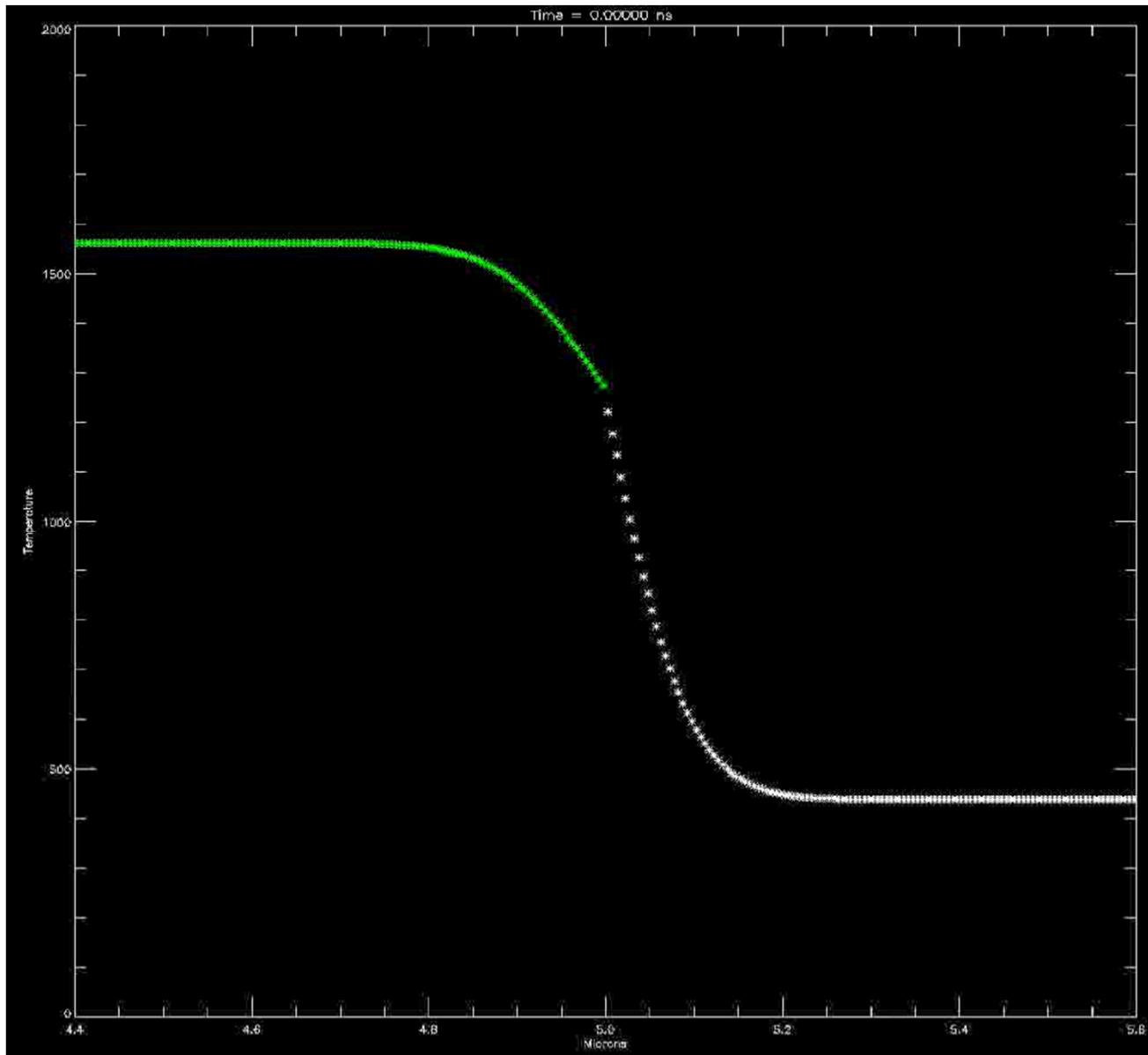
$$P_1 = 250 \text{ GPa}$$

$$\rho_1 = 5.362 \text{ g/cc}$$

$$T_{b1} = 415 \text{ K}$$

$$\kappa_1 = 0.1 \text{ W/mK}$$

