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**Extreme Material
Dynamics Experiments
on SNL's Z Machine**



Dr. P. Kalita

**Joint CDAC & CMEC
Invited Seminar**

02-22-23



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Acknowledgments

- EOS design: S. D. Crockett & S. P. Rudin – LANL
- AIMD calculations: K. R. Cochran – SNL

SNL Management: C. Seagle, T. Mattsson, D. Sinars

Z machine:

- **Z Experiments: M. Knudson, S. Root, T. Ao – SNL**
- **Z hardware design: C. Blada, J. Jackson**
- **Z pulsedshaping: H. Hanshaw**
- **Z Velocimetry: E. Scoglietti, J. Gluth,**
- **Z Target Fabrication Team: G. Smith, J. Taylor, A. Romero**
- **Z Machine Operations Team**

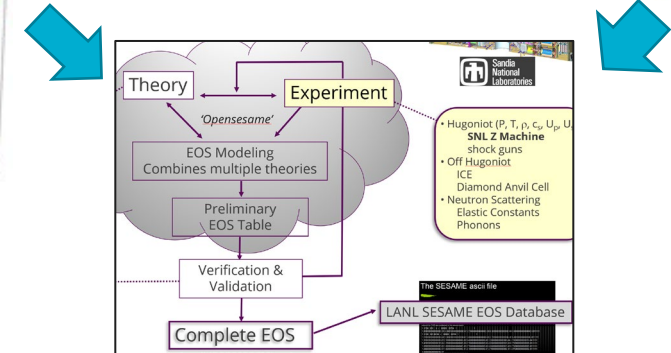
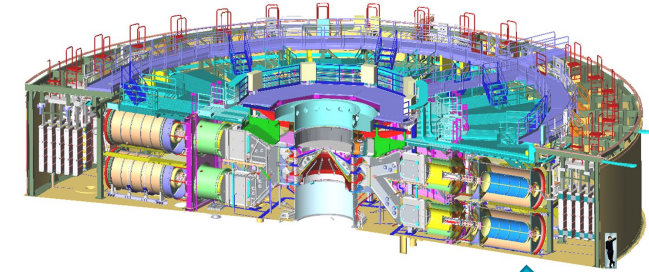
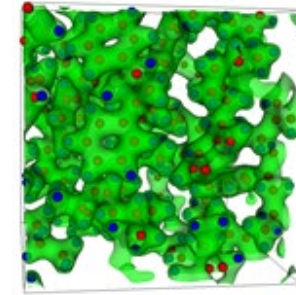
SNL is managed by NTESS, LLC under contract DE-NA0003525.

Work at Los Alamos National Laboratory is supported by the US DOE through contract number 89233218NCA000001.



Outline

- Intro about SNL
- Shock compression
- Z machine and shock experiments
- E.g. 1: Shock and re-shock of PMMA polymer to 1 TPa
- E.g. 2: Platinum as a shock standard to 2 TPa.
- E.g. 3: Ti64 alloy shocked to 1.2 TPa and a broad range EOS



Equation of State: In physics and thermodynamics, an EOS is a constitutive equation describing the state of matter under a given set of physical conditions. It provides a mathematical relationship between two or more of that matter's state functions, such as its temperature, pressure, volume, or internal energy.

<https://www.lanl.gov/org/ddste/alldsc/theoretical/physics-chemistry-materials/sesame-database.php>

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A federally funded research and development center managed and operated by National Technology & Engineering Solutions of Sandia, LLC.

Sandia is the largest of the 17 U.S. Department of Energy's national laboratories

- ~14,920 employees in FY21
- >13,000 located in Albuquerque, New Mexico, USA
- ~1800 located in Livermore, California, USA
- ~\$4.5B budget in FY21



ADVANCED SCIENCE & TECHNOLOGY

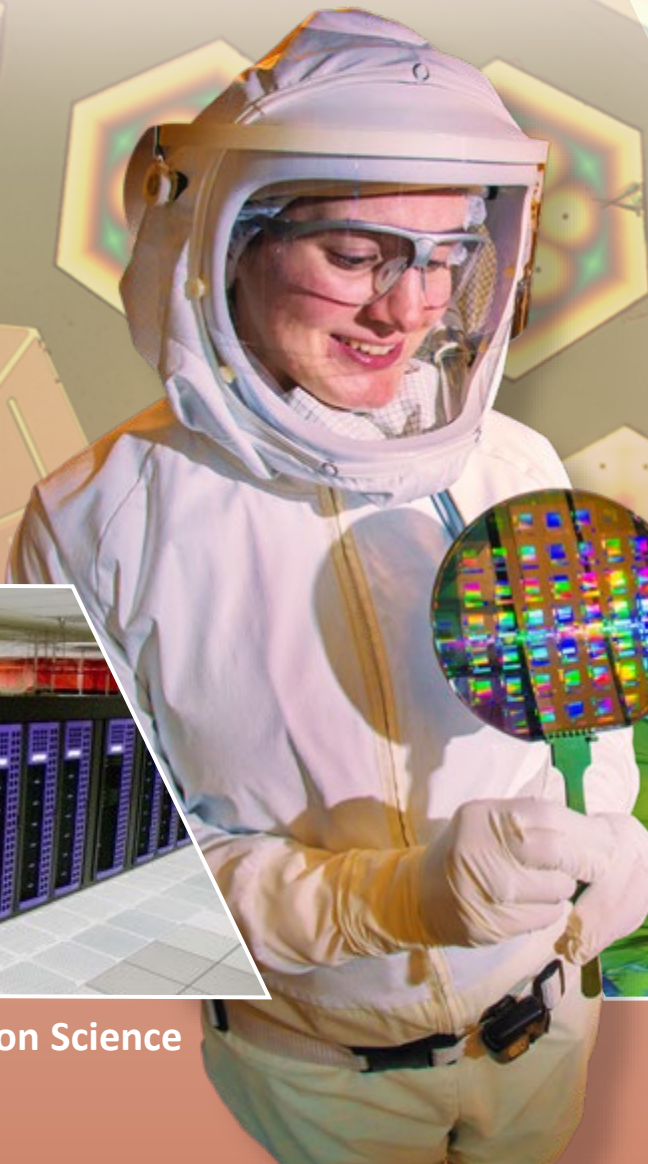


Sandia maintains seven Research Foundations in key areas of science

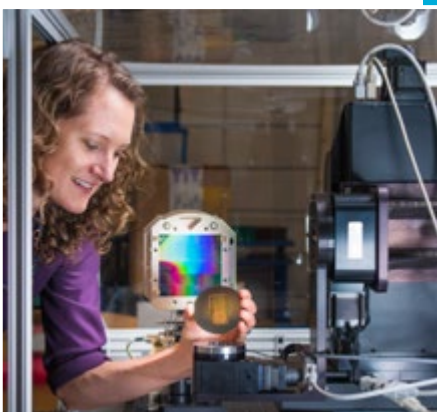
Nanodevices & Microsystems



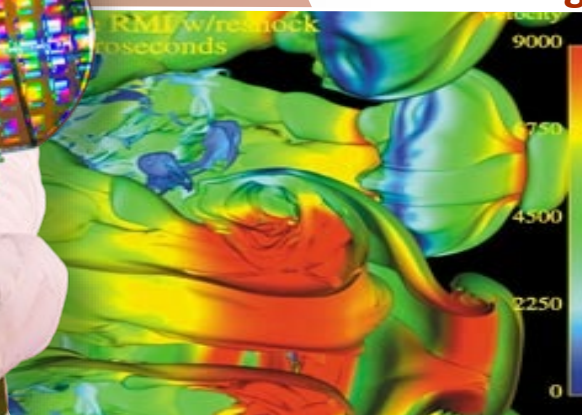
Computing & Information Science



Radiation, Electrical, and High Energy Density Science



Materials Science



Engineering Science

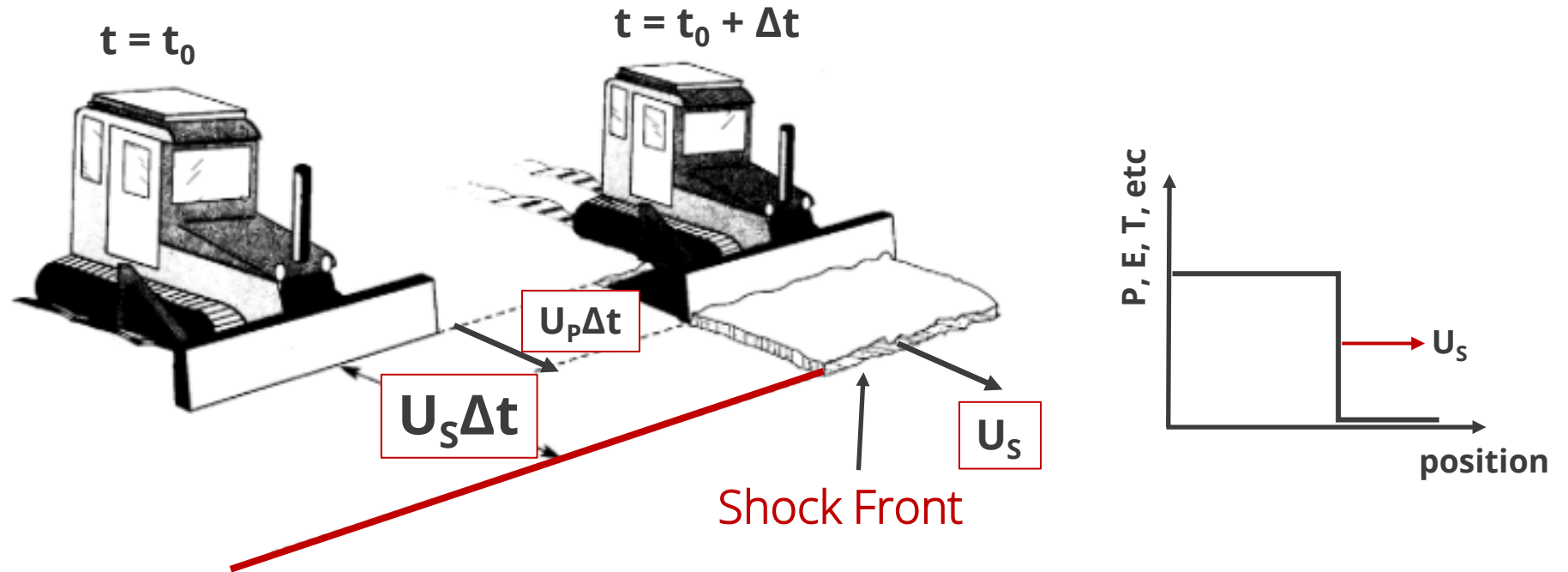


Earth Science



Bioscience

Shock Compression: what is a Shock Wave?



- Shock wave: A propagating discontinuity in pressure, density, energy, etc.
- The pressure, density, energy are increased behind the shock front
- The material velocity behind the shock front is the *particle velocity*, U_p
- **The shock wave velocity, U_s , is greater than the sound speed in the undisturbed material**
- In real life, shock waves are not perfect discontinuities



Shock Event: the Rankine-Hugoniot Equations

Conservation of Mass

$$\rho_0(U_S - U_0) = \rho_1(U_S - U_1)$$

Conservation of Momentum

$$P_1 - P_0 = \rho_0(U_S - U_0)(U_1 - U_0)$$

Conservation of Energy

$$E_1 - E_0 = \frac{1}{2}(P_1 + P_0)(V_0 - V_1)$$

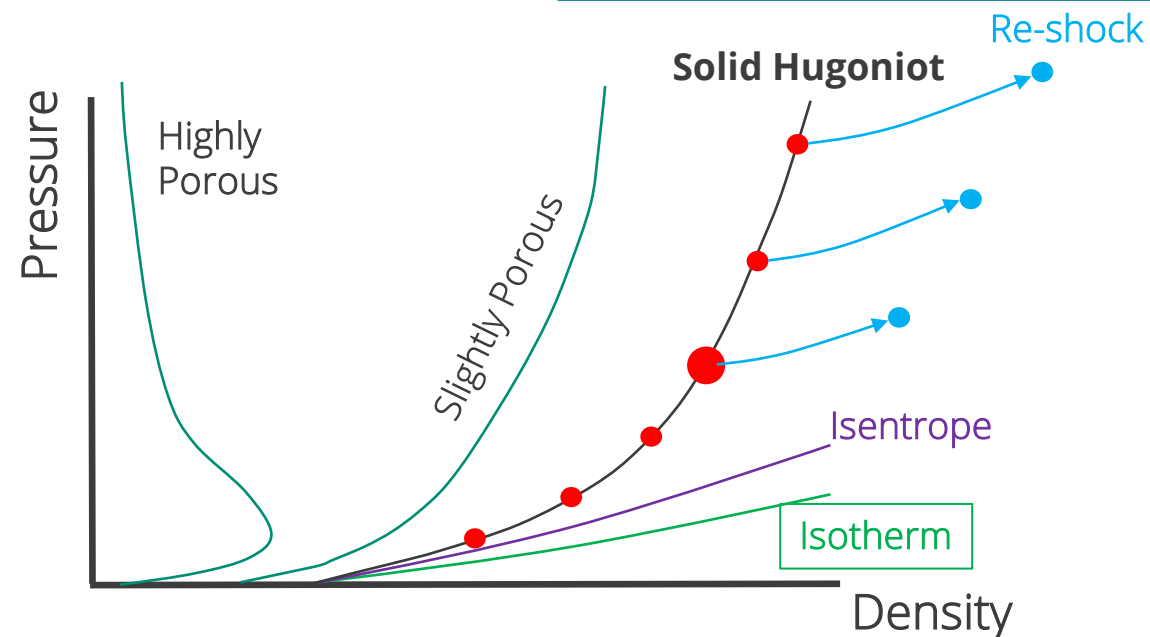
$$U_0, P_0 = 0$$

$$\frac{\rho}{\rho_0} = \frac{U_S}{U_S - U_P}$$

$$P = \rho_0 U_S U_P$$

$$E - E_0 = \frac{1}{2}P(V_0 - V)$$

- We have 3 equations, but 5 unknowns: $U_p - U_s - \rho - P - E$
- Need to experimentally determine two unknowns
- The Hugoniot equations do not explicitly contain temperature
- Not a complete equation of state: $E(P, V)$ – need T
- *The equations are based on a specific initial state*



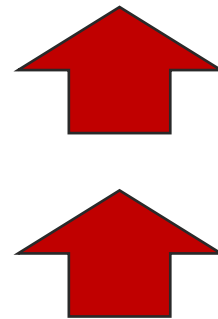
- **The Hugoniot is not a path in space**
- **Hugoniot is defined by a specific initial state**



How to find experimentally a Hugoniot State?

