SAND2024-16382C

Shock-ramp compression of MgO up to 390 GPa on Sandia's Z Machine

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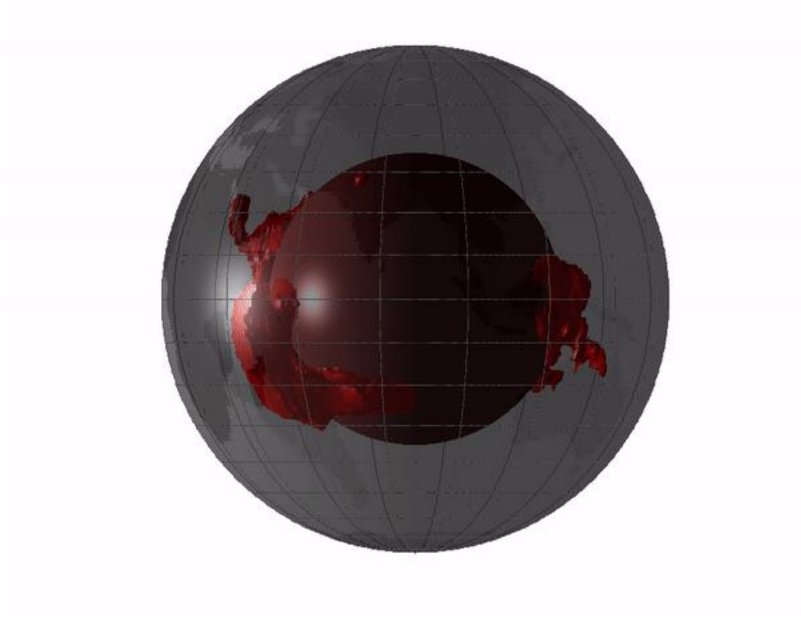
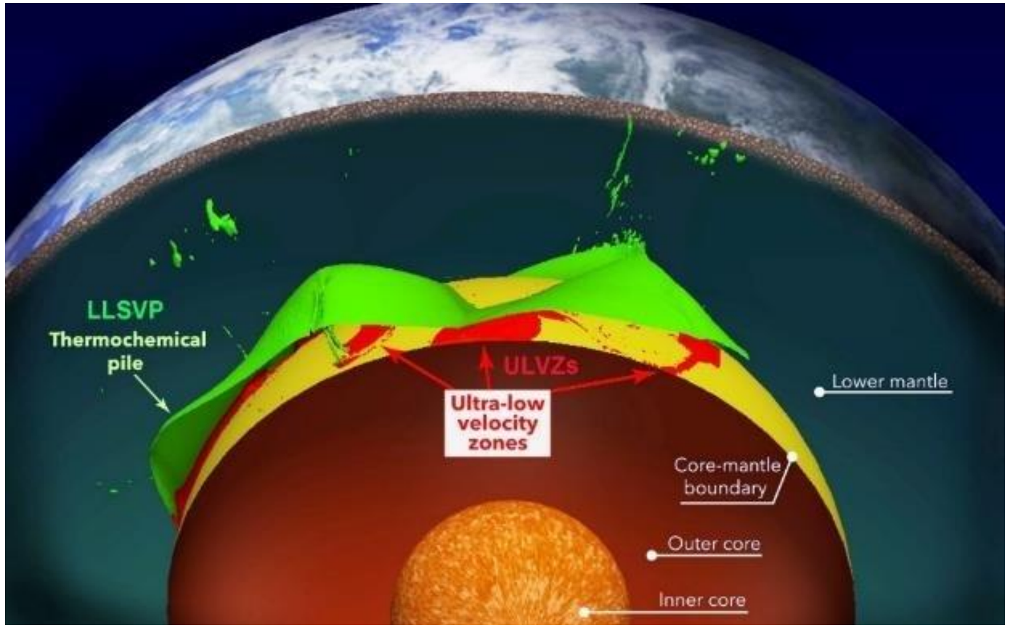
Why study MgO up to Earth's core conditions?