# Thermal conduction at D2/LiF interface



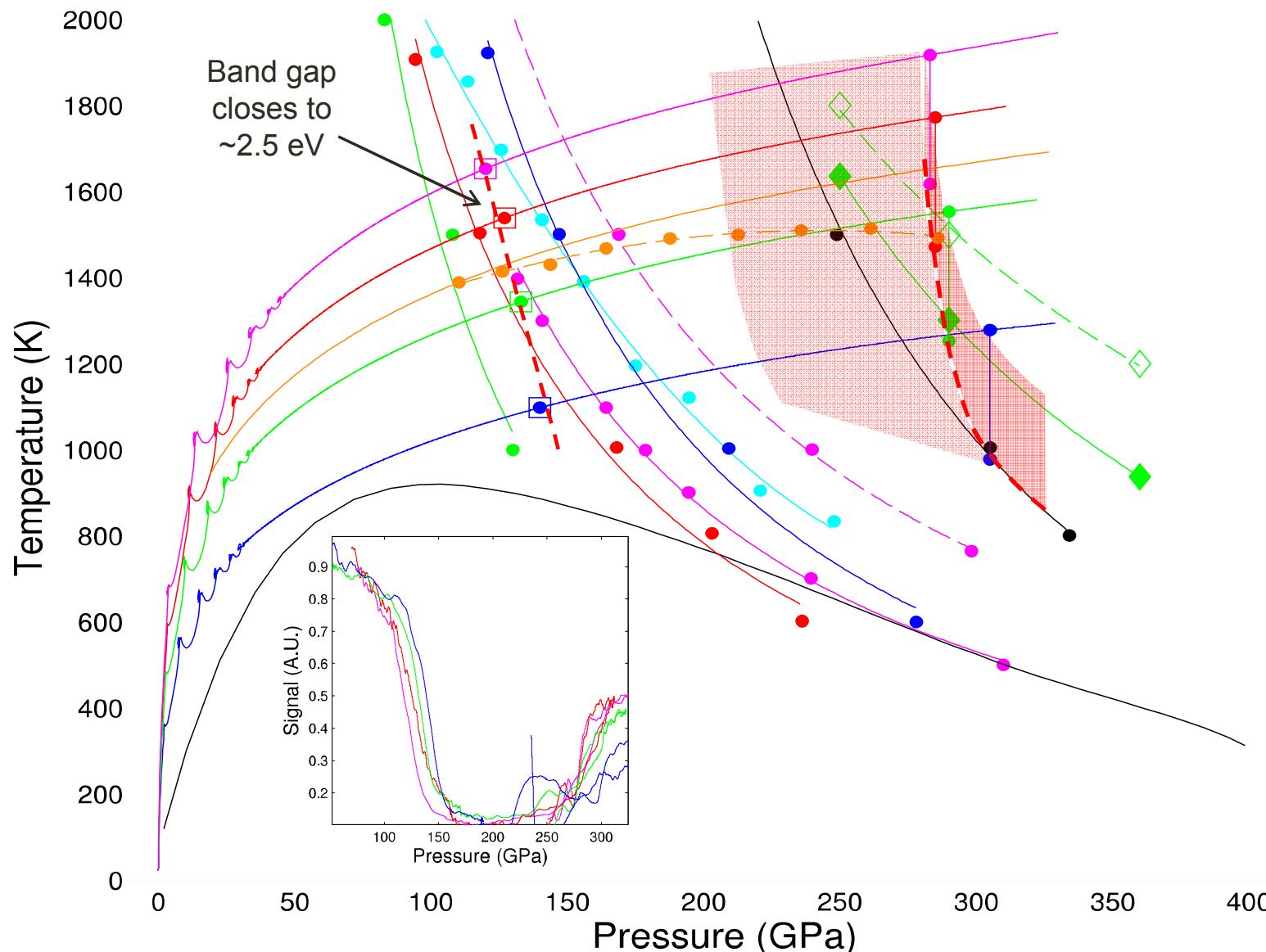
deuterium

$P_2 = 300 \text{ GPa}$   
 $\rho_2 = 2.080 \text{ g/cc}$   
 $T_{b2} = 1562 \text{ K}$   
 $\kappa_2 = 25 \text{ W/mK}$