- Initiate a shock wave in a sample
- U_S and U_P are the easiest to measure
 - cannot always measure both
- Development of Hugoniot **standards for Impedance Matching (ex: Al, Ta)**
- $U_S = F(U_P) \rightarrow U_S = C_0 + S_1 U_P$
- P and U_P at an interface are equal

Target/sample



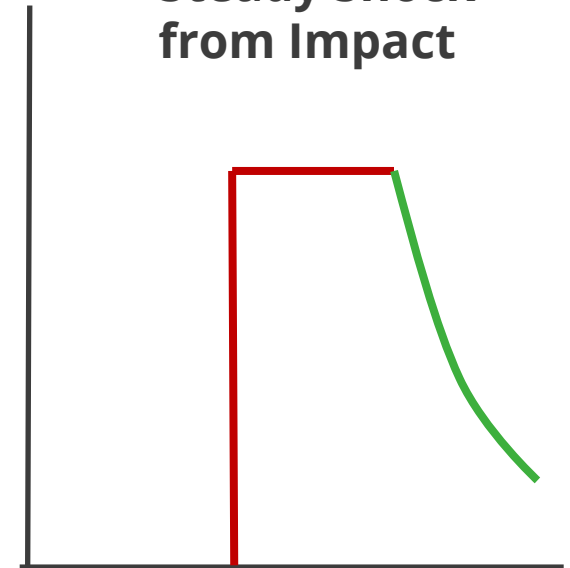
Impactor/Flyer

$$\frac{\rho}{\rho_0} = \frac{U_S}{U_S - U_P}$$

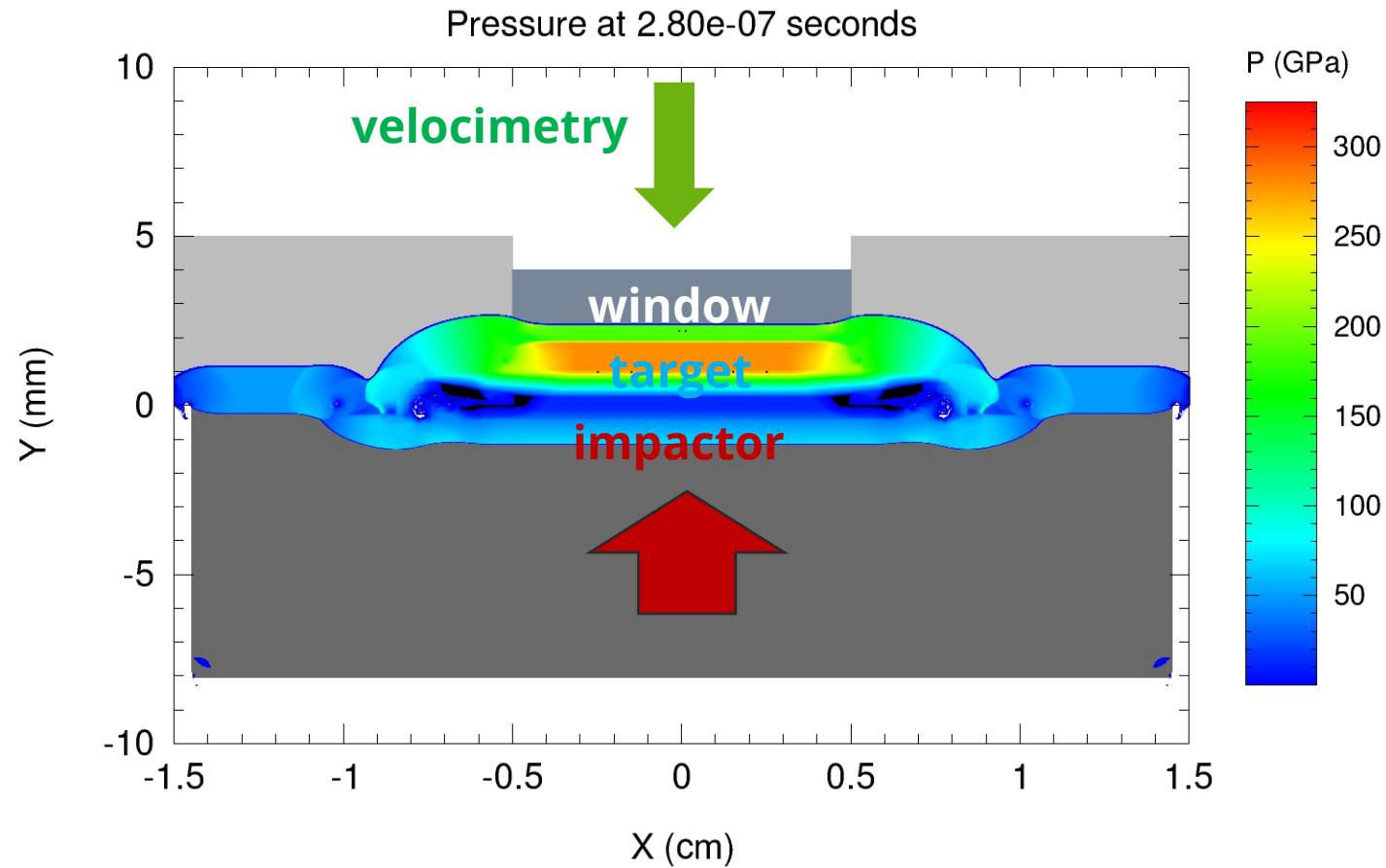
$$P = \rho_0 U_S U_P$$

$$E - E_0 = \frac{1}{2} P (V_0 - V)$$

Steady Shock from Impact

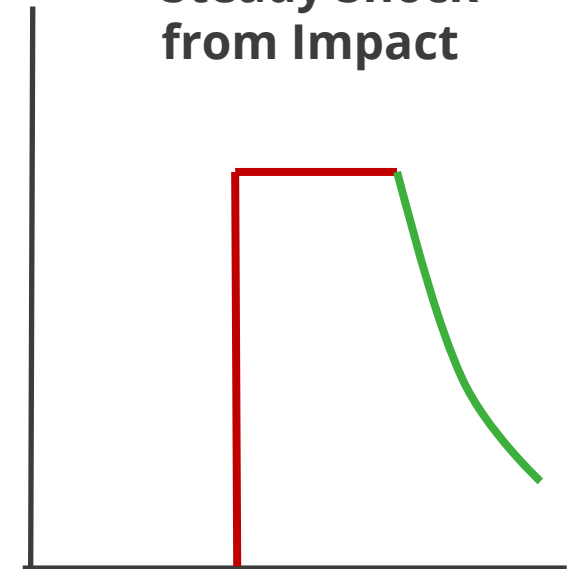


Shock wave propagation: a simulation



CTH hydrocode simulation

Steady Shock
from Impact





Z is one of three flagship HEDP facilities in the U.S.



Lawrence Livermore National Laboratory

National Ignition Facility (NIF)

- Largest Laser on Earth
- Primary facility for Laser Indirect Drive fusion
- 400 TW / 1.8 MJ (Max Power & Energy)



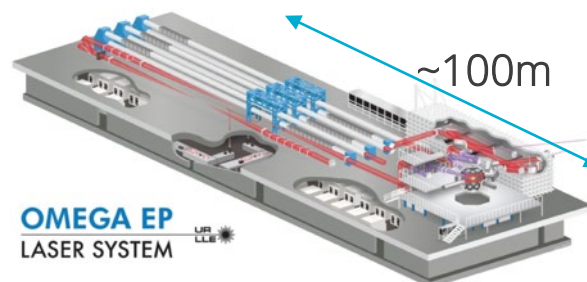
~235m



University of Rochester

OMEGA Laser Facility

- High shot-rate academic laser facility
- Primary facility for Laser Direct Drive fusion
- 20 TW/.03 MJ (Max Power & Energy)



~100m

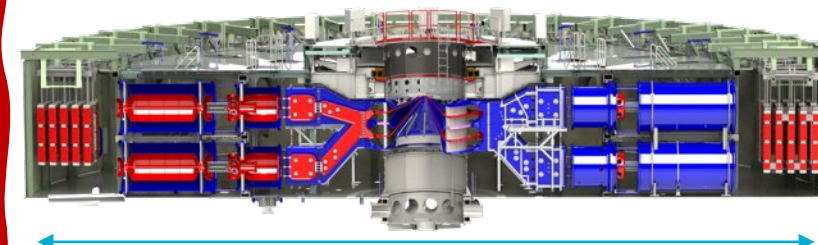
OMEGA EP
LASER SYSTEM



Sandia National Laboratories

Z Facility

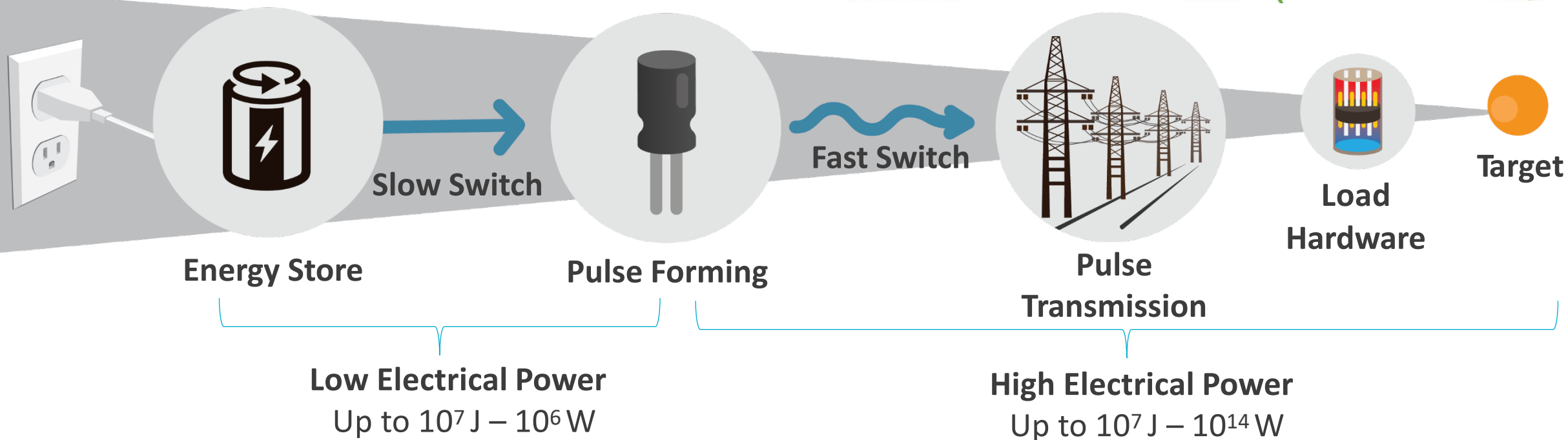
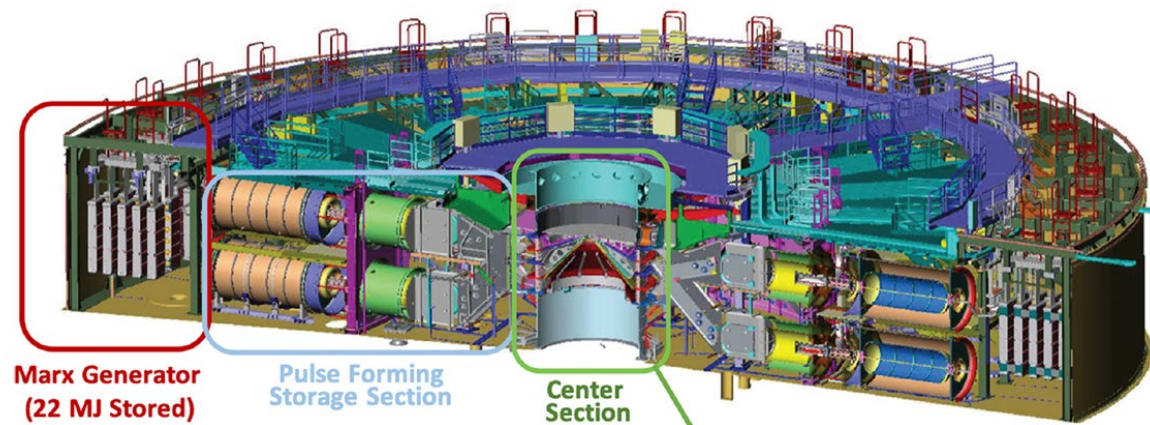
- Largest Pulsed Power Facility on Earth
- Primary facility for Magnetic Direct Drive fusion
- 80 TW / 3 MJ (Max Power & Energy)



33 m



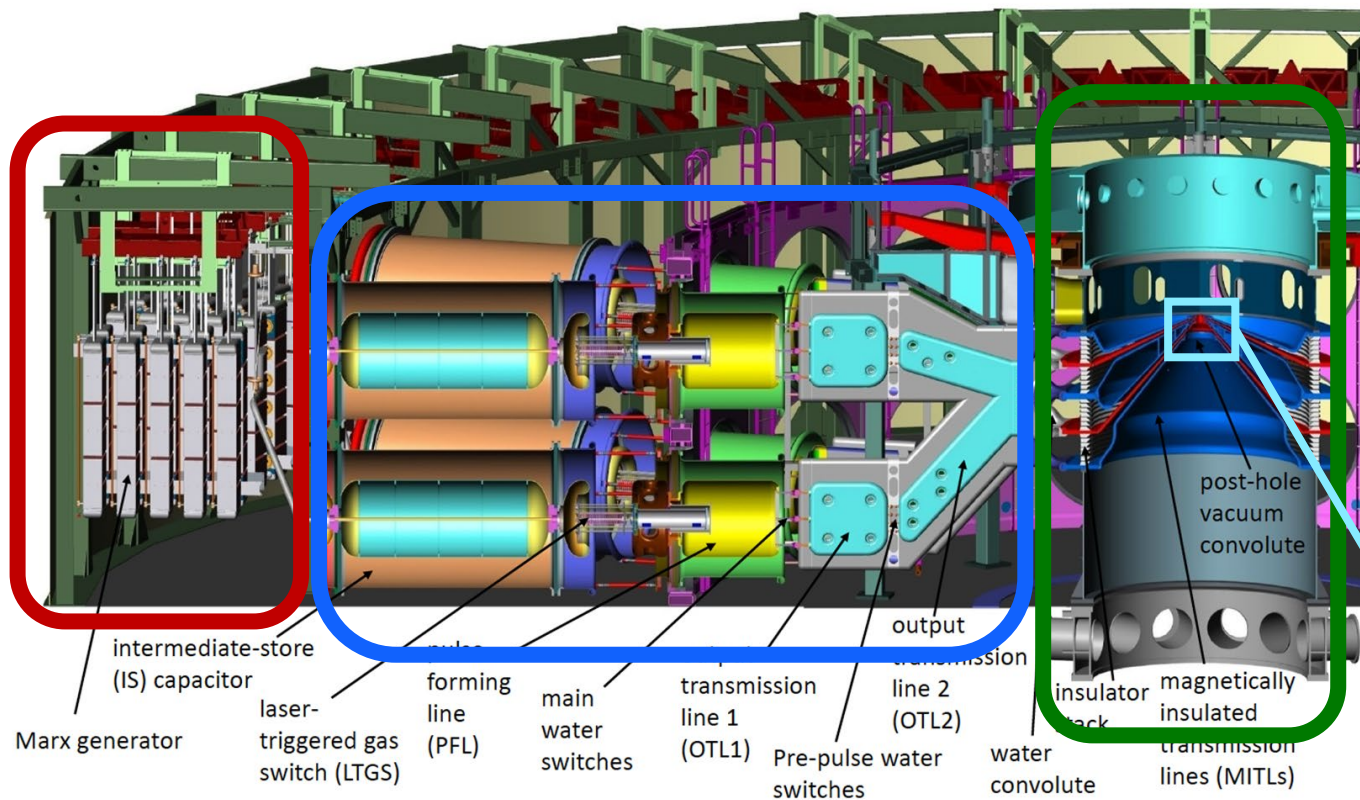
Pulsed Power: how does it work?