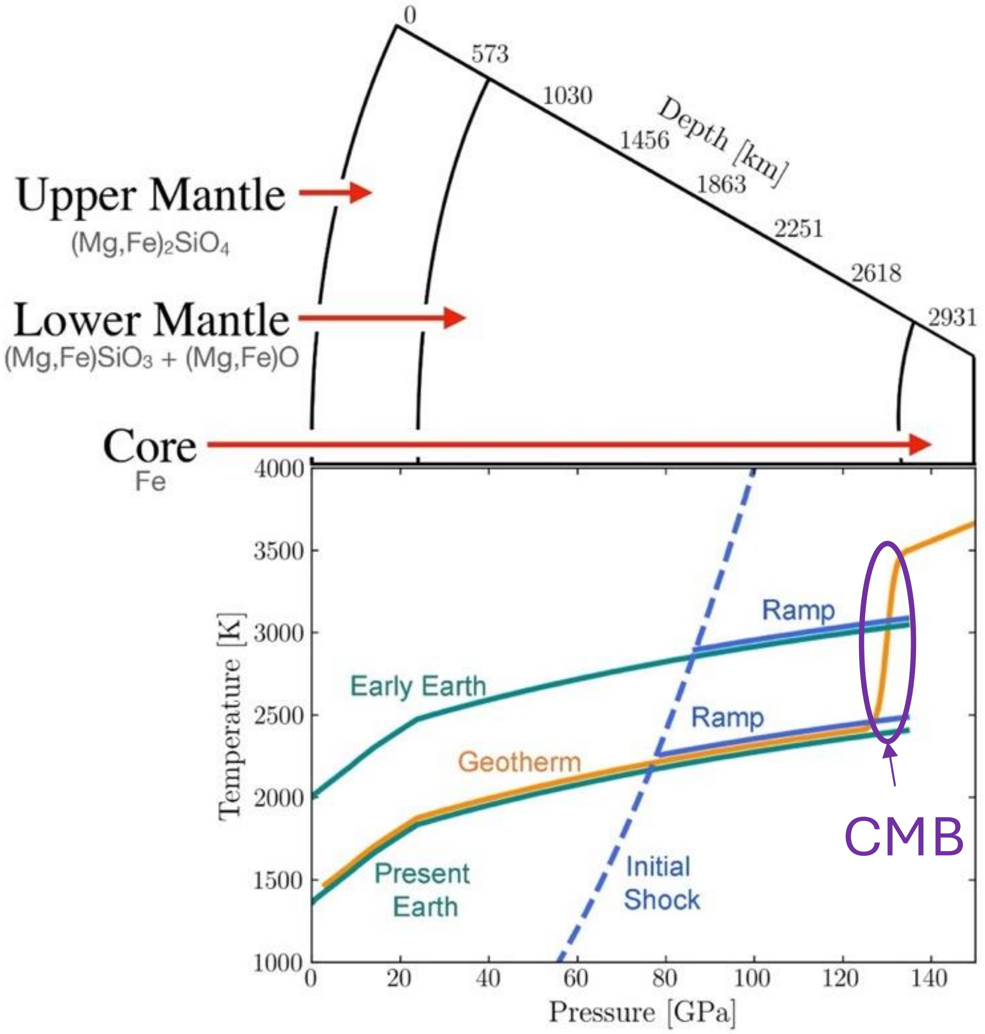


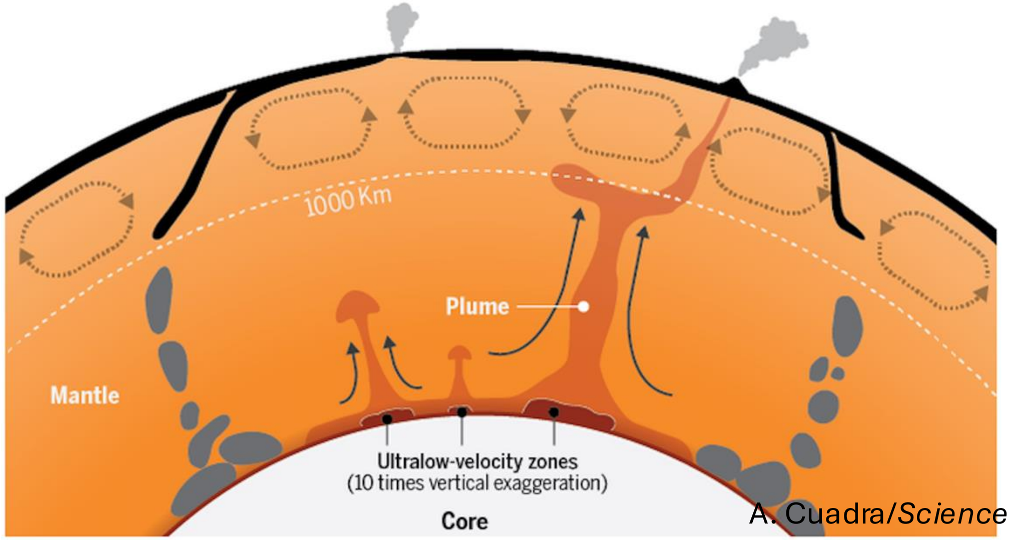
Credit: Sanne Cottaar



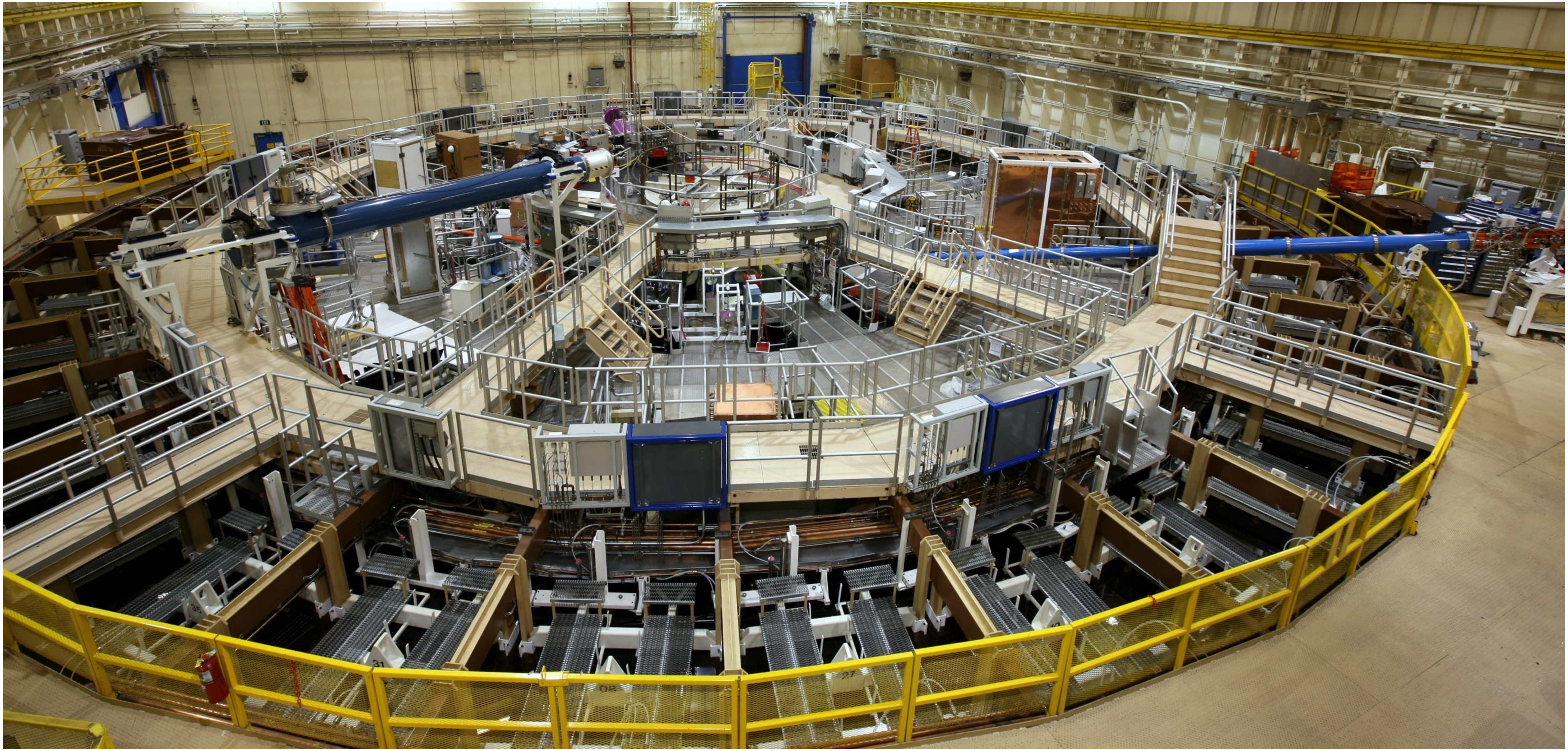
Cutaway of Earth's interior showing schematic locations of an LLSVP and ULVZs on the core-mantle boundary. Image courtesy of E. Garnero/M. Li, ASU.

MgO & (Mg,Fe)O shock-ramp experiments on Z





- *Motivation*: Can Fe-enrichment account for Earth's ULVZs?
- *Goal*: First direct measurements of sound speeds of (Mg,Fe)O following isentropic paths similar to the geotherm



DFT calculations guiding shock and ramp

Josh Townsend

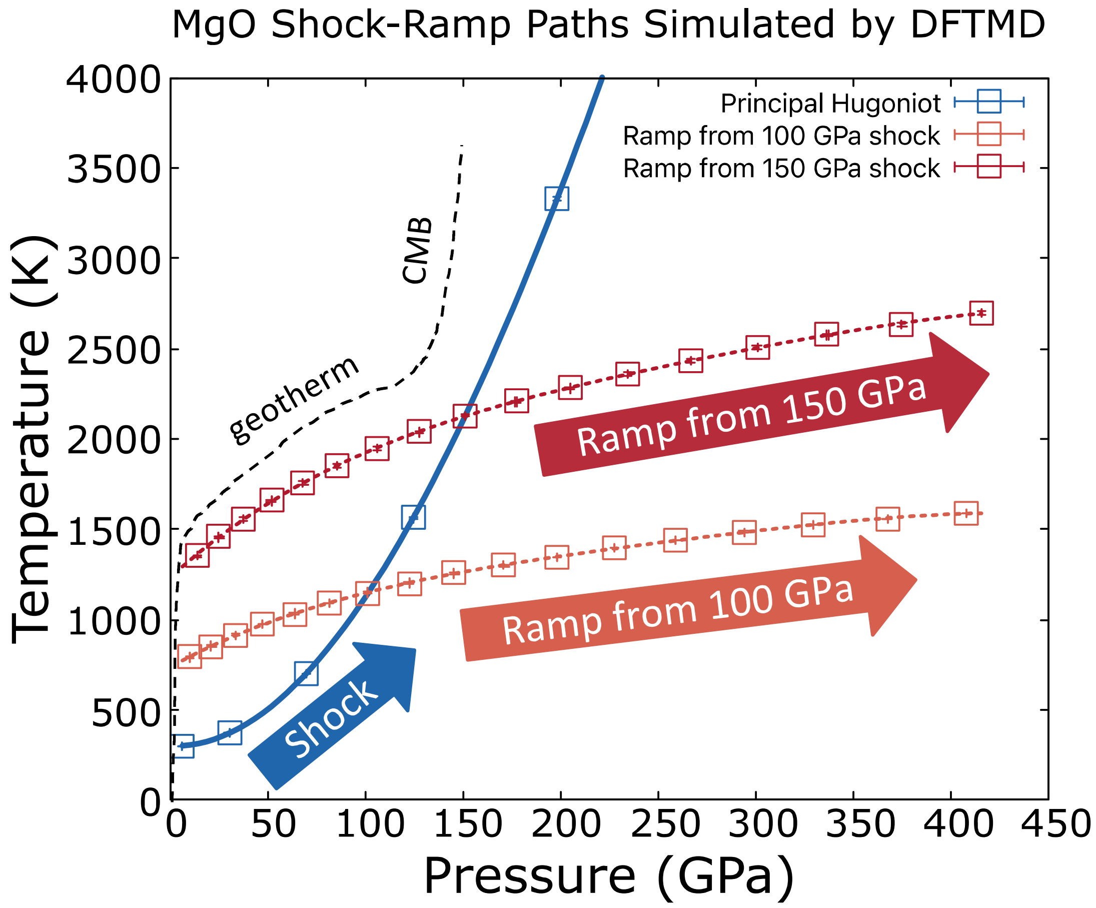
- MgO B1
- MD calculations using Quantum Espresso
- 64 atoms supercell