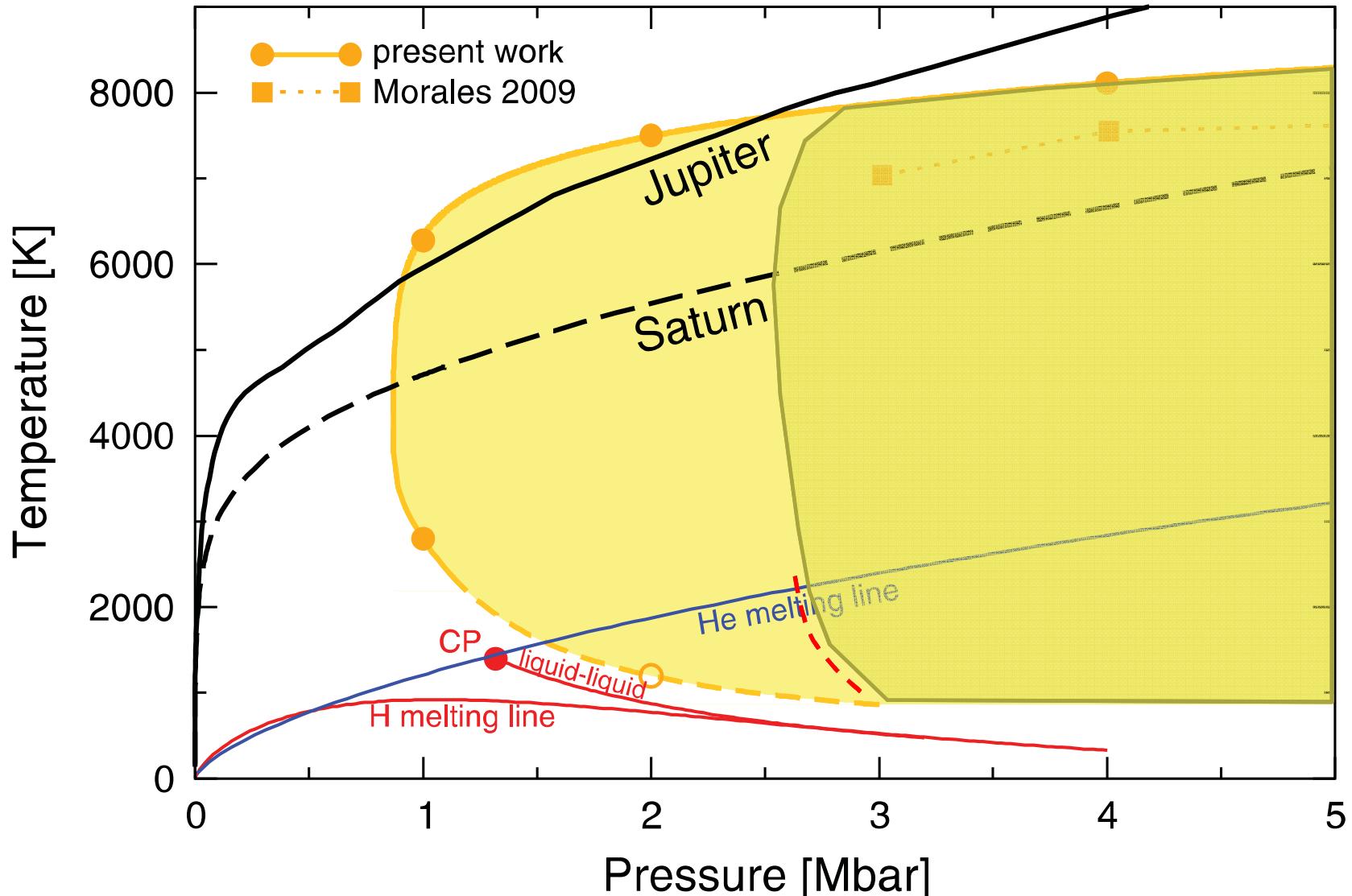
LiF

$P_2 = 300 \text{ GPa}$   
 $\rho_2 = 5.547 \text{ g/cc}$   
 $T_{b2} = 438 \text{ K}$   
 $\kappa_2 = 0.1 \text{ W/mK}$

# Possible location of the LL-IMT in deuterium



# H-He de-mixing appears to be precipitated at low T and P by metallization in hydrogen



# Conclusions

- Shock-ramp technique enables experimental access to the region of phase space where the liquid-liquid, insulator-metal transition (LL-IMT) has been proposed for hydrogen
  - Temperature of the adiabat controlled by magnitude of initial shock
  - $P(t)$  in the experiments determined from the LiF equation on state
- Experiments above  $\sim 250$  GPa show clear evidence of metallization of deuterium
  - Very abrupt increase in reflectivity to  $\sim 50$ -60%
  - Pressure state well above numerous first principles predictions
  - Indications suggest that the transition is first order
- Interpretation of the experimental results is complicated
  - Thermal conduction likely very important at the deuterium / LiF interface

# Future Directions

- Continued analysis of existing data
  - Evaluate effects of thermal conduction using QMD estimates for thermal conductivity of the molecular and atomic fluids
  - Detailed QMD calculations in the vicinity of the transition to estimate the temperature drop due to latent heat
  - Compare measured reflectivity with QMD predictions for optical properties of the atomic fluid
  - Compare observed band gap closure with QMD predictions for various functionals
- Attempt temperature measurements
  - Plan to use a novel reflectivity based temperature measurement to investigate the phase transition
  - Method is not yet calibrated, but could provide sign of  $dT/dP$
- Experiments on hydrogen
  - Attempt to observe pressure difference for the transition due to zero-point energy effects

## Experiment Design/Analysis

Marcus Knudson

Ray Lemke

Kyle Cochrane

Devon Dalton

Dustin Romero

## Diagnostics

Charlie Meyer

Jeff Gluth

Devon Dalton

Anthony Romero

Dave Bliss

Alan Carlson

# Acknowledgements

## QMD Calculations

Mike Desjarlais

Andreas Becker

Winfried Lorenzen

Ronald Redmer

## Planetary Modeling

Nadine Nettelmann

Andreas Becker

Ronald Redmer



## Pulse Shaping

Ray Lemke

Jean-Paul Davis

Mark Savage

Ken Struve

Keith LeChien

Brian Stoltzfus

Dave Hinshelwood

Entire Z crew

University of Rostock