Pulsed power compresses electrical energy in both space and time to produce short bursts of high power.



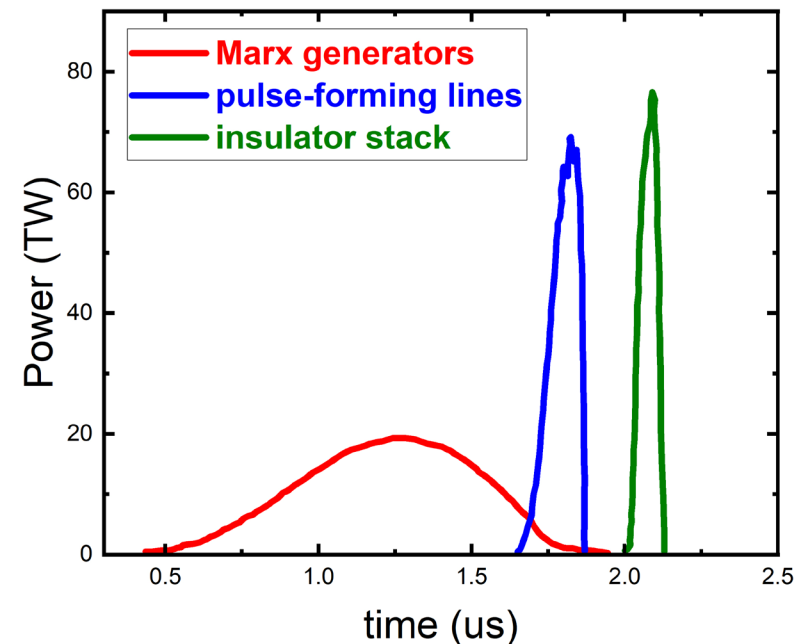
the largest pulsed power facility in the world today: the 80-TW “Z” machine at Sandia