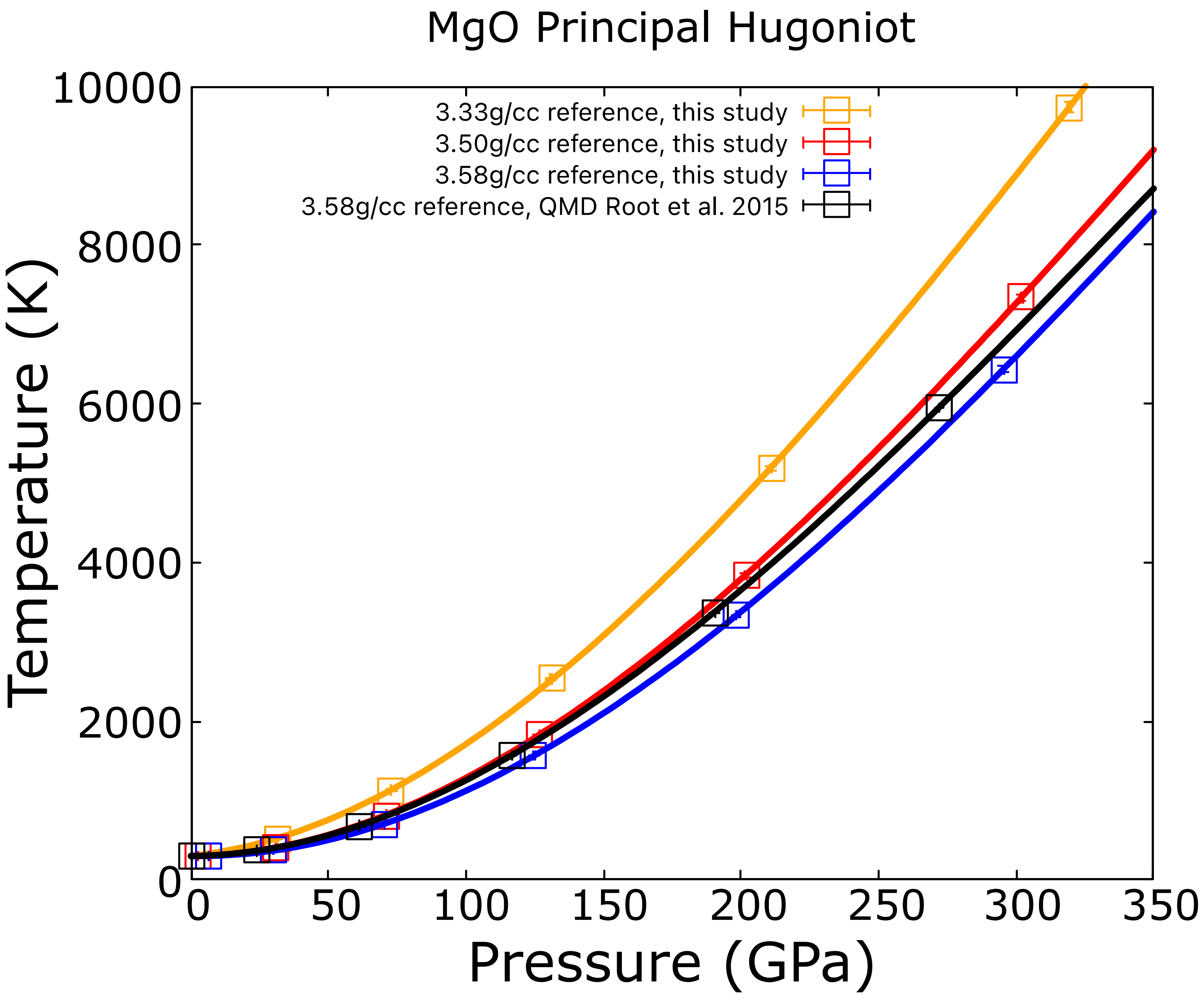
<u>Rankine-Hugoniot relations</u>

$\rho_0 U_S = \rho(U_S - u_p)$

$P - P_0 = \rho_0 (U_S - u_0)(u_p - u_0)$

$E - E_0 = 1/2(P + P_0)(V - V_0)$

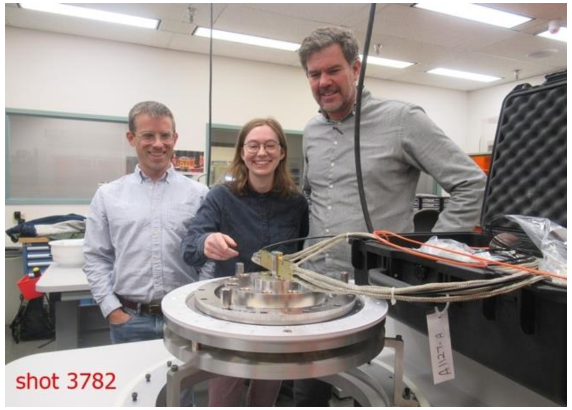


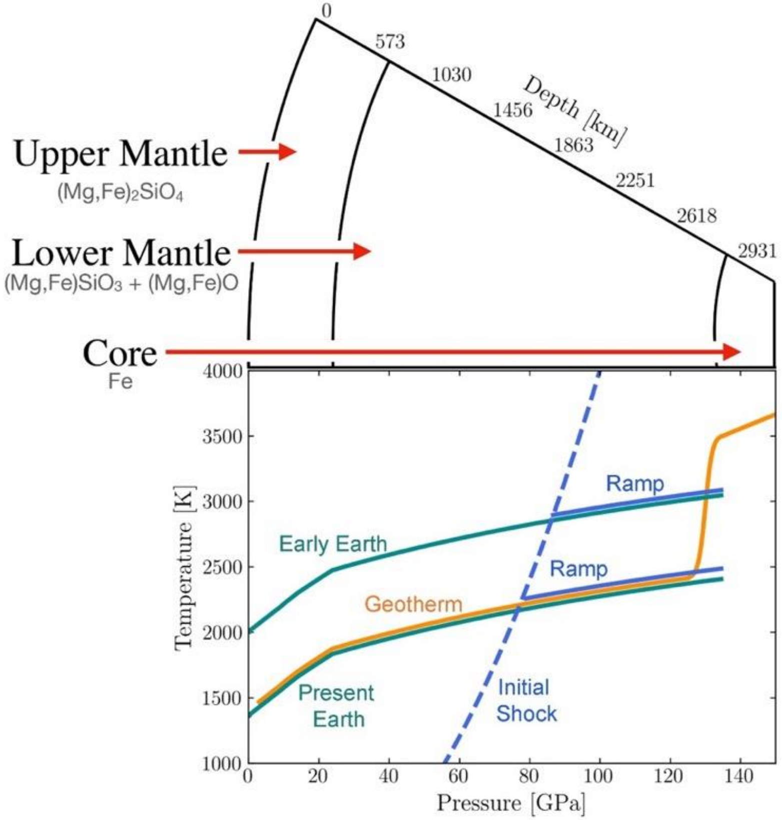

MgO Principal Hugoniot
3.33g/cc reference, this study
3.50g/cc reference, this study
3.58g/cc reference, this study
3.58g/cc reference, QMD Root et al. 2015
Temperature (K)
Pressure (GPa)
0
2000
4000
6000
8000
10000
0
50
100
150
200
250
300
350

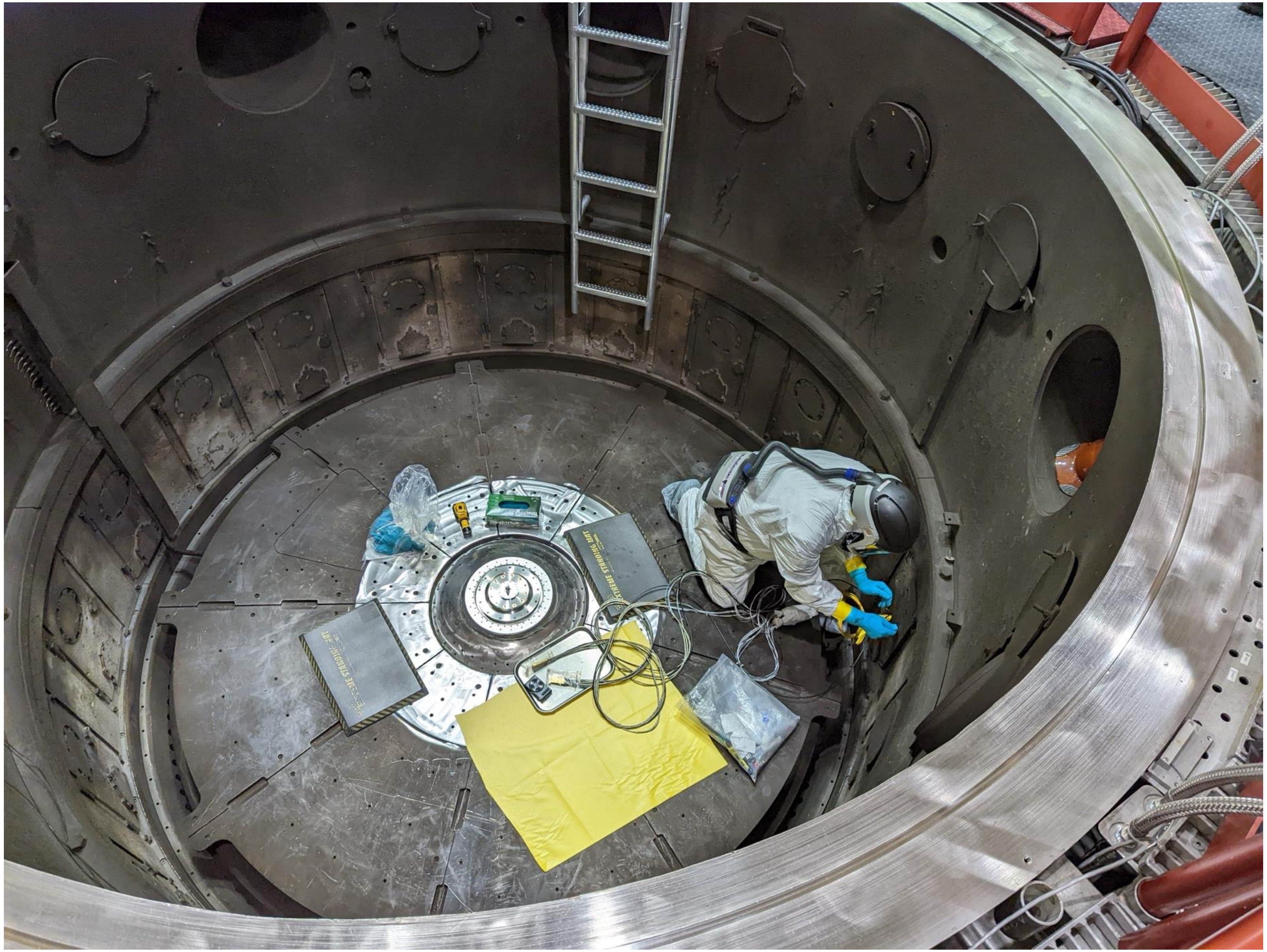
Z experiments

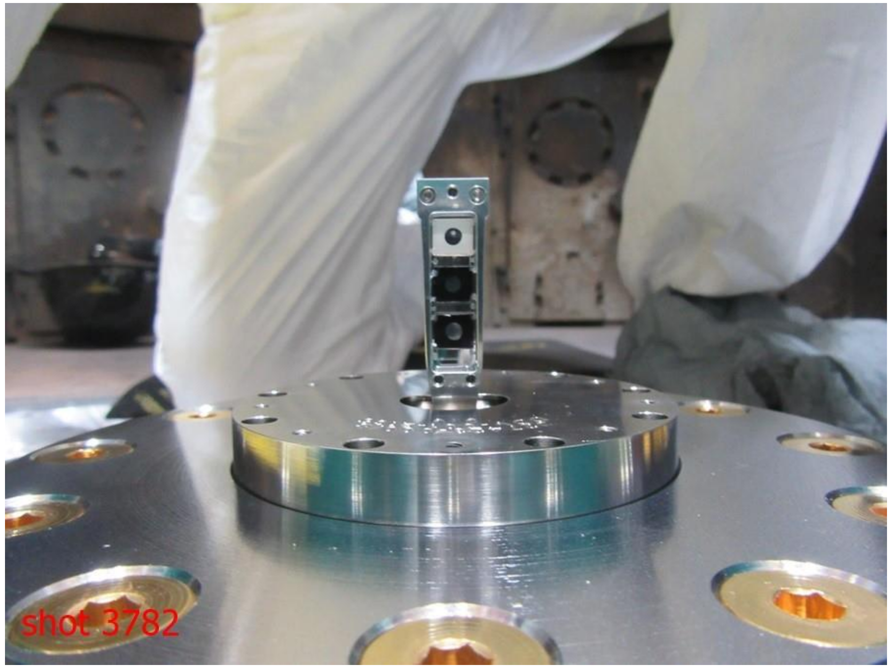
fp0	fp25	fp50
MgO	$(Mg_{0.75}Fe_{0.25})O$	$(Mg_{0.5}Fe_{0.5})O$
End Member	Bulk Mantle	Fe-enriched