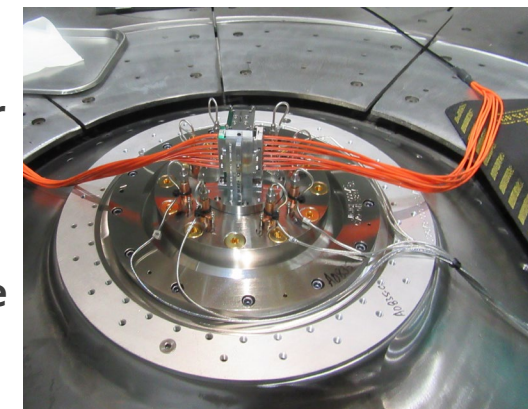
**36 Marx Banks
(22 MJ stored)**

**Pulse forming
storage section**
18 independently triggerable groups
of 2 transmission lines

**Center
section**



the “load” for
a DMP shock
compression
experiment
with multiple
samples



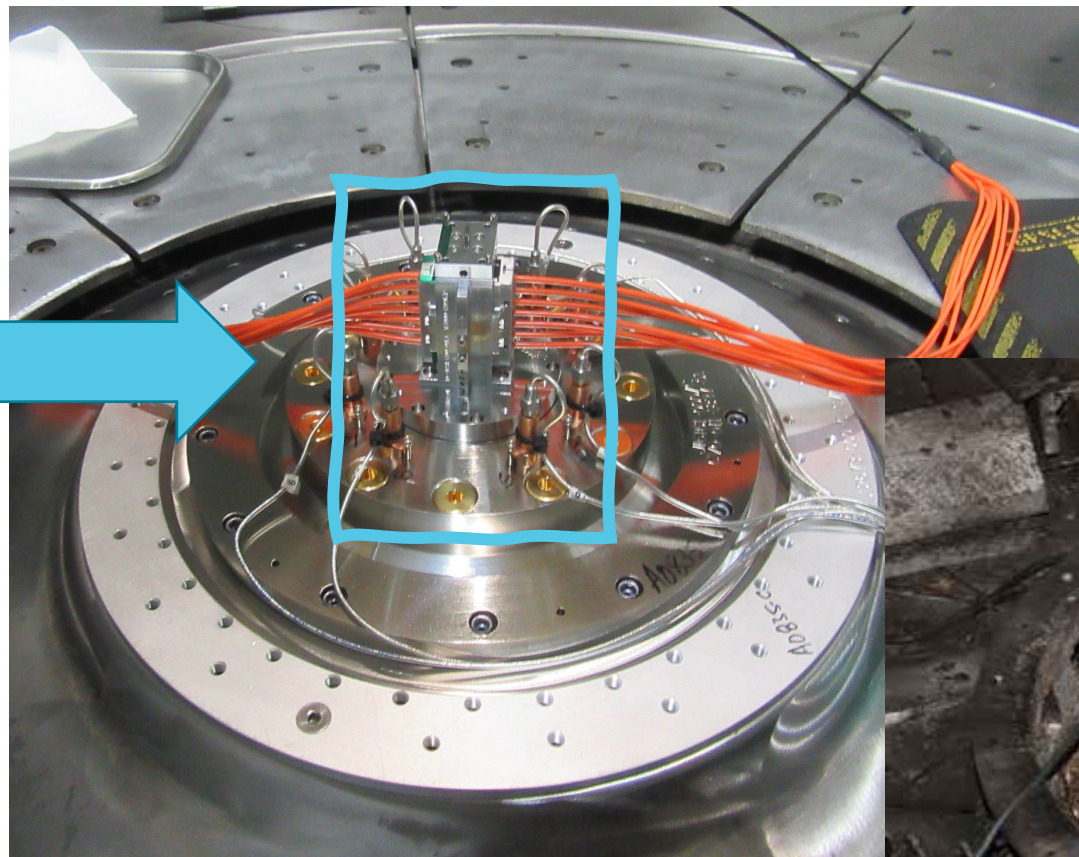


Z experiments release the energy of a few sticks of dynamite



before

after



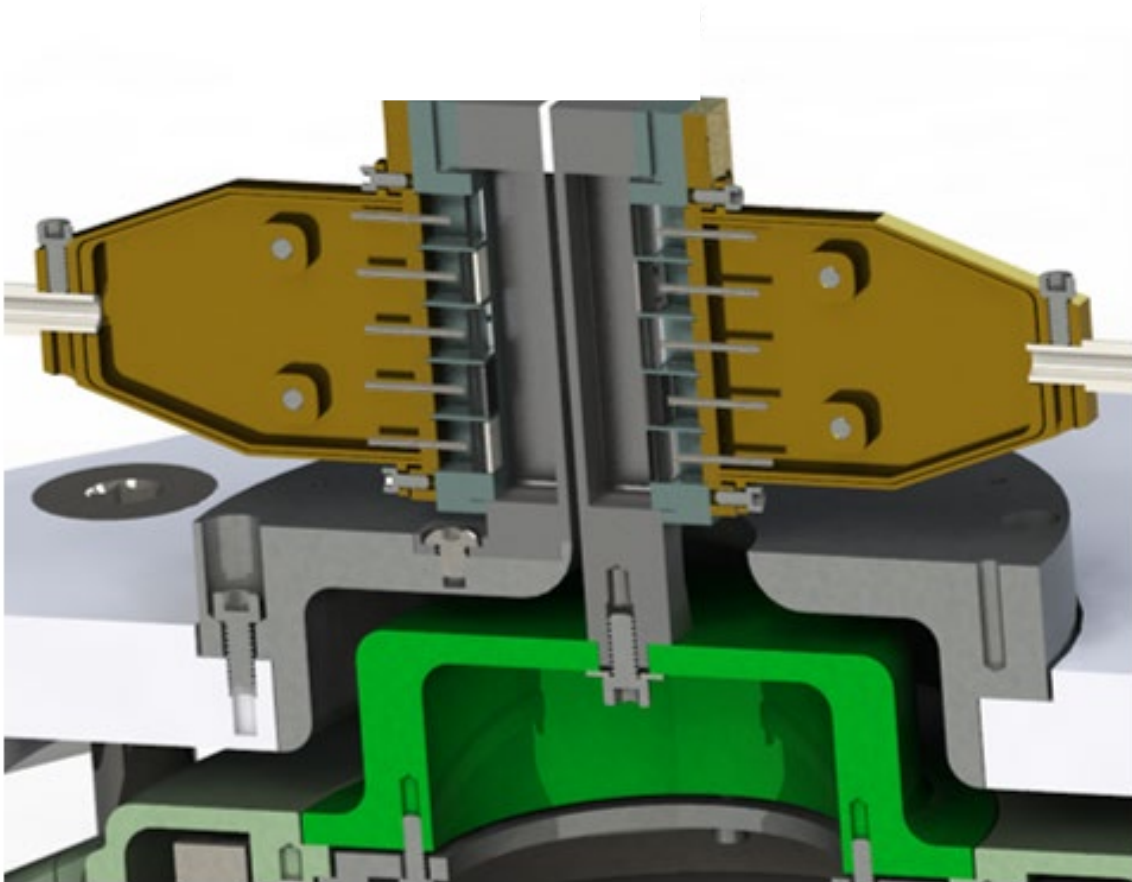
Load with column of samples



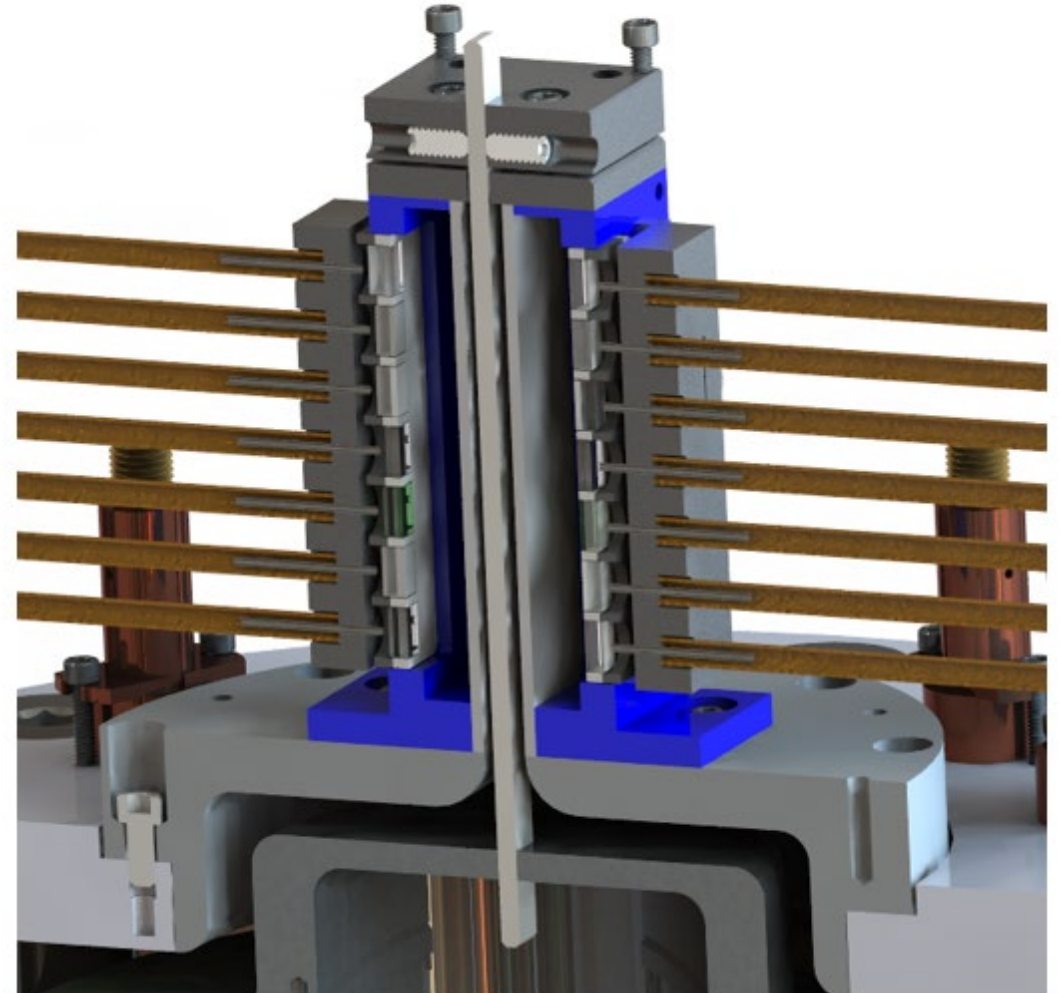


Hugoniot shock experiments on Z Machine: 2 load geometries

2-sided **STRIPLINE** flyer velocities up to ~40 km/s



COAXIAL two flyer velocities 9-25 km/s



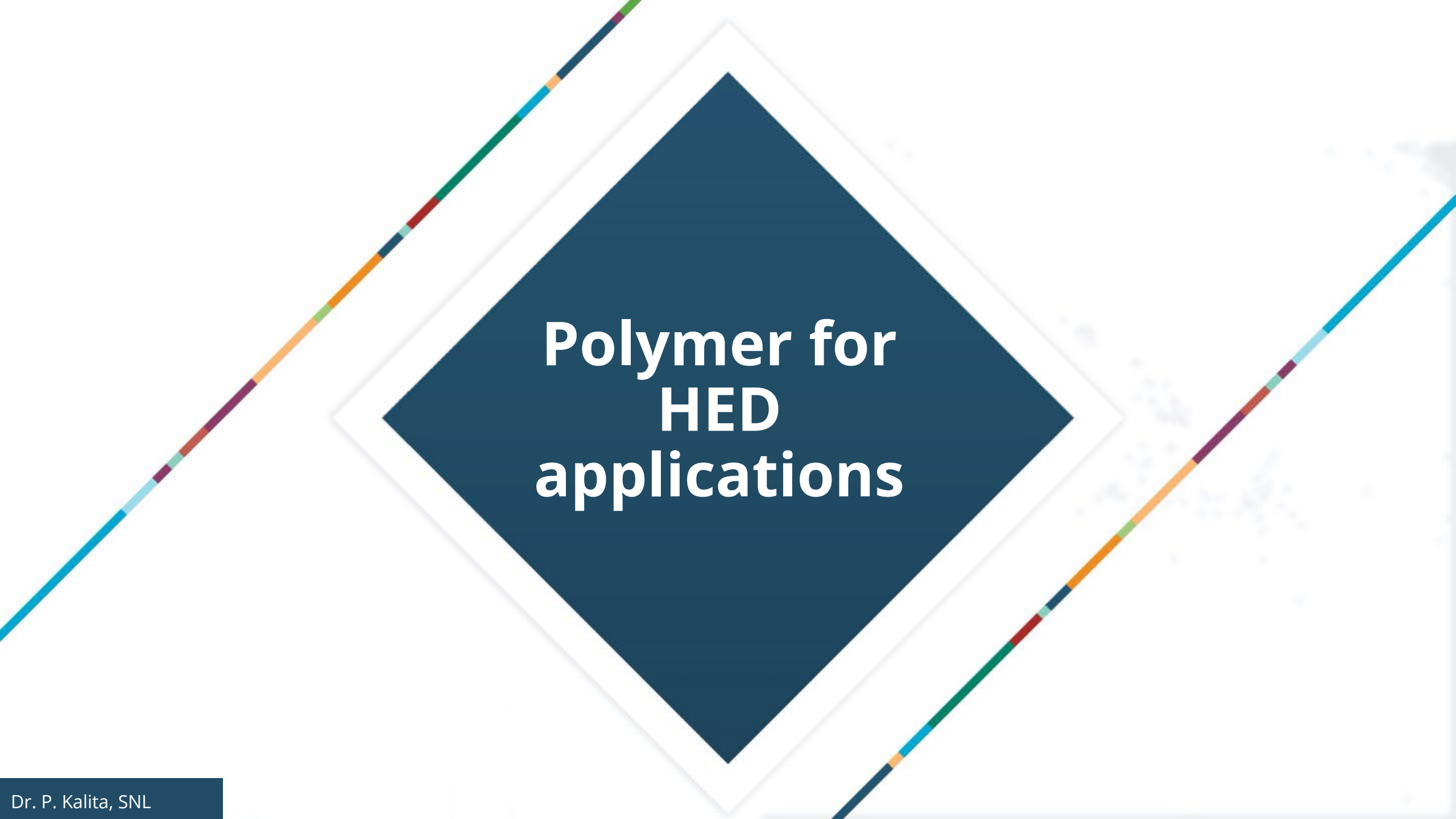


Al flyers: V_F



Al flyers: V_F





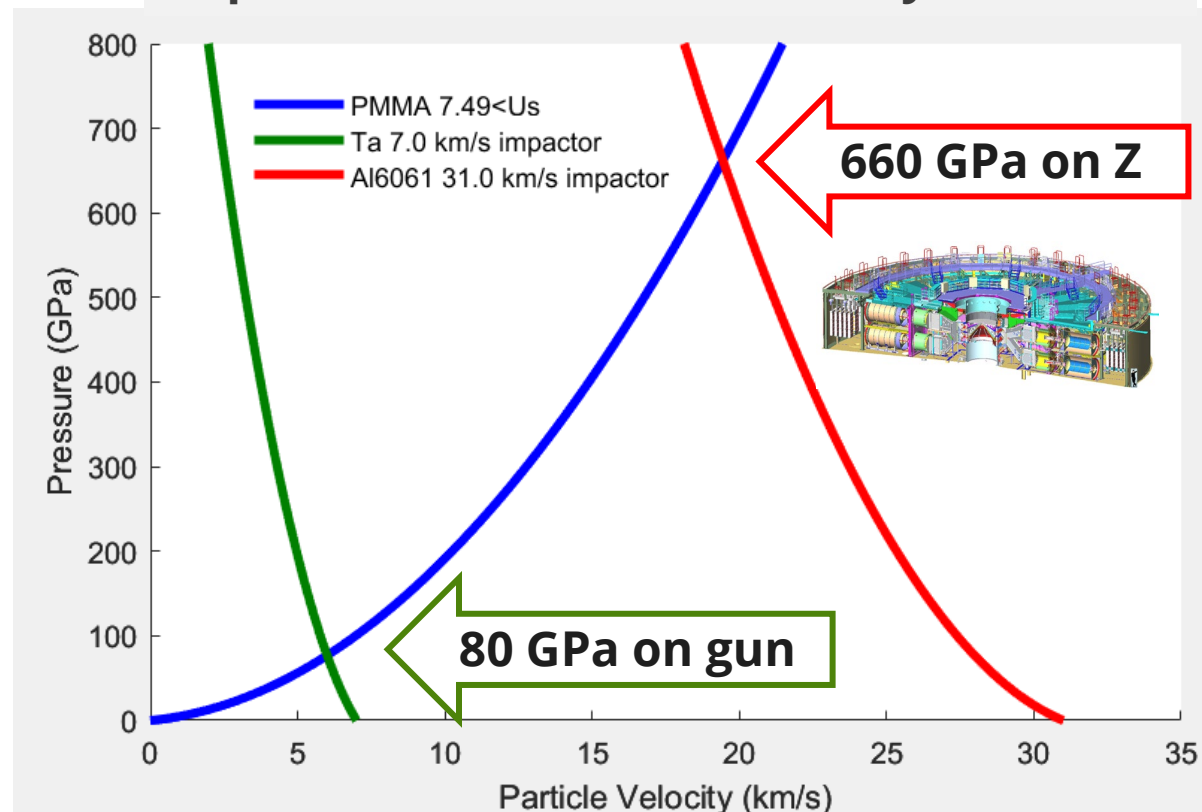
Polymer for HED applications



Example #1: PMMA polymer

- PMMA, Plexiglass® or Lucite®
- PMMA, belongs to the family of hydrocarbon polymers used in a wide variety of practical applications
- HED - High Energy Density facilities use these polymers in dynamic compression at extreme P
- existing Equation of State (EOS) of PMMA are benchmarked up to ~130 GPa at most!
- extrapolation is risky: the higher the pressure, the riskier the extrapolation of an EOS.
- **no data on Hugoniot above ~130 GPa**

Impedance mismatch & velocity in action



- Acoustic impedance: reference density \times the speed of sound
- A polymer is a very low impedance material!
- Tantalum is a very high impedance impactor
- The **impedance difference** between flier and sample determines how much shock pressure will be generated

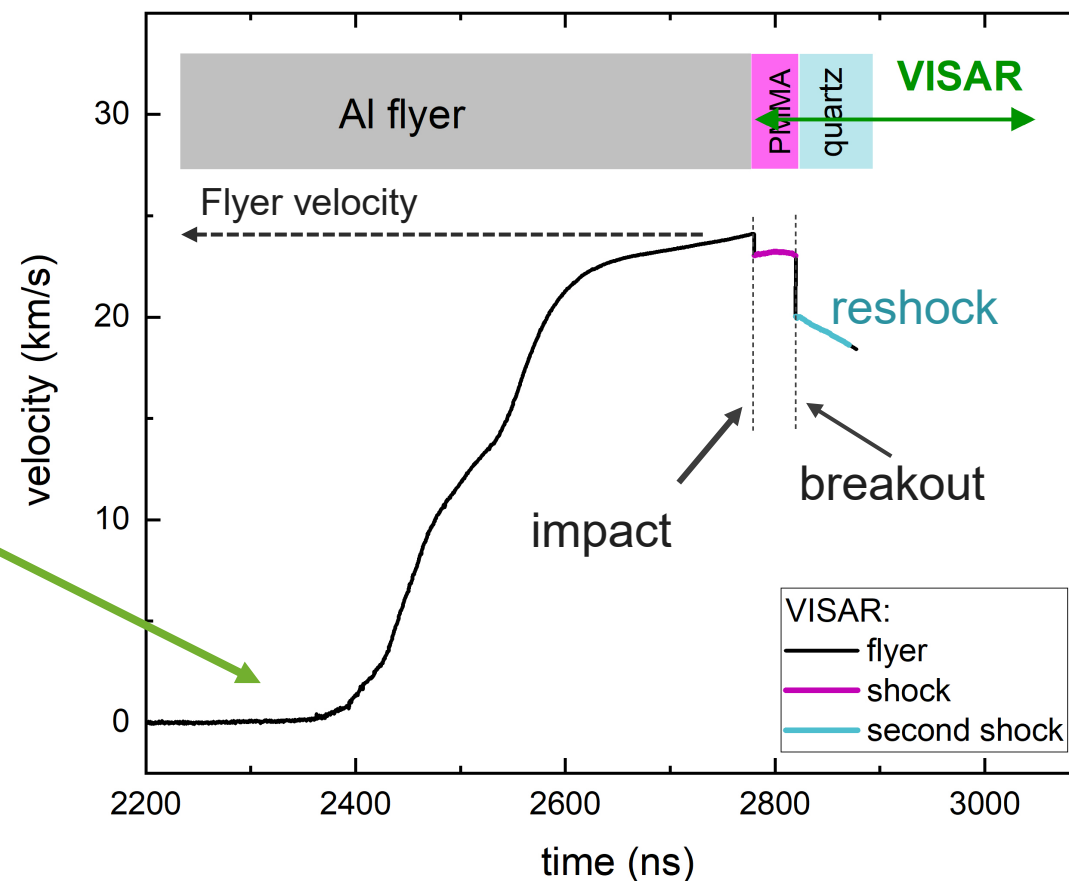
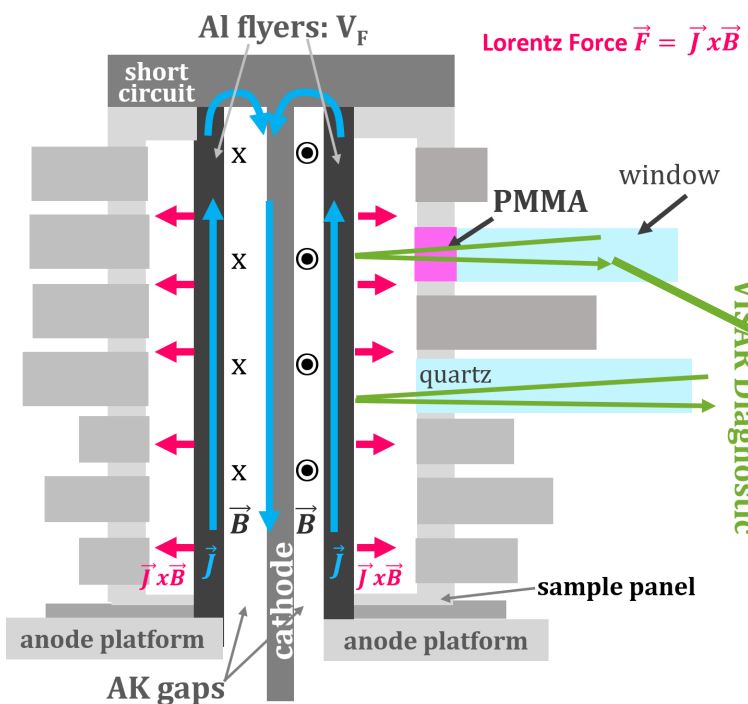


PMMA - Hugoniot shock experiments on Z

Our key diagnostic: VISAR (532nm)

Velocity interferometer system for any reflector

Asymmetric coaxial config. 9-25 km/s





PMMA - Hugoniot shock experiments on Z

Our key diagnostic: VISAR (532nm)

Velocity interferometer system for any reflector

PMMA sample:
experimental $U_s \rightarrow$ reflective shock front

Rankine-Hugoniot eq.

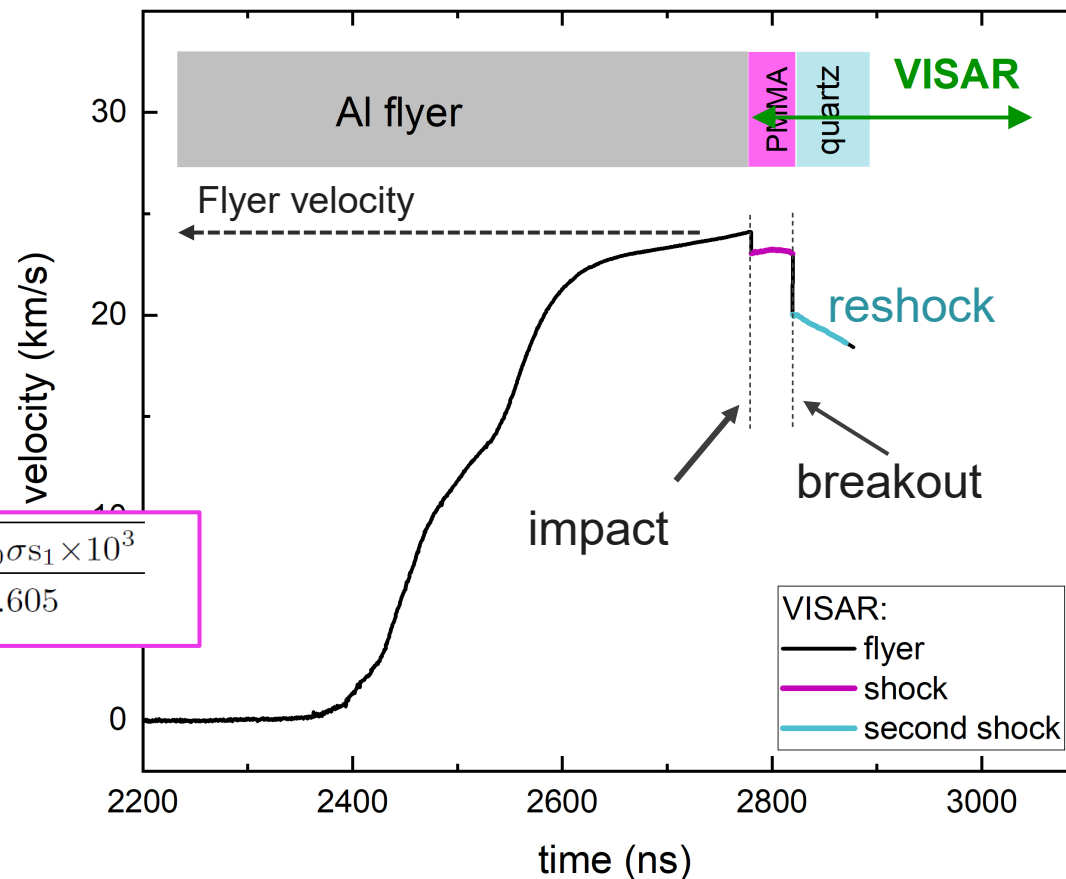


Monte-Carlo **impedance matching** with Al flyer



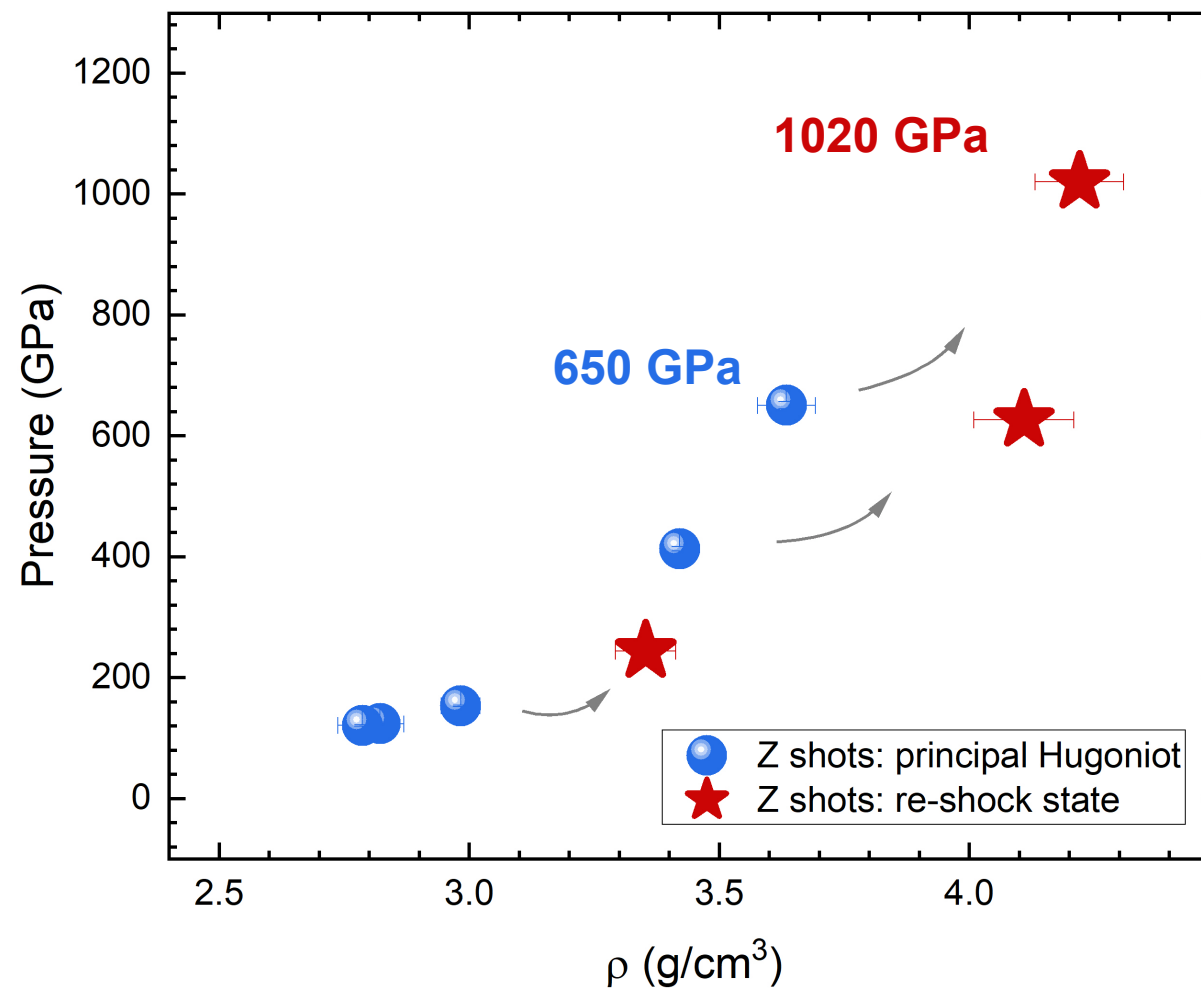
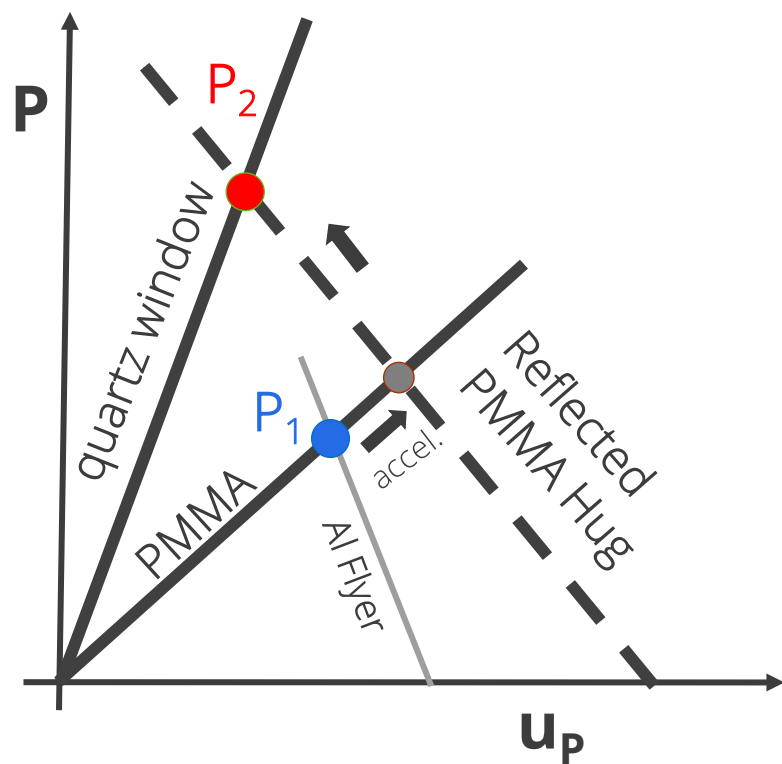
Flyer	C_0 (km/s)	s_1	$\sigma C_0 \sigma s_1 \times 10^3$
Al	6.322 ± 0.231	1.188 ± 0.020	—4.605

PMMA sample: U_p, P, ρ





PMMA Shock Hugoniot & re-shock states





Hugoniot data form Z vs existing EOSs

Two fits to US – UP data:

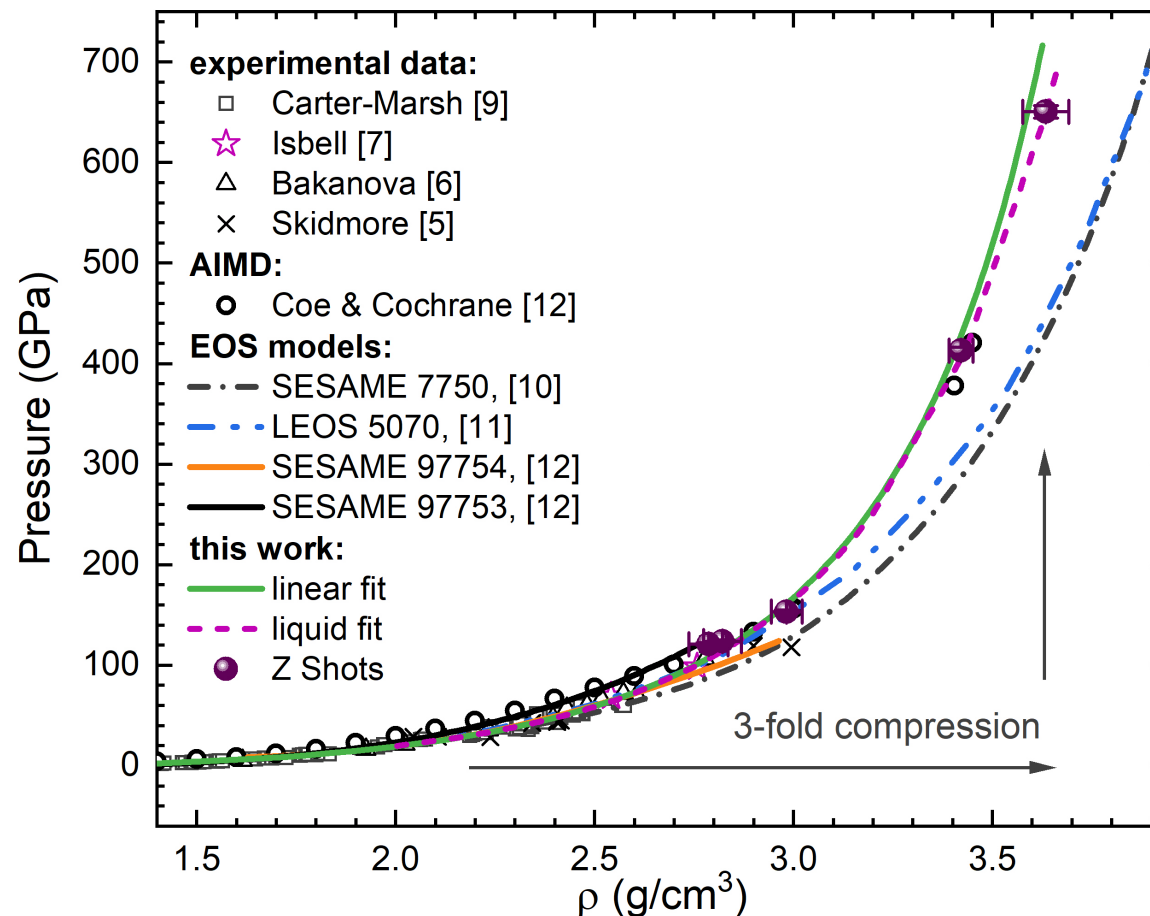
- Linear fit
- Liquid fit

TABLE VI. PMMA Hugoniot linear fit parameters and covariance matrix elements for $U_S = C_0 + S_1 u_P$ up to 650 GPa.

C_0 (km/s)	S_1	$\sigma_{C_0}^2 \times 10^4$	$\sigma_{S_1}^2 \times 10^5$	$\sigma_{C_0 S_1} \times 10^5$
2.855 ± 0.021	1.344 ± 0.005	4.59	2.36	-8.47

TABLE IV. The modified, universal liquid fit $U_S = A + Bu_P - Cu_P \exp(-Du_P)$ parameters for the PMMA Hugoniot up to 650 GPa.

A (km/s)	B	C	D (km/s) ⁻¹
3.18 ± 0.72	1.32 ± 0.04	0.19 ± 0.4	0.30 ± 0.14





PMMA – takeaways




- new direct measurements of shock states for PMMA polymer
- pressure and density along the principal Hugoniot are extended from **120 to 650 GPa**.
- Re-shock states up to **1020 GPa**, which corresponds to **~3.5-fold compression** of PMMA
- the Z data are significantly stiffer than the existing EOS models
- This work shows clear evidence for the **need to revisit the wide-ranging PMMA EOS tables** for experimental and modeling applications

Journal of Applied Physics

Shock compression of poly(methyl methacrylate) PMMA in the 1000 GPa regime: Z machine experiments

Cite as: J. Appl. Phys. **133**, 035902 (2023); <https://doi.org/10.1063/5.0128681>

Submitted: 29 September 2022 • Accepted: 16 December 2022 • Published Online: 19 January 2023

 Pat Kalita,  Marcus D. Knudson,  Tom Ao, et al.



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CrossMark



Platinum standard



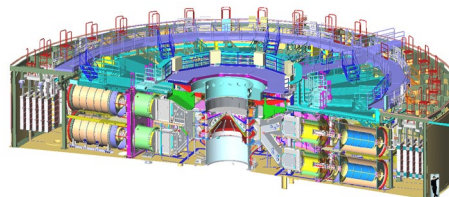
Example #2: Platinum shock standard at multi-TPa pressures

- Cutting edge shock compression research is moving towards ever increasing pressure or stress states into > TPa range
- Experiments at extreme pressures allow to test numerical methods, physics theories and uncover exotic matter behaviors.
- Existing Equation of State (EOS) standard materials are limited to < 0.5 TPa,
 - no data on Pt Hugoniot above 670 GPa
 - Shockless compression to 1 TPa
- Extrapolation is risky: at shock $P > 1$ TPa significant uncertainties.

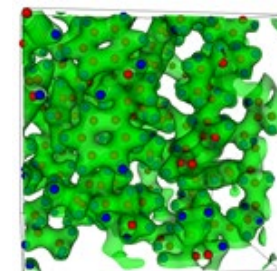
- We conducted a series of shock compression experiments on Pt up to 2 TPa = 20 Mbar = 20 million atm on **SNL Z machine** combined with **DFT-AIMD** calculations and with **design of a broad range Hugoniot EOS**
- **Our work establishes Platinum as a shock compression standard to > 2 TPa**

SNL
shock experiments on Pt
on Sandia's Z machine
up to 2177 GPa = 2.17 TPa

SNL
ab initio molecular
dynamics (AIMD)
simulations on Pt



SNL & LANL
broad range multiphase
EOS design for Pt
SESAME 3732





Pt standard: DFT calculations of the cold curve & AIMD calculations of the Hugoniot EOS



DFT cold curve - 0K:

- Exchange correlation energy computed with **PBEsol** or with **AM05** functional and a **16-electron pseudopotential**
- results are in **excellent agreement** with literature data and with the independently developed **SESAME EOS**
- DFT also validated by calculating the elastic constants and phonon dispersion (using AM05 potential)

AIMD - ab initio molecular dynamics simulations:

- generate a tabular EOS directly useable in a hydrodynamics code
- 16-electron pseudopotential, **PBEsol**, and the Mermin's generalization of the **Kohn-Sham** equations to finite T
- good agreement between **DFT** and **SESAME** Hugoniot and with principal isentrope
- **DFT melt transition is upper bound in T**
- **SESAME EOS melt density is consistent with DFT**

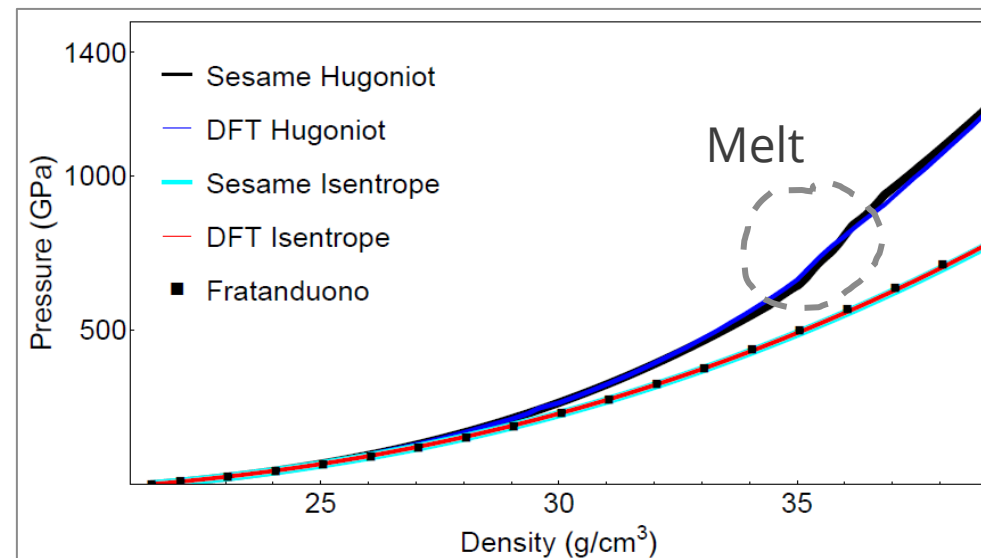


FIG. 7. Hugoniot calculated from DFT and SESAME EOSs. The isentrope is virtually identical in pressure/density space. The DFT calculated isentrope values compare well with experimental data [23].