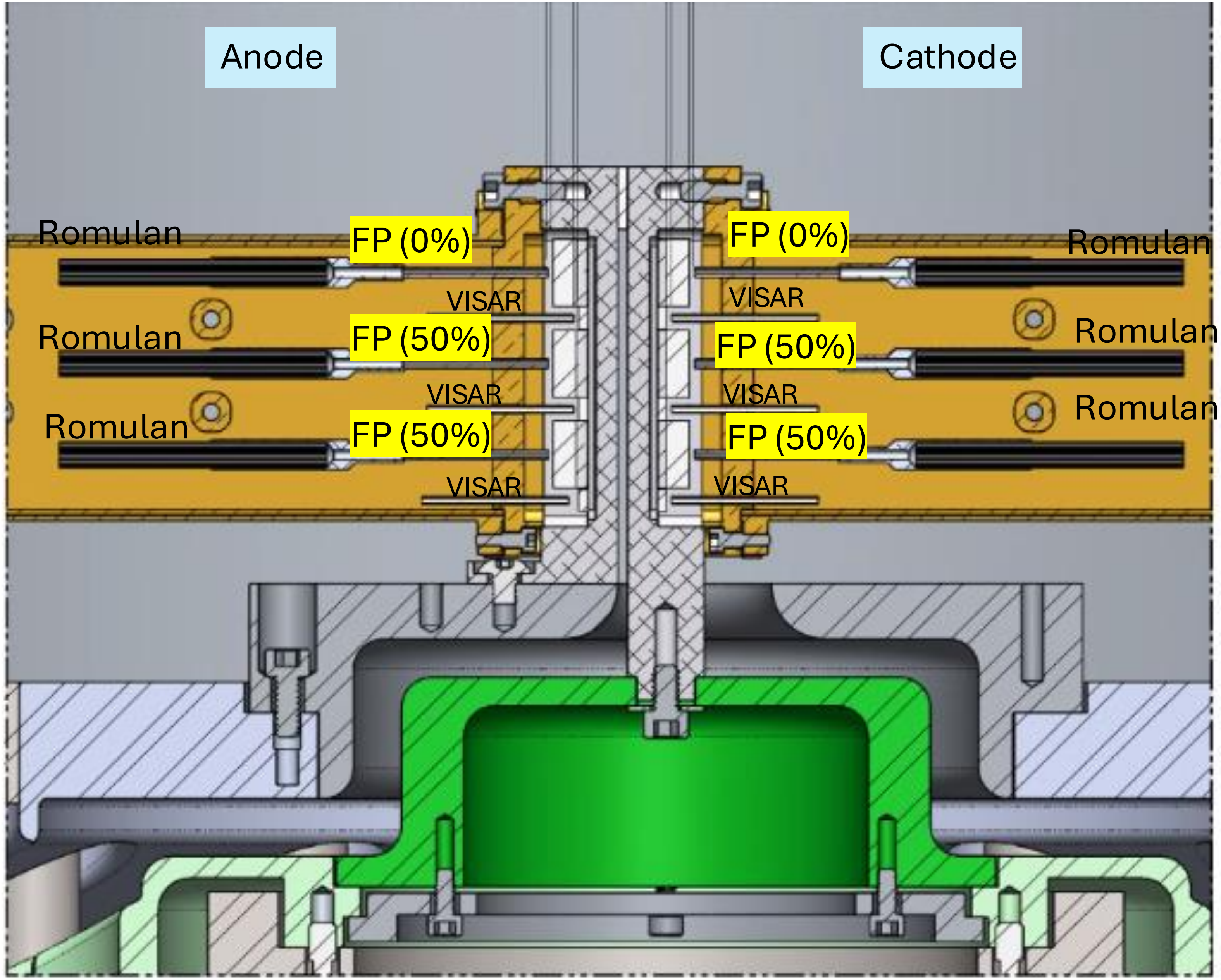
experiment	shock pressure	compositions
Z3894	90 GPa	fp50 & MgO
Z3809	90 GPa	fp25 & MgO
Z3865	150 GPa	fp25 & MgO
Z3866	150 GPa	fp50 & MgO

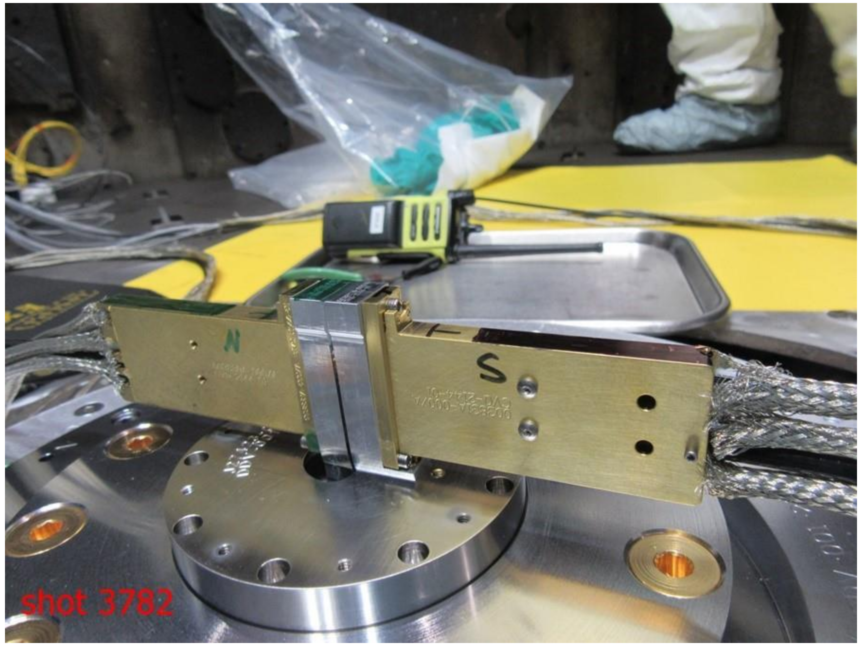




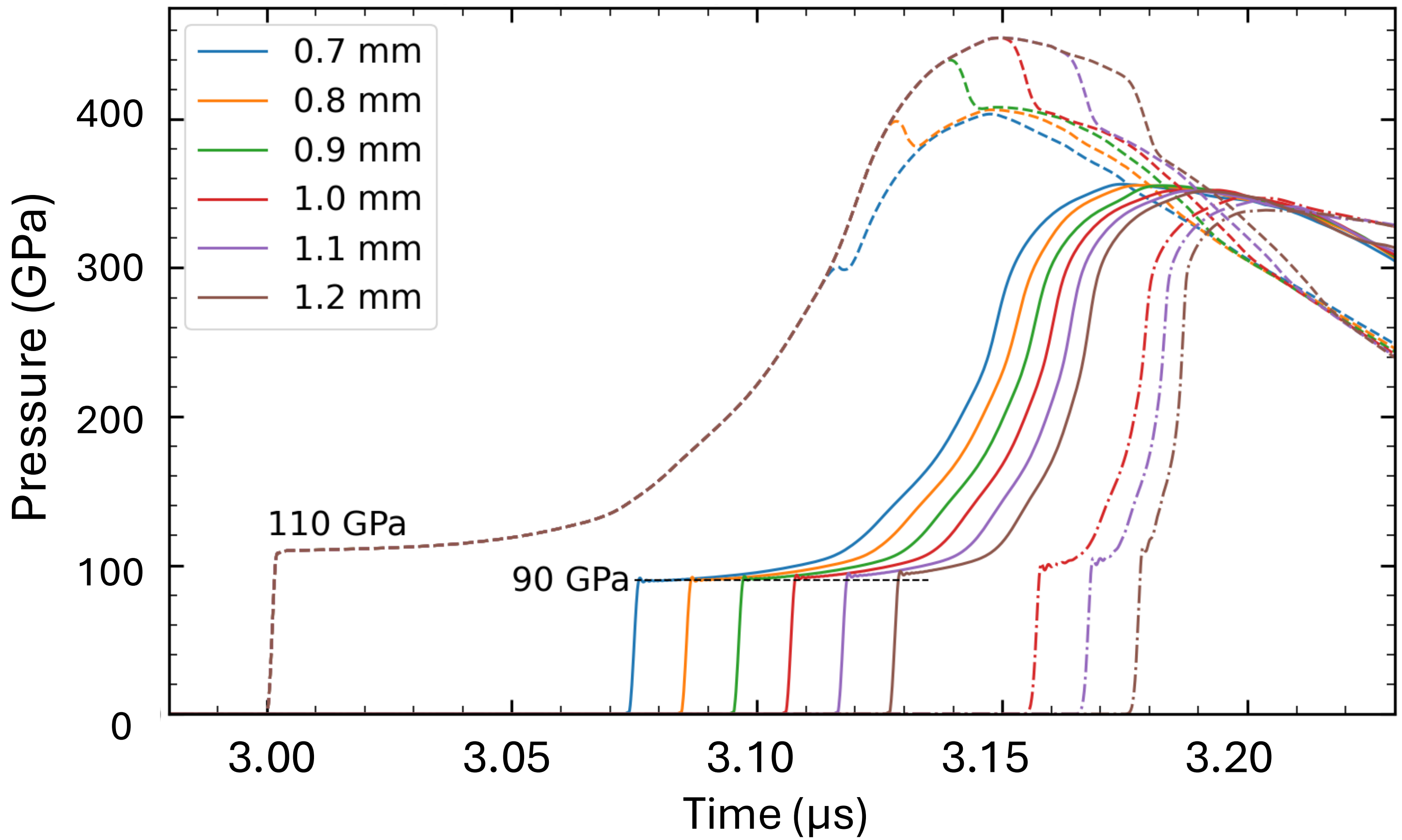



shot 3782


Anode
Cathode
Romulan
FP (0%)
FP (0%)
Romulan
VISAR
VISAR
Romulan
FP (50%)
FP (50%)
Romulan
VISAR
VISAR
Romulan
FP (50%)
FP (50%)
Romulan
VISAR
VISAR