[23] = Fratanduono et al., Science 372, 1063–1068 (2021).



Pt standard: Broad-Range Multi-Phase EOS Design

Helmholtz
free energy

$$F(T, V) = F_{cold}(V) + F_{ion}(T, V) + F_{electron}(T, V)$$

**cold curve
contribution**

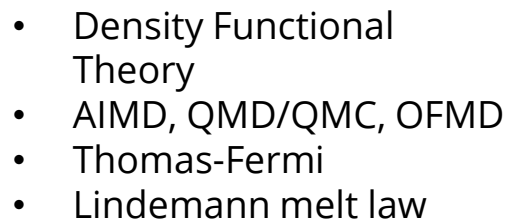
**cold + thermal
ionic contribution**

**thermal electronic
contribution**

Development of SESAME EOS 3732

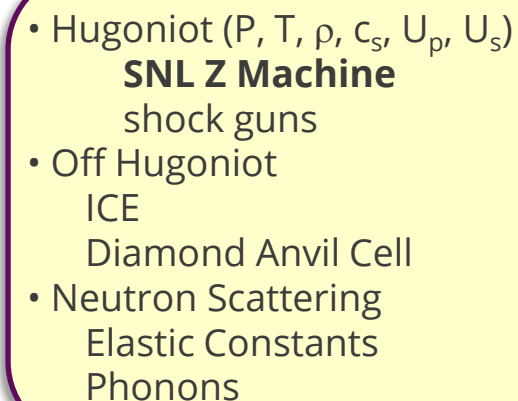
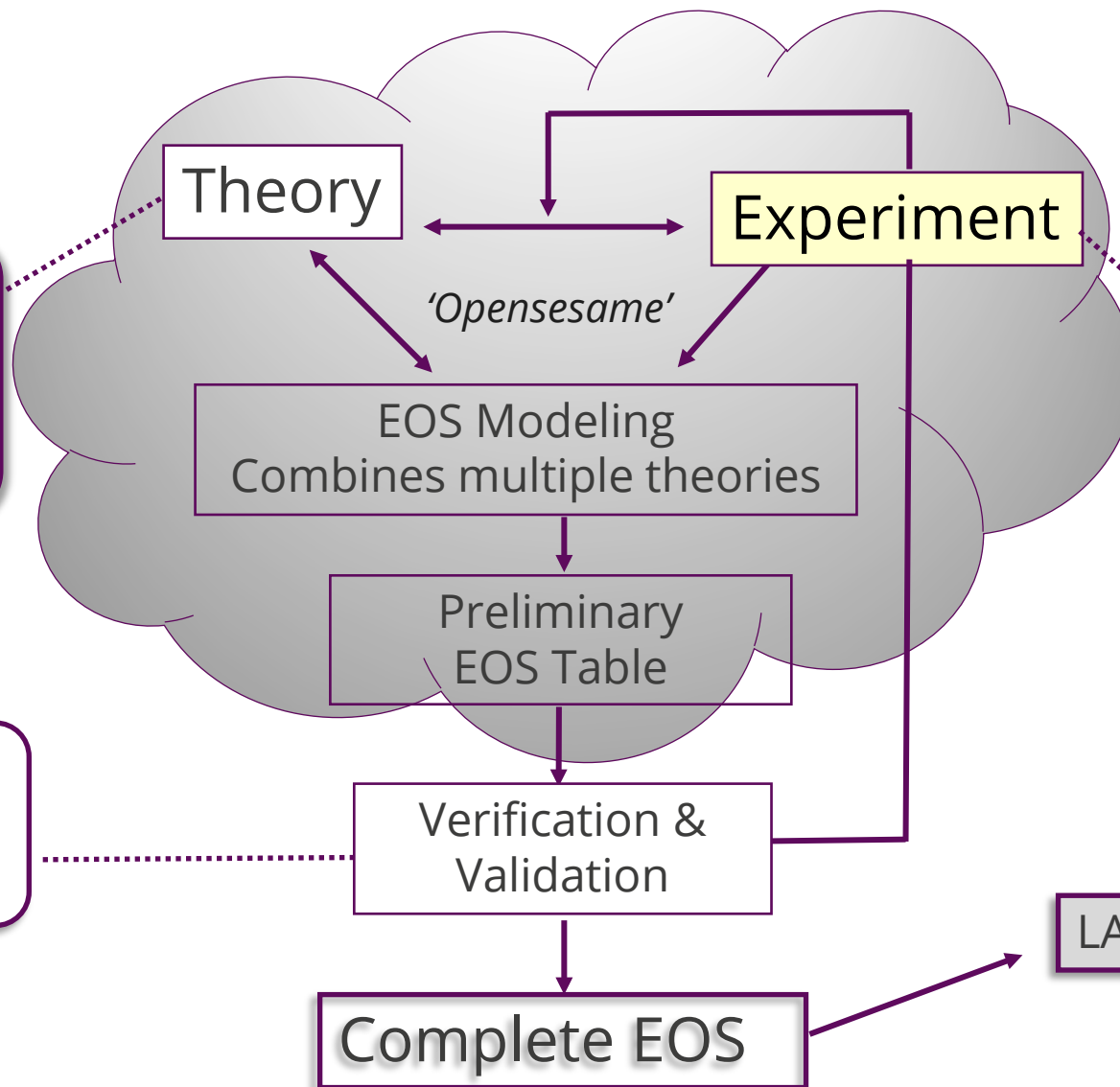
- standard decomposition of Helmholtz free energy
- **Cold curve**
 - determined via Mie-Grüneisen approximation by matching a quadratic to experimental data
 - intercept of the quadratic was fixed to match the adiabatic bulk modulus from ultrasonic data
- **Ion thermal component**
 - used Debye approximation for solid and corrected Debye for fluid
 - Grüneisen gamma Γ parameter and ref. Debye T in ion thermal model is set by matching **isobaric expansion data** and **specific heat** data
 - derivative of Γ with density obtained by matching to RT DAC data
- **electron thermal component** was determined using the **Thomas-Fermi-Dirac** model
- melt transition used Lindemann Melt Law.

SESAME EOS
development
implemented in
LANL code:
'Opensesame'



VASP, RSPT, Wien2K,
Quantum Espresso

- Hydrocode Simulation
- Additional Experiments
- Refined Theories



The SESAME ascii file

LANL SESAME EOS Database

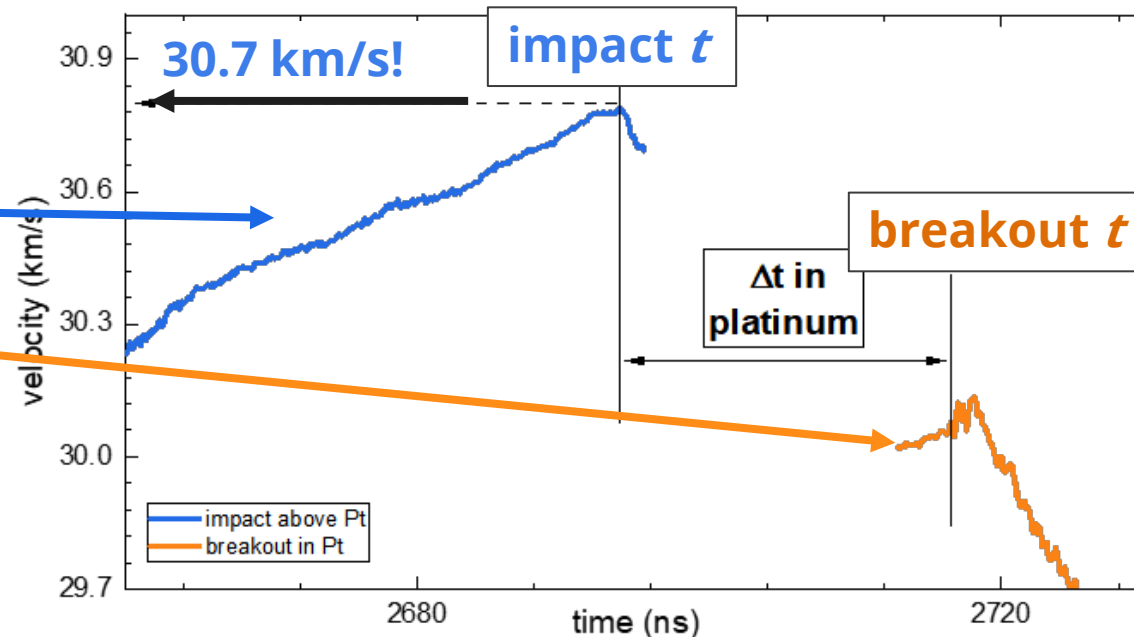
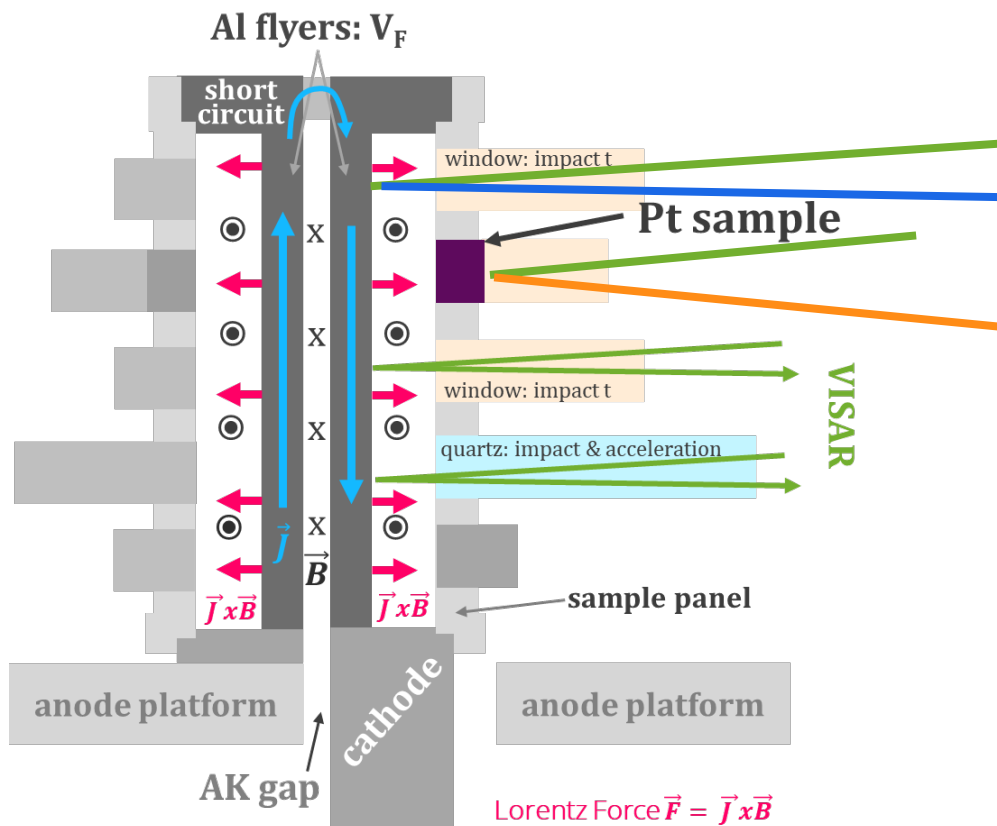
[illegible]



Hugoniot shock experiments on SNL Z Machine: 2 geometries

Our key diagnostic: VISAR (532nm)

Velocity interferometer system for any reflector



$$\text{experimental } U_s = \text{thickness} / \Delta t$$

Monte-Carlo impedance matching with Al flyer

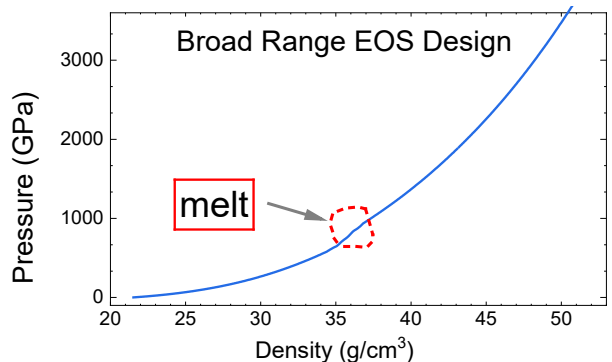
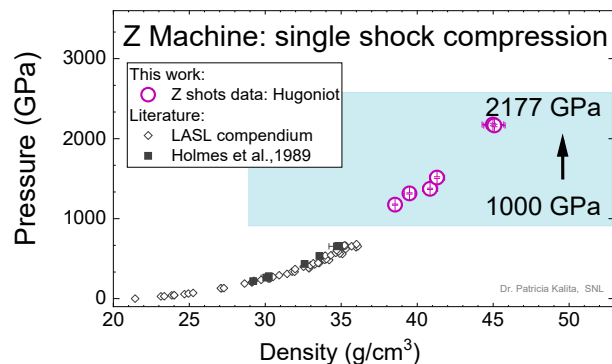
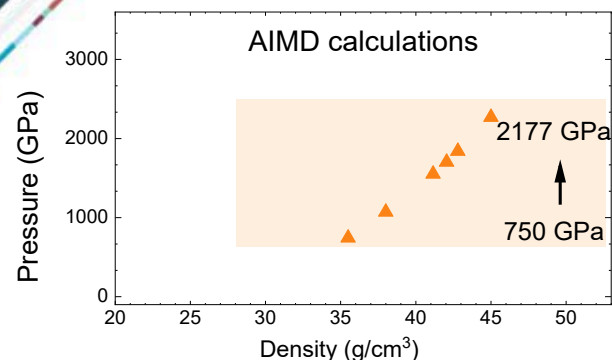
Pt sample: U_p , P , ρ

Flyer	$C_0(\text{km/s})$	s_1	$\sigma C_0 \sigma s_1 \times 10^3$
Al	6.322 ± 0.231	1.188 ± 0.020	-4.605

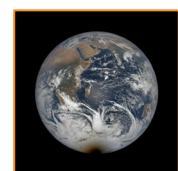


Pt: New experimental Hugoniot to 2.2 TPa + AIMD simulations + SESAME 3732 EOS

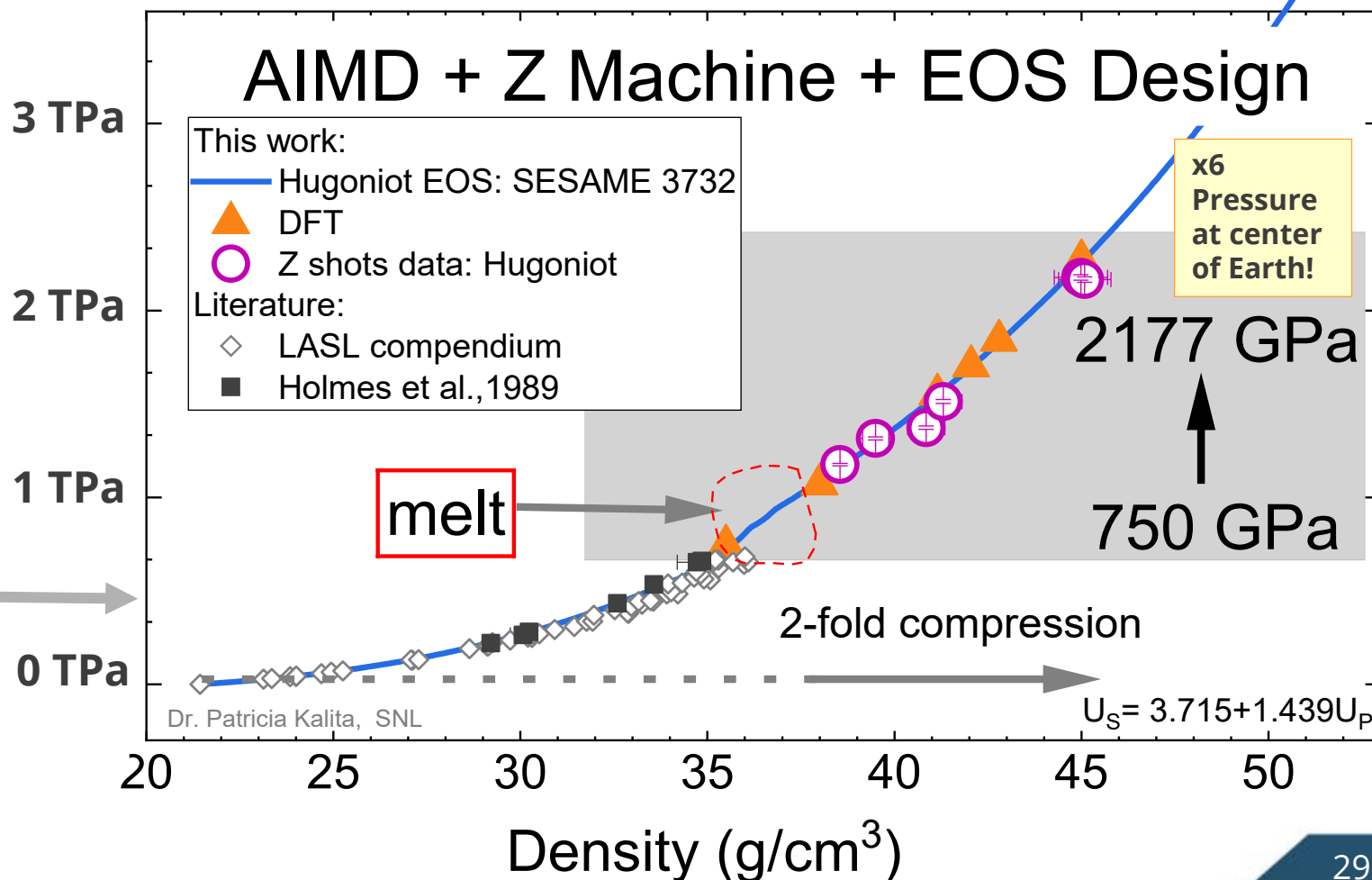
Establishing Platinum as a shock compression standard to more than 2 TPa.



Pt compressed to $> 2 \text{ TPa}$ =
 20 Mbar = 20 million atm.

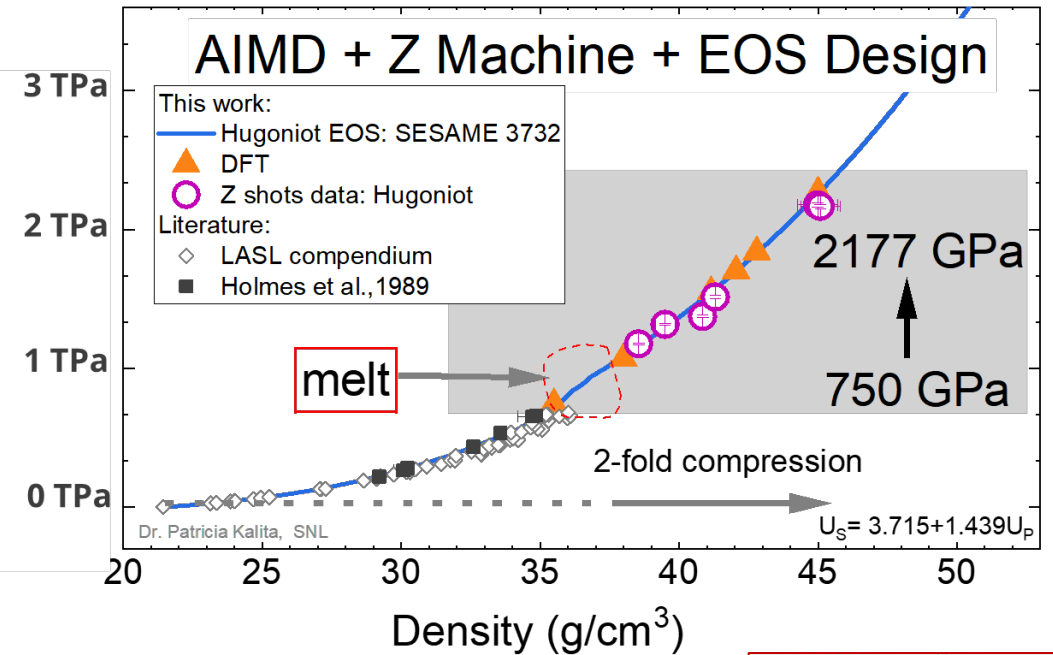


Earth



Pt standard - Takeaways

- Our multi-TPa EOS of platinum allows to use Pt as a dependable high impedance standard in shock experiments
- We experimentally constrained the Pt standard up to 2.2 TPa using shock compression
- we carried out AIMD simulations
- we designed a new EOS for Pt: SESAME 3732
- Achieved record shock pressure on Z machine



PHYSICAL REVIEW B

covering condensed matter and materials physics

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Platinum equation of state to greater than two terapascals: Experimental data and analytical models

Kyle R. Cochrane, Patricia Kalita, Justin L. Brown, Chad A. McCoy, Jeffrey W. Gluth, Heath L. Hanshaw, Edward Scoglietti, Marcus D. Knudson, Sven P. Rudin, and Scott D. Crockett
Phys. Rev. B **105**, 224109 – Published 17 June 2022



Shock compression of Ti64 alloy

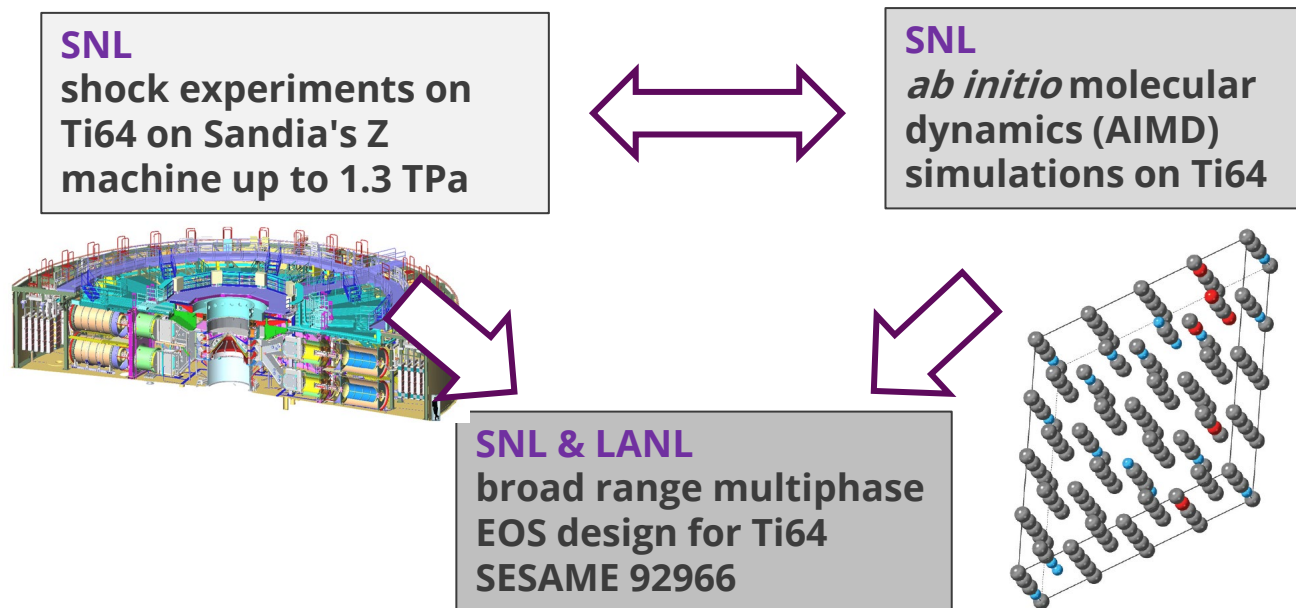


Example #3: Ti64 alloy

- **Ti-6Al-4V** (Ti 90wt%, Al 6wt%, V 4wt%), or Ti64
- the most widely used of titanium alloys
- multitude of commercial & industrial applications
- for use in extreme conditions - defense, aerospace, or nuclear industries - it is paramount to have a good description of the mechanical response of the **Ti64 alloy** to extreme P and T
- yet the **Ti64 alloy** is much less studied, compared with pure **titanium**
- no shock data on **Ti64 alloy** > 250 GPa
- extrapolation of EOS without benchmarking to experimental data is risky

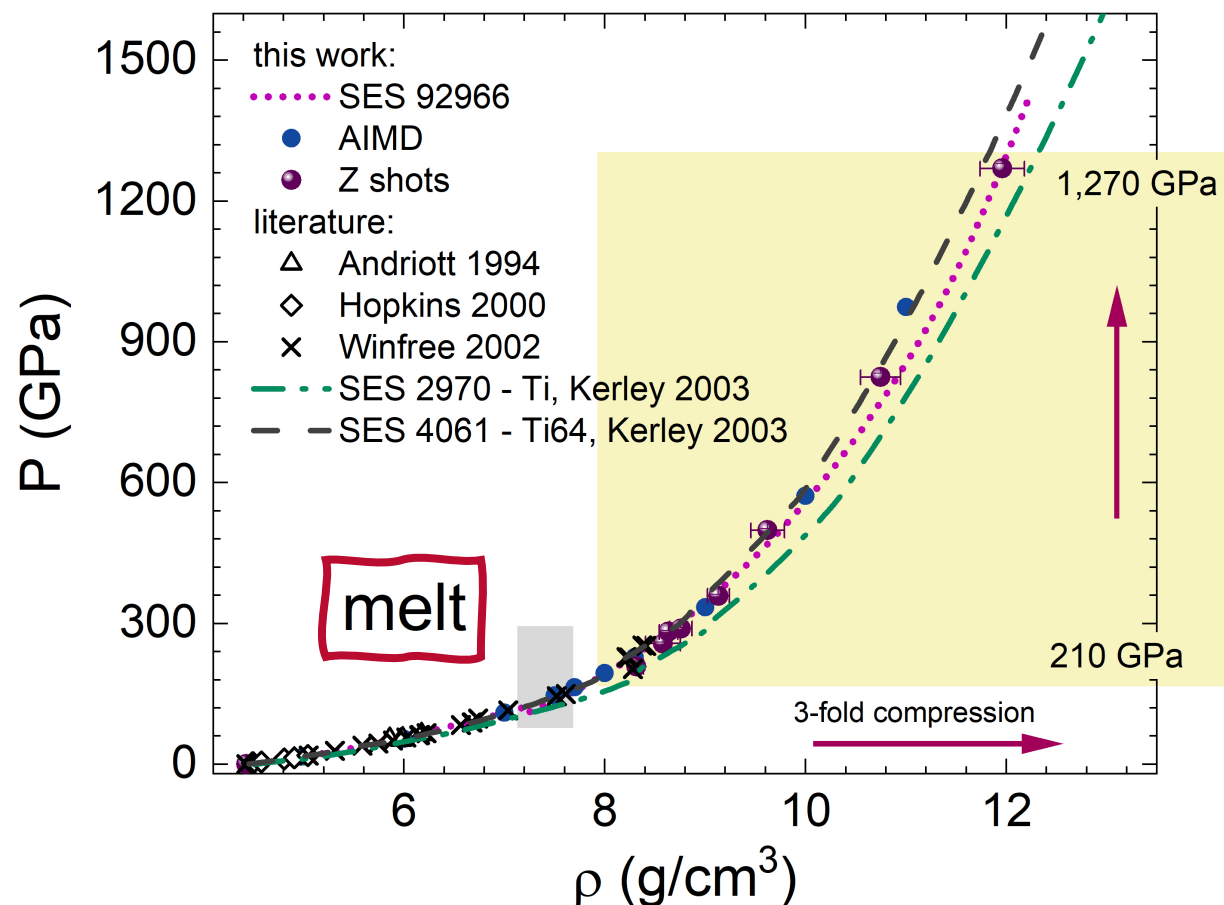
We conducted:

- a series of shock compression experiments on Ti64 up to 1.3 TPa on **SNL Z machine**
- combined with **DFT-AIMD** calculations
- and with **design of a broad range Hugoniot EOS**