shot 3782

Predicting shock-ramp path

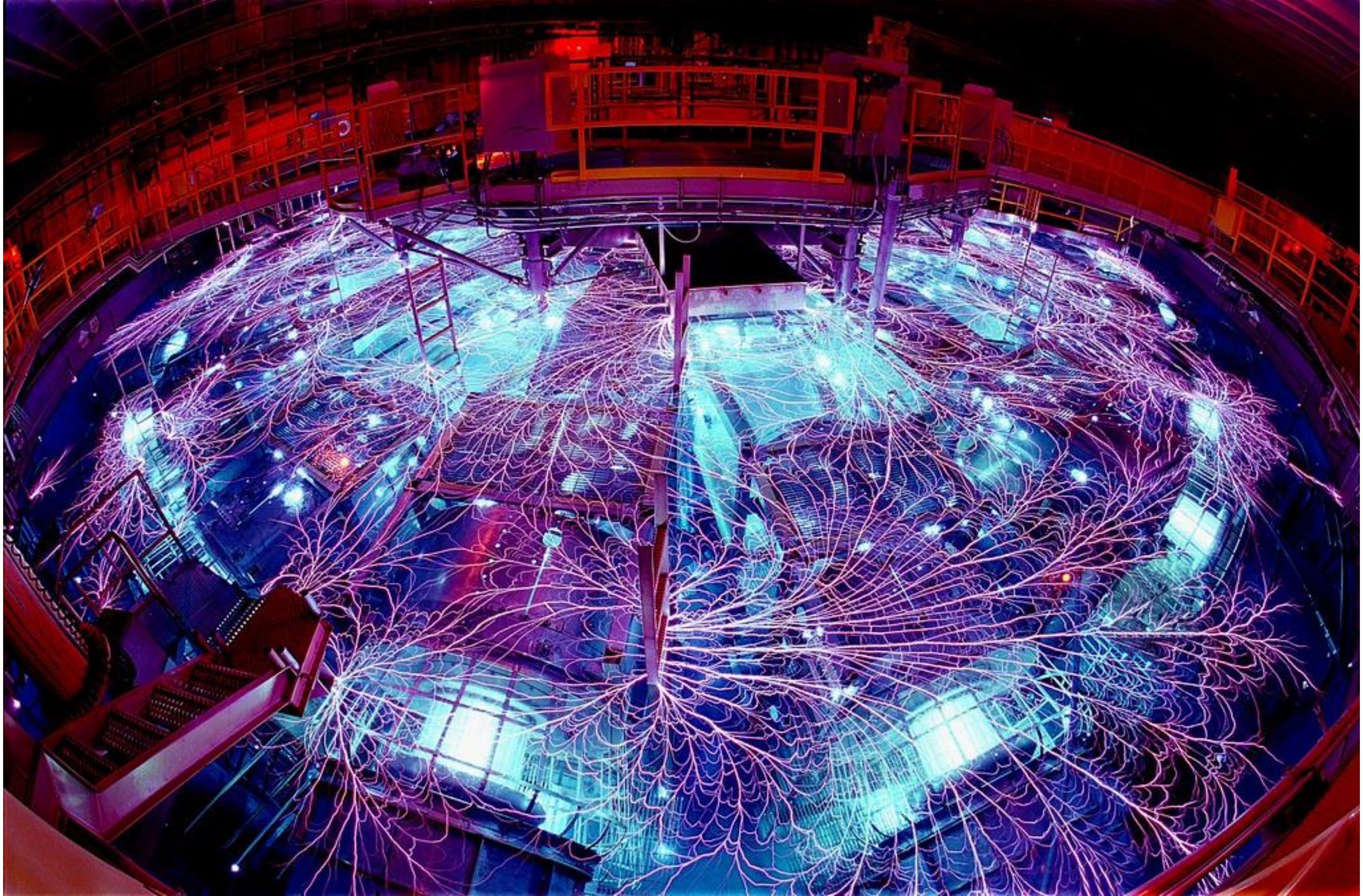


Jean-Paul Davis

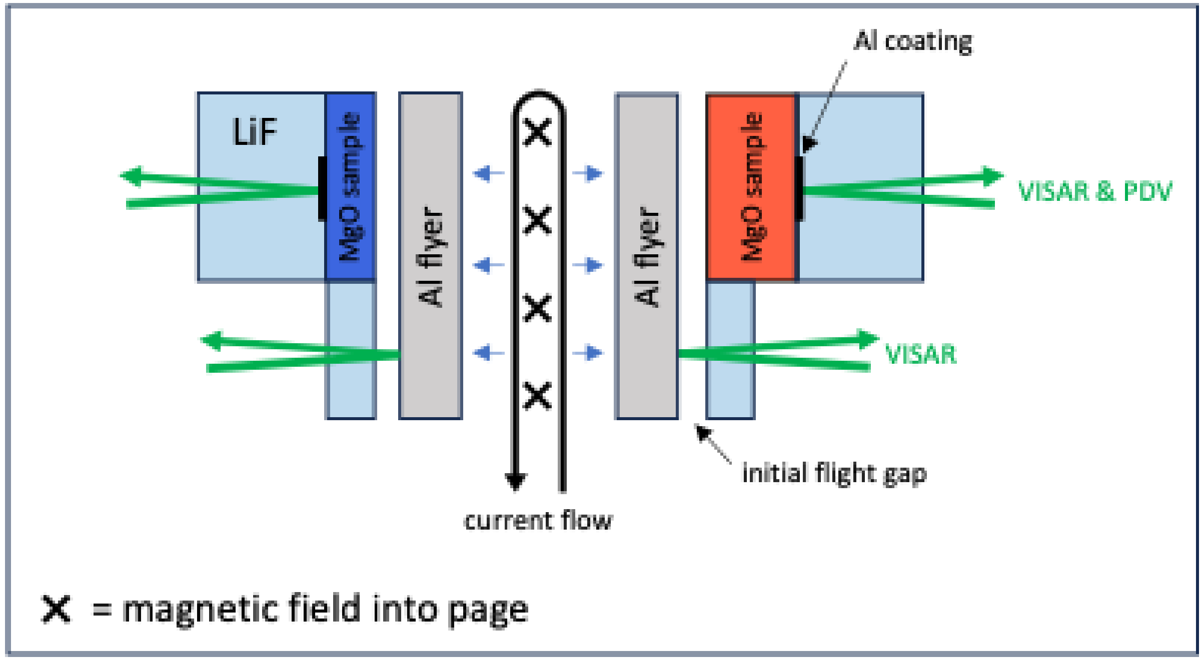
Sakun Duwal

Prediction:

- **Shock to ~90 GPa**
- **Ramp to ~ 350 GPa**



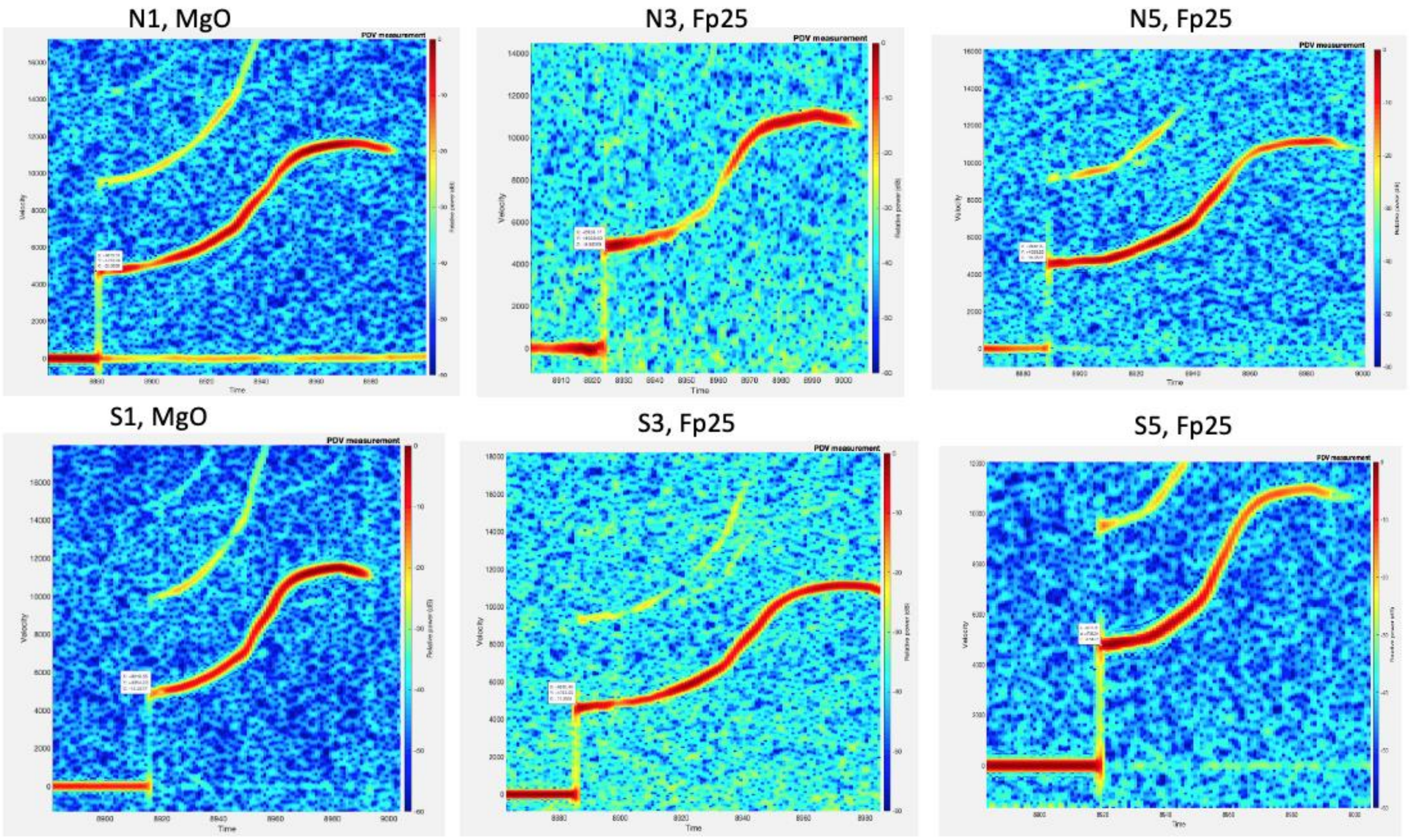
Measurements on the Z machine

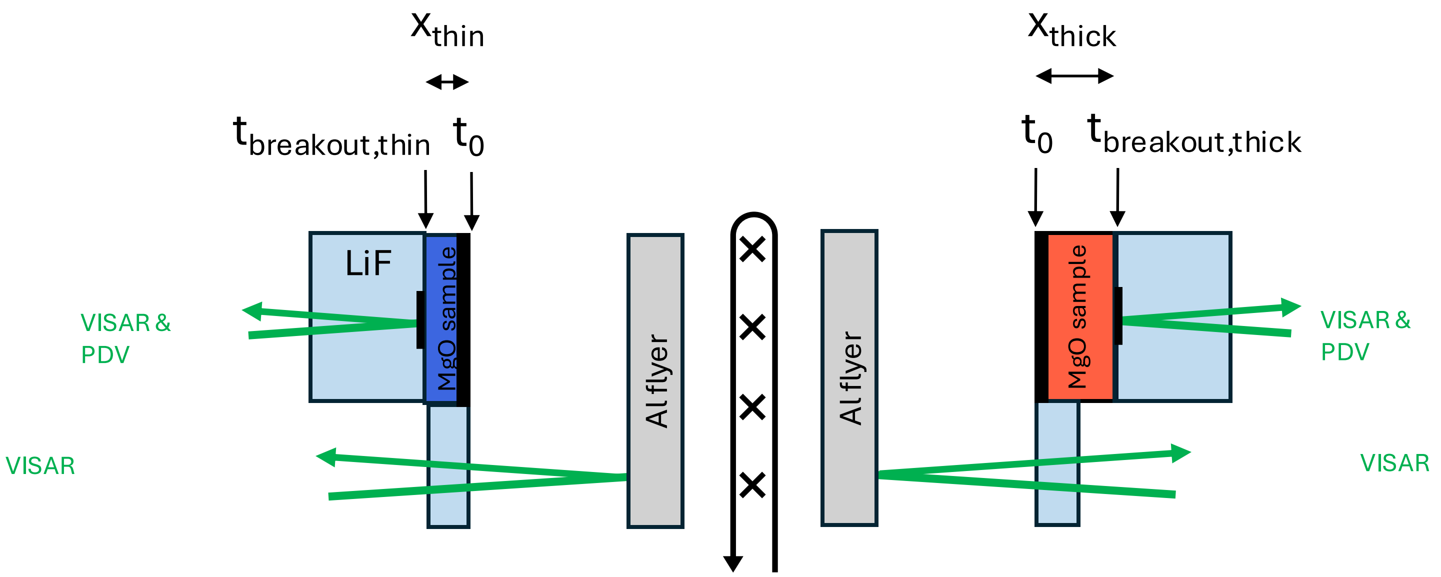


Diagnostics

- Velocity interferometer system for any reflector (VISAR)
- Photon Doppler velocimetry (PDV)

PDV velocimetry profiles

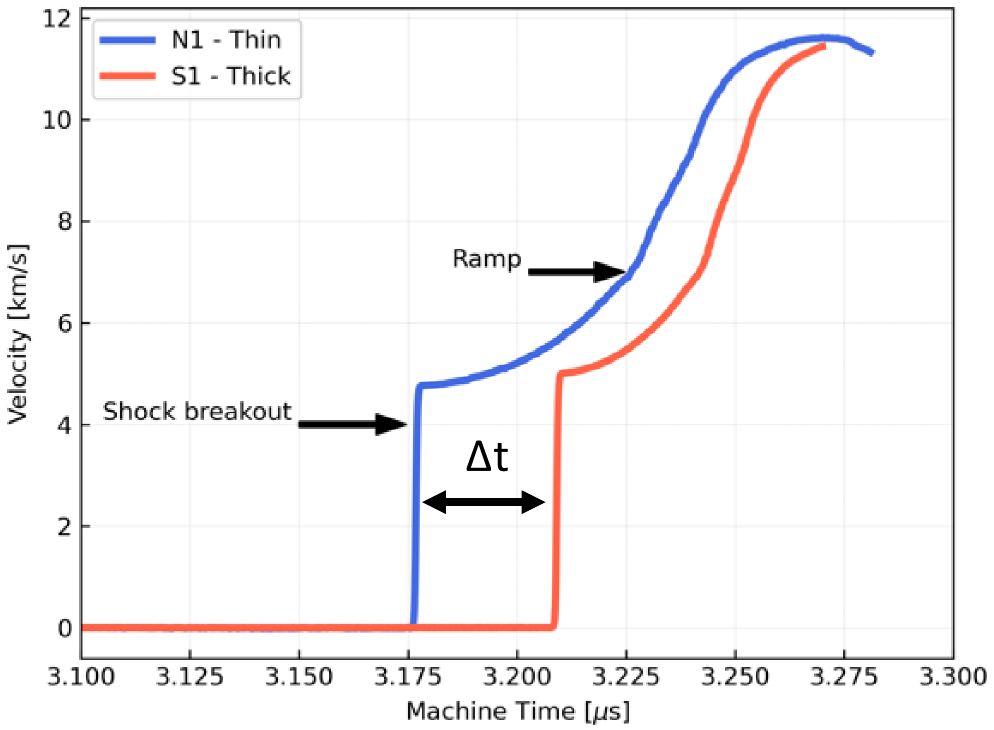


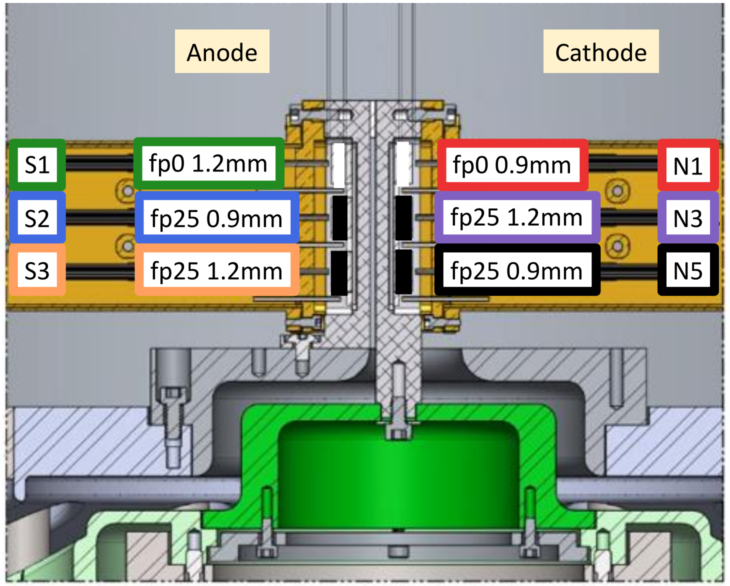


$$u_s = \frac{\Delta x}{\Delta t}$$

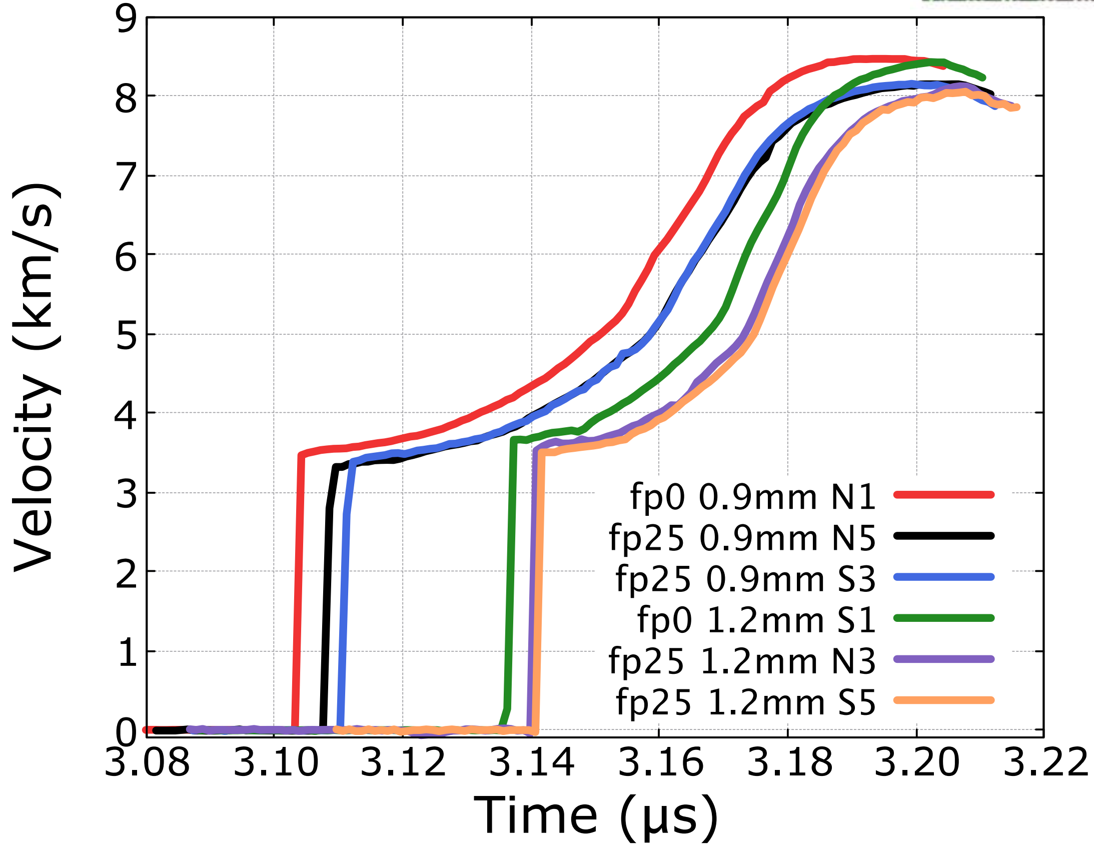
$\Delta t = t_{breakout,thick} - t_{breakout,thin}$

Δx = thick sample thickness – thin sample thickness

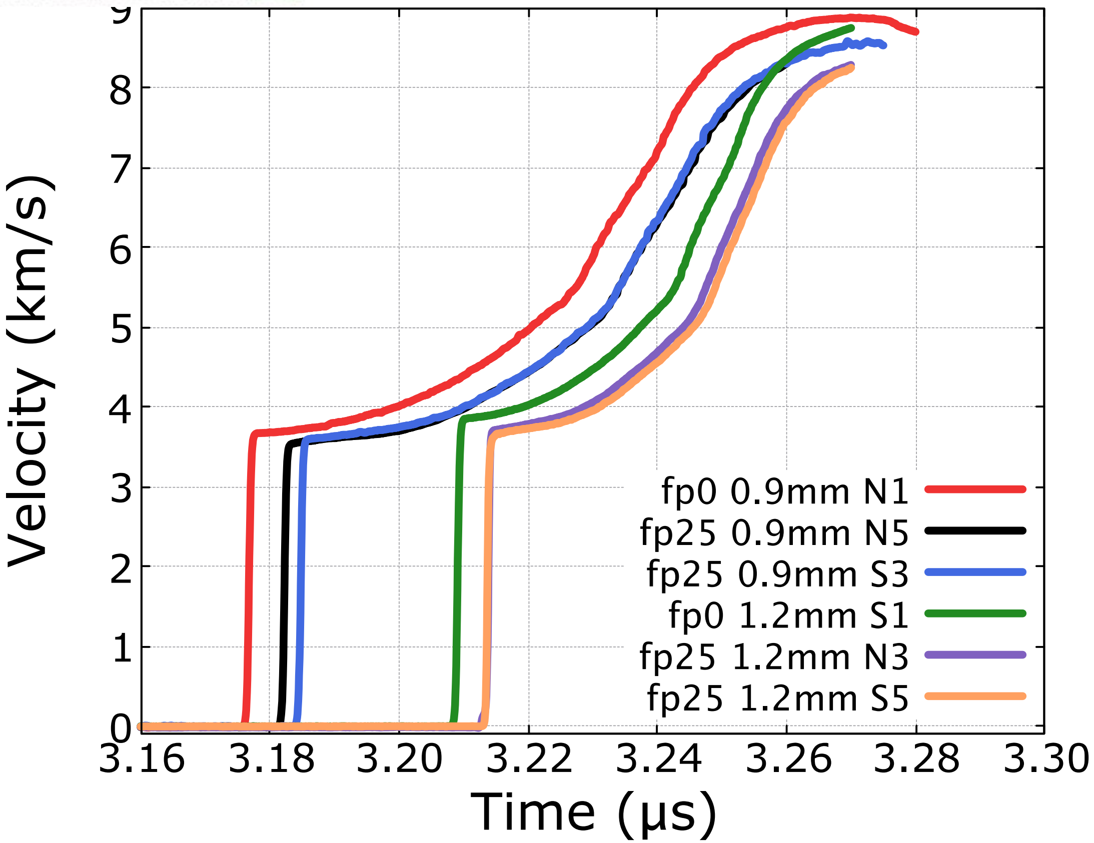



Anode
Cathode
S1
fp0 1.2mm
S2
fp25 0.9mm
S3
fp25 1.2mm
fp0 0.9mm
N1
fp25 1.2mm
N3
fp25 0.9mm
N5

PDV

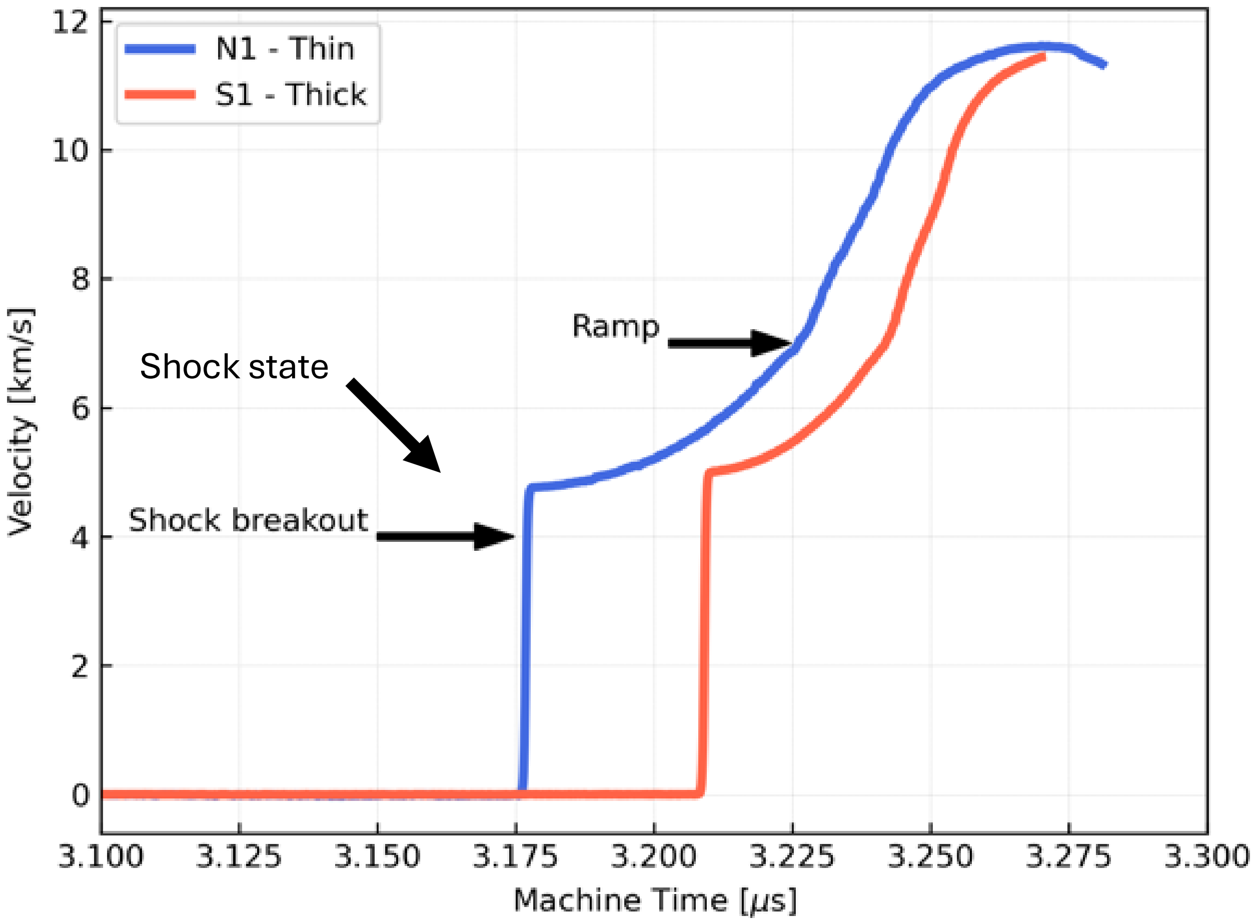

Velocity (km/s)
Time (μs)
0
1
2
3
4
5
6
7
8
9
3.08
3.10
3.12
3.14
3.16
3.18
3.20
3.22
fp0 0.9mm N1
fp25 0.9mm N5
fp25 0.9mm S3
fp0 1.2mm S1
fp25 1.2mm N3
fp25 1.2mm S5

VISAR


Velocity (km/s)
Time (μs)
0
1
2
3
4
5
6
7
8
3.16
3.18
3.20
3.22
3.24
3.26
3.28
3.30
fp0 0.9mm N1
fp25 0.9mm N5
fp25 0.9mm S3
fp0 1.2mm S1
fp25 1.2mm N3
fp25 1.2mm S5

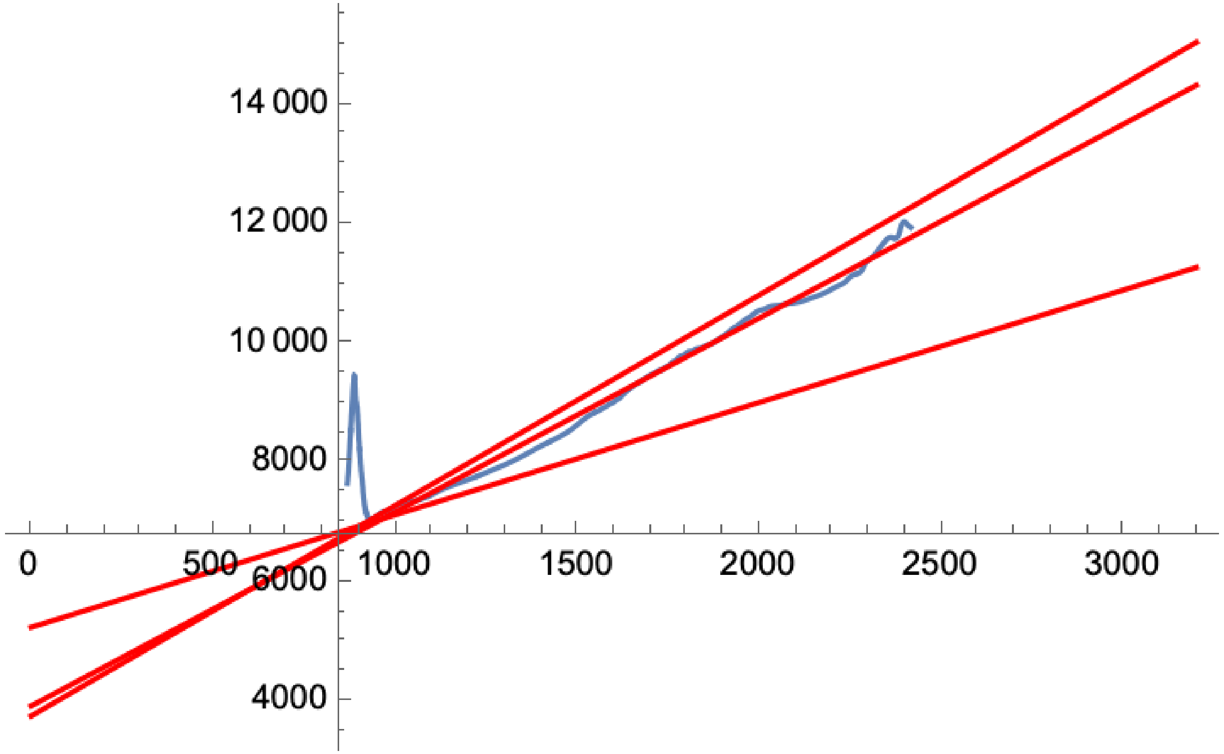
Velocimetry analysis

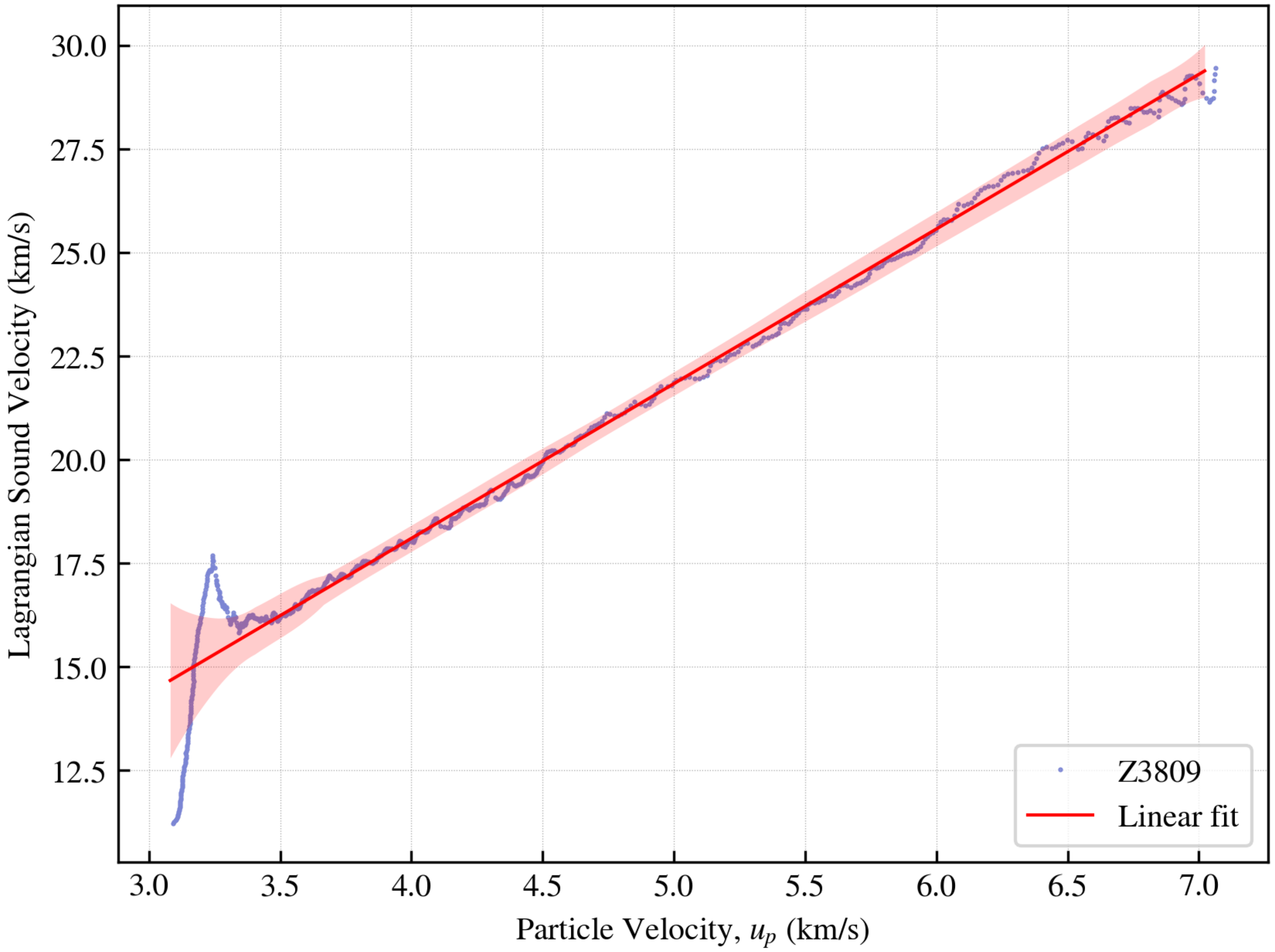
- Average PDV and VISAR data to minimize uncertainty
- Correct velocities for the LiF windows
- Calculate the shock state given a Hugoniot state guess
  - This is the state that we begin the ramp and Lagrangian analysis



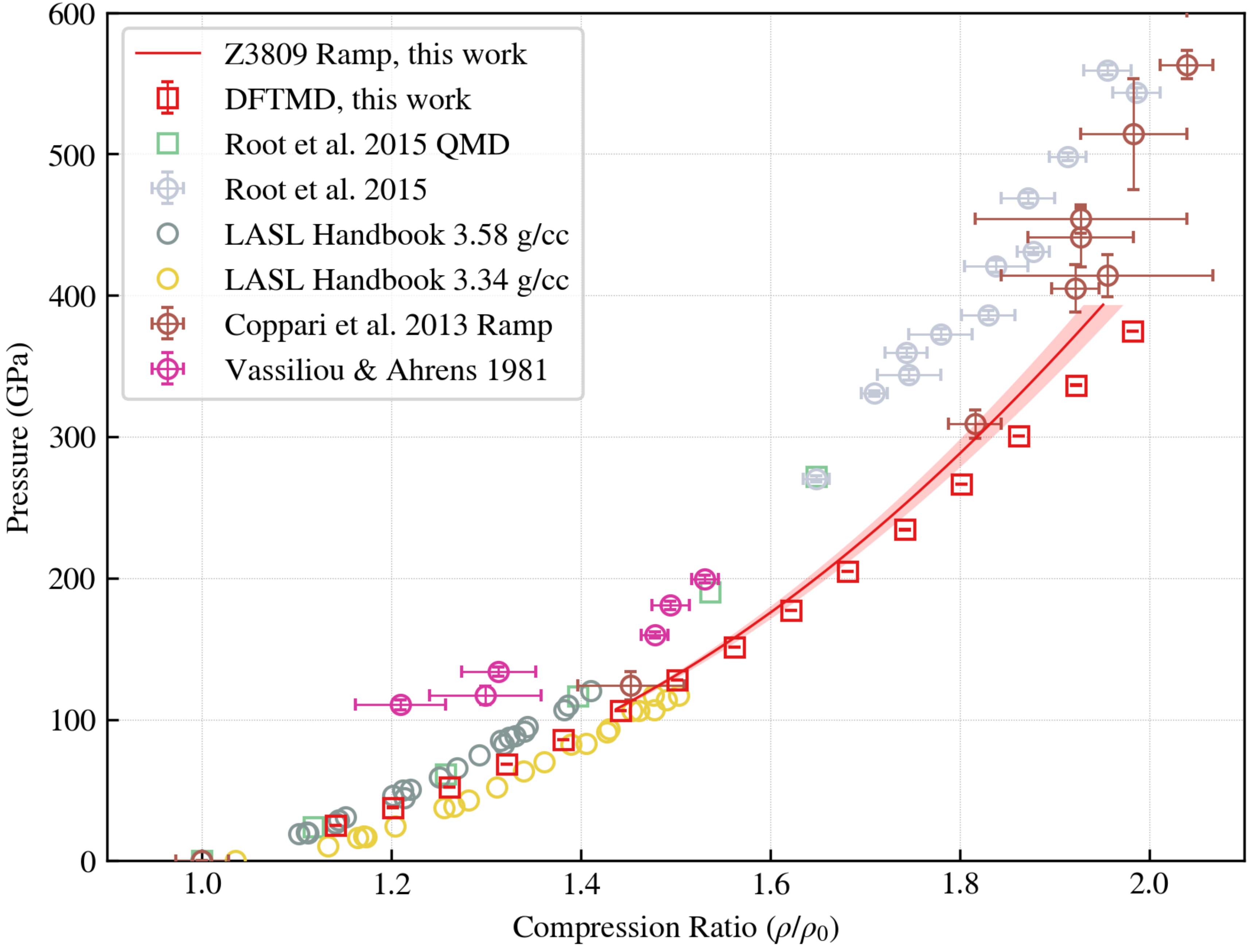
Iterative Lagrangian Analysis (ILA)

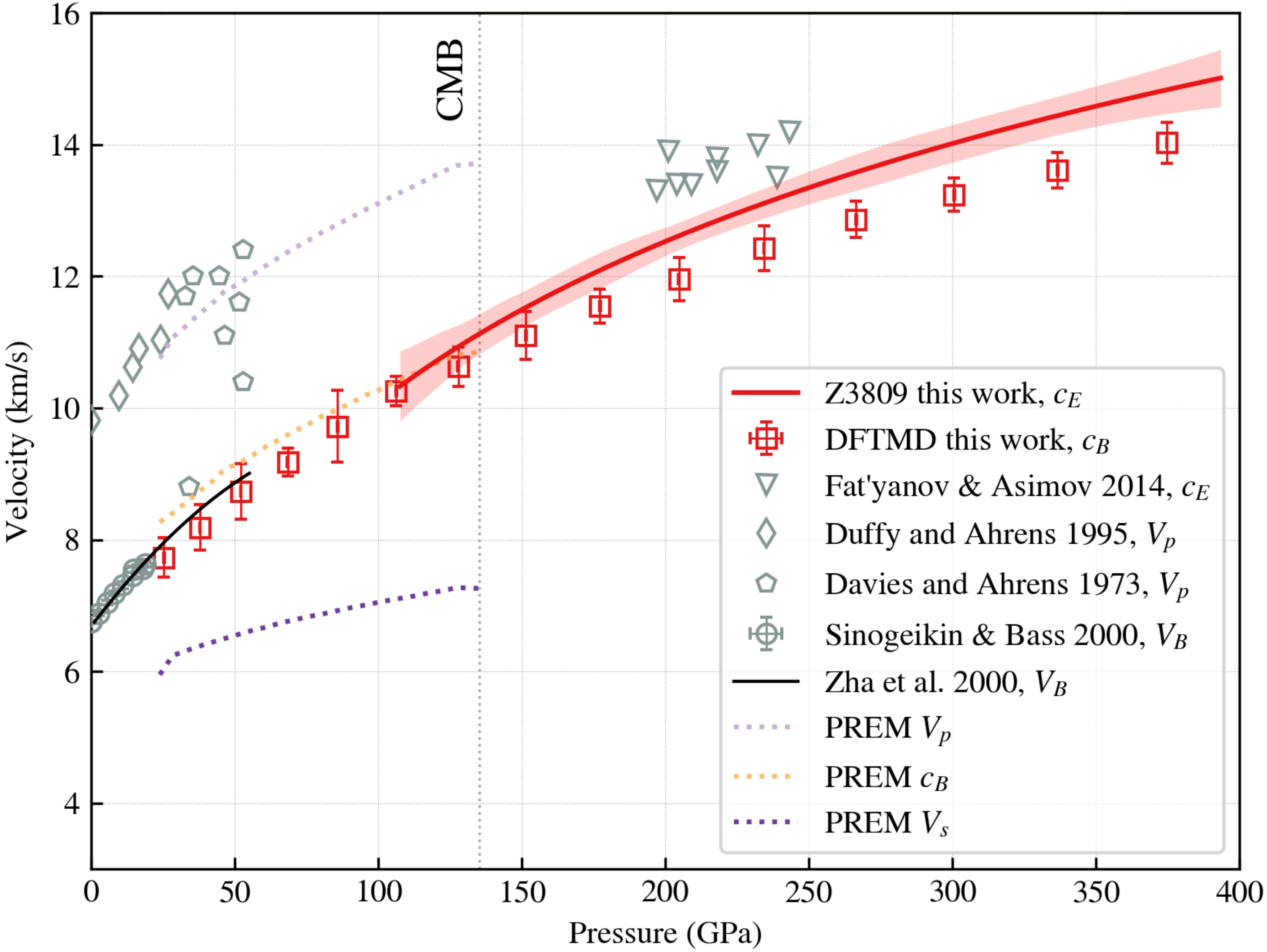
- Lagrangian Analysis
- Reiterate until minimal change in EOS for each iteration





Lagrangian Sound Velocity (km/s)
Particle Velocity, u_p (km/s)
30.0
27.5
25.0
22.5
20.0
17.5
15.0
12.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
Z3809
Linear fit


Z3809 Ramp, this work
DFTMD, this work
Root et al. 2015 QMD
Root et al. 2015
LASL Handbook 3.58 g/cc
LASL Handbook 3.34 g/cc
Coppari et al. 2013 Ramp
Vassiliou & Ahrens 1981
Pressure (GPa)
Compression Ratio (ρ/ρ_0)
0
100
200
300
400
500
600
1.0
1.2
1.4
1.6
1.8
2.0



CMB
Velocity (km/s)
Pressure (GPa)
0
50
100
150
200
250
300
350
400
4
6
8
10
12
14
16
Z3809 this work, c_E
DFTMD this work, c_B
Fat'yanov & Asimov 2014, c_E
Duffy and Ahrens 1995, V_p
Davies and Ahrens 1973, V_p
Sinogeikin & Bass 2000, V_B
Zha et al. 2000, V_B
PREM V_p
PREM c_B
PREM V_s