Ti64 alloy: AIMD + Z Machine up to 1.3 TPa + SESAME 92966 EOS

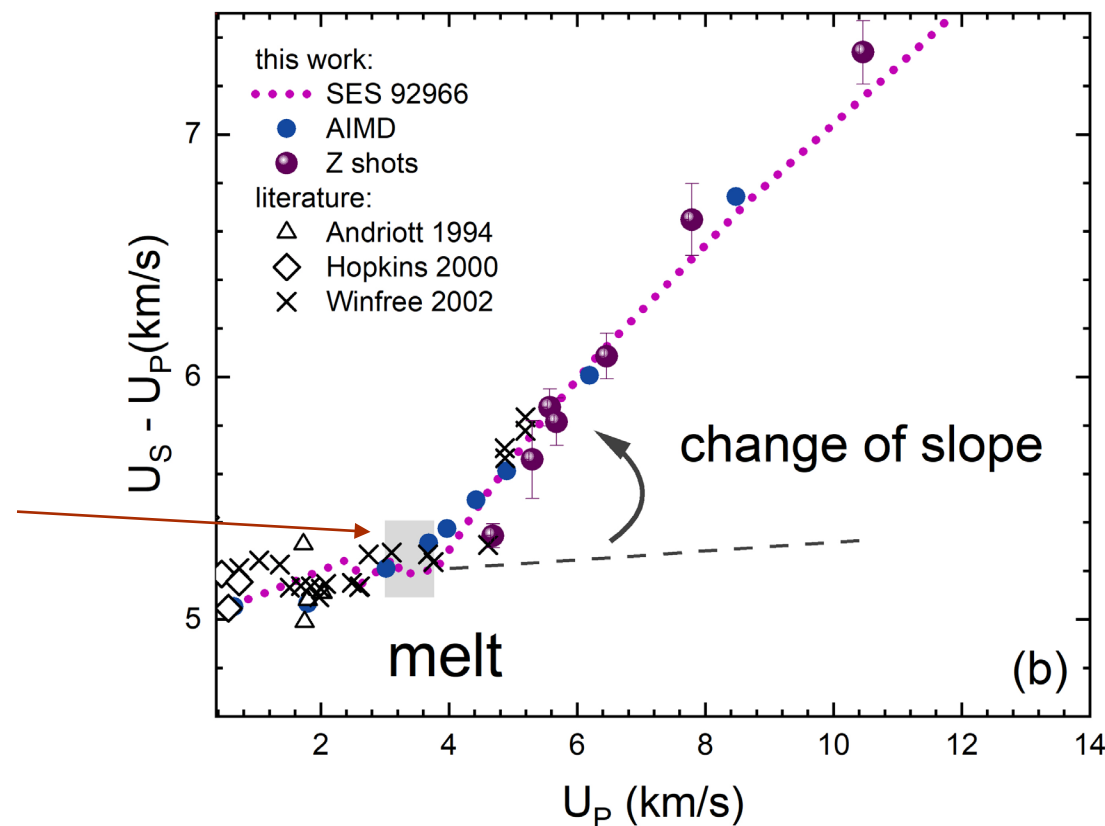
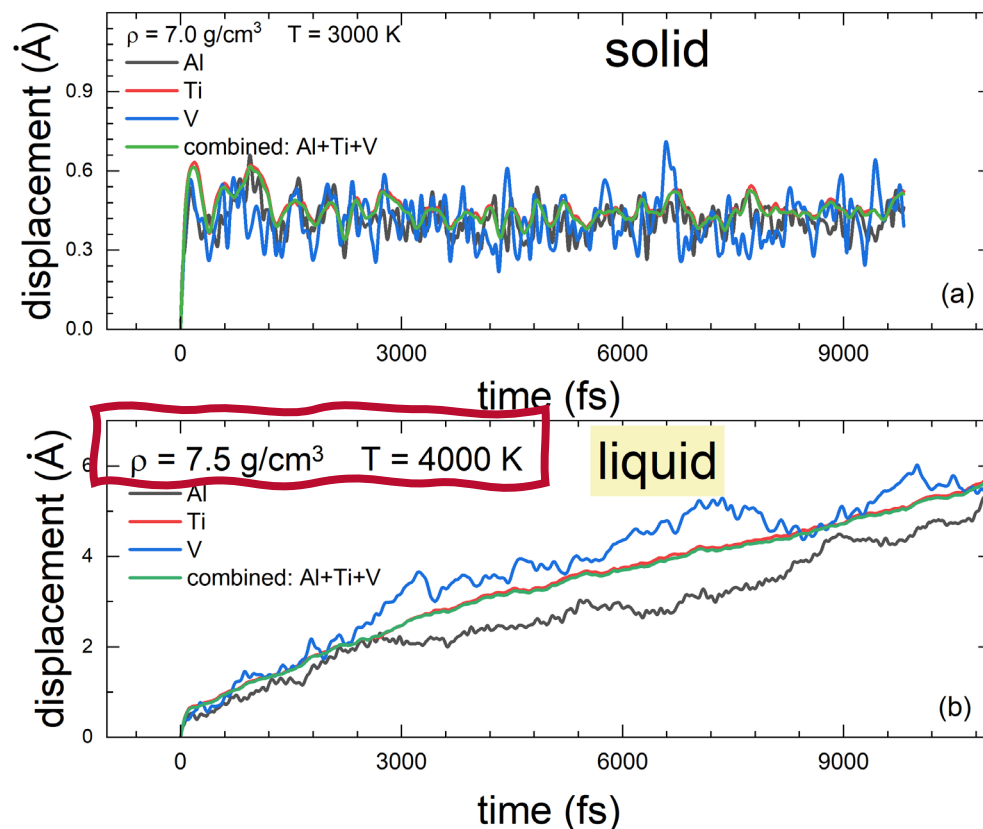


density accuracy
better than 2%

Ti64 compressed to > 1.3 TPa = 13 Mbar = 13 million atm.



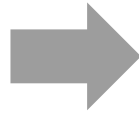
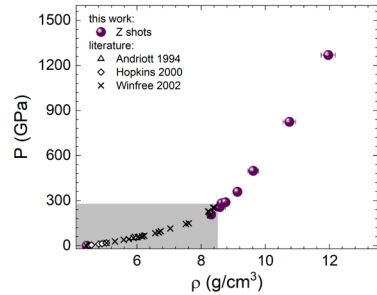
Ti64: AIMD + Z Machine demonstrate melt on Hugoniot



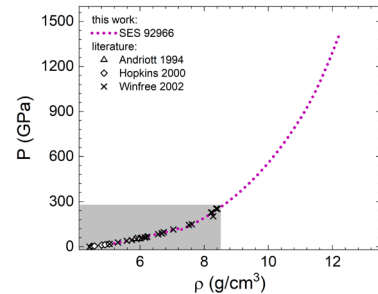
- Melt boundary on Hugoniot in disagreement with literature EOS
- previously shock melt was proposed at 6000–6800 K and 182–207 GPa
- our work shows shock melt on the Hugoniot is $\sim 4000 \text{ K}$ and $\sim 140 \text{ GPa}$

Final product: broad-range phase diagram for Ti64 alloy

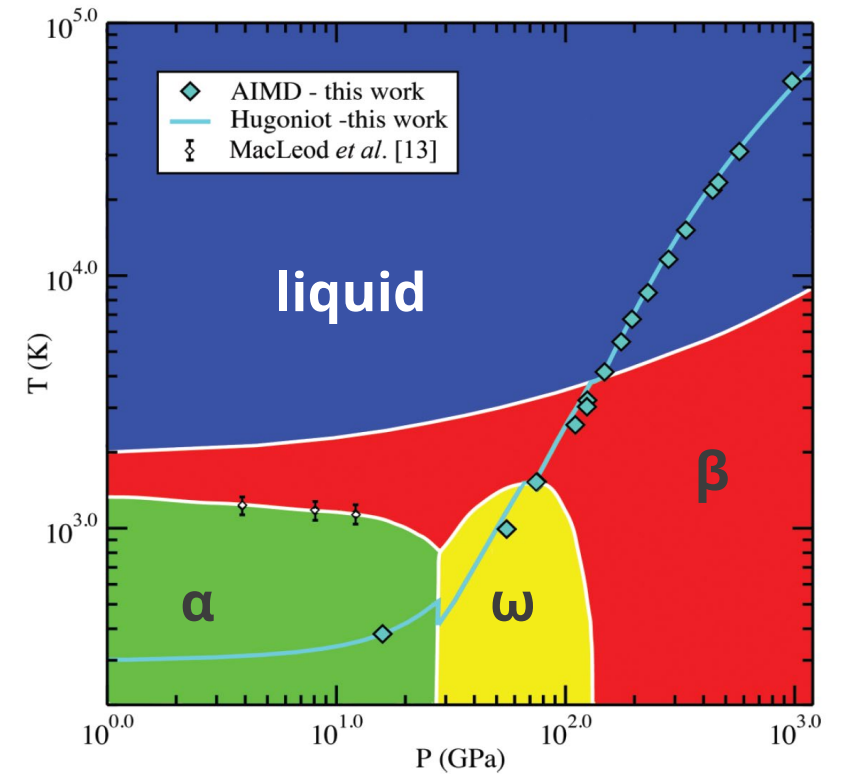
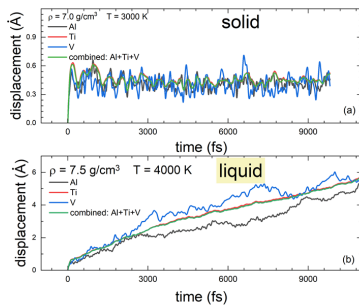
Z machine experiments



New SESAME EOS



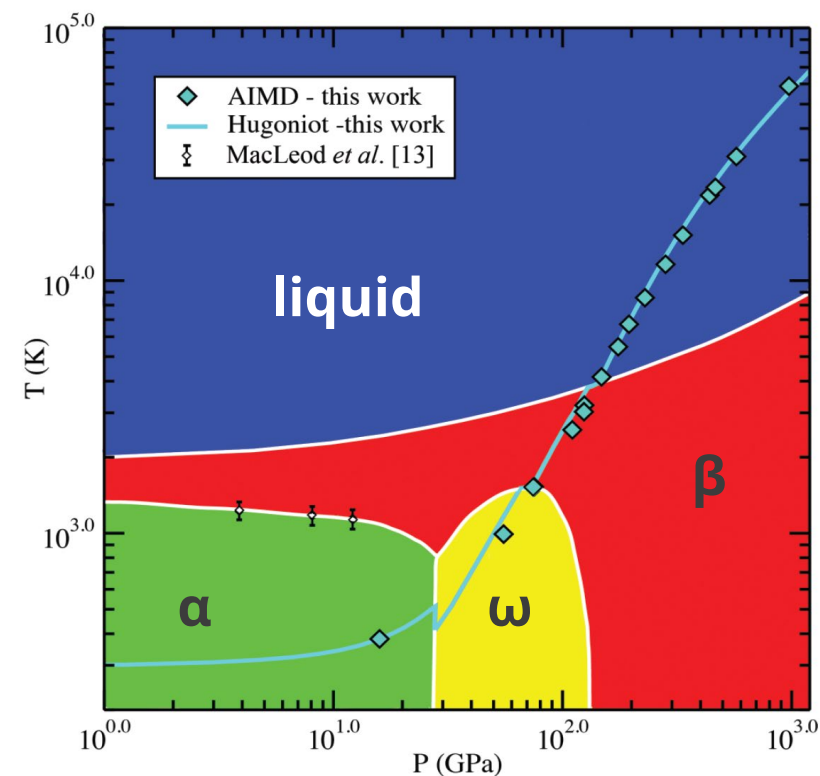
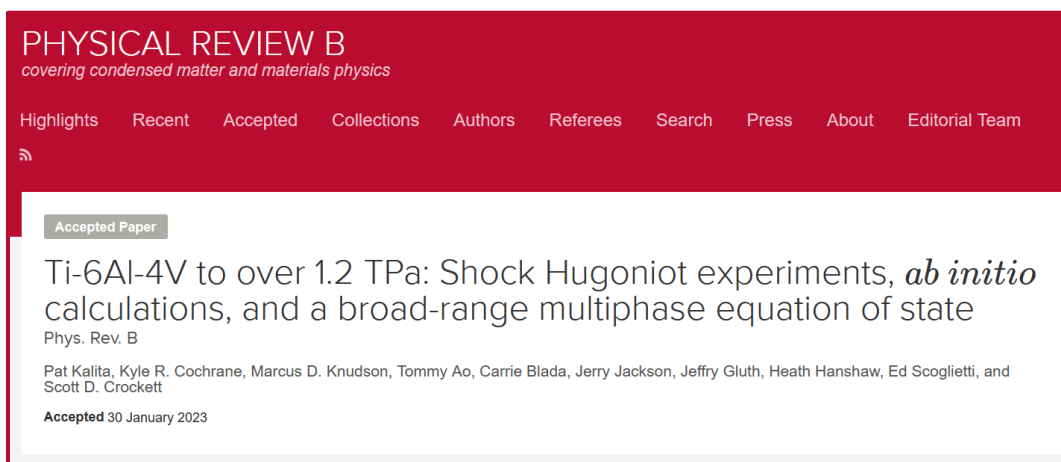
AIMD calculations





Ti64 alloy: Takeaways

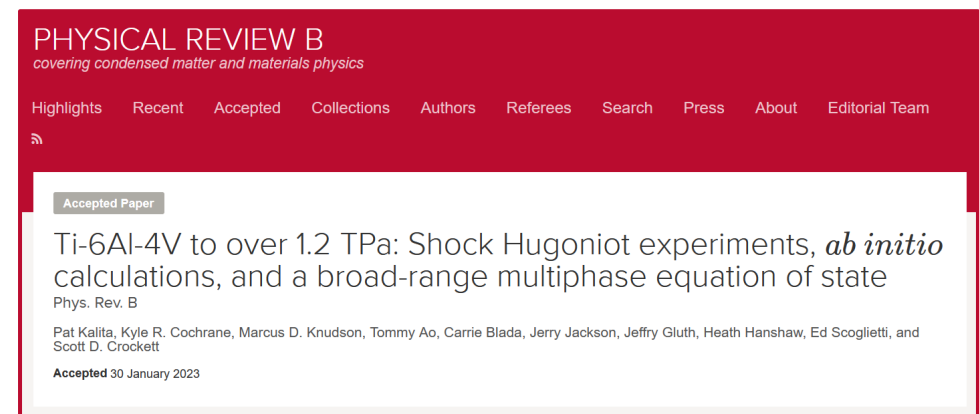
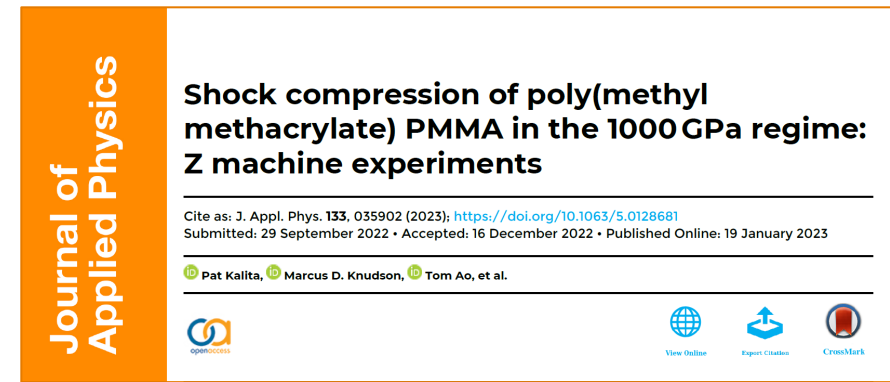
- New shock Hugoniot data are from the Sandia Z machine 0.21 TPa - 1.27 TPa
- our AIMD calculations in excellent agreement with Z data
- Shock melt on Hugoniot is lower than previously calculated
- we developed a high-fidelity, multiphase EOS of Ti64, SESAME EOS 92966, spanning a broad range of T and P
- Hugoniot $U_s(u_p)$ can be used in dynamic experiments



Conclusions

- Z is an “engine of discovery” for a wide range of HED science
- ~1/3 of our Z shots are dynamic material properties experiments
- Cutting edge shock compression research is moving towards ever increasing pressure or stress states into > TPa range
- Shock experiments on Z allow to understand the high P-T behavior of materials and...
- ...create accurate equation of state models based on experimental data

<https://journals.aps.org/prb/accepted/3c07c090J741fd4061ee3b303fa03d1fb33f395c3>
<https://journals.aps.org/prb/abstract/10.1103/PhysRevB.105.224109#>
<https://aip.scitation.org/doi/10.1063/5.0128681>



Backup slides

Sandia's Z Pulsed Power Facility

The Earth's largest pulsed power machine: The central focus of today's talk

Z Building

An aerial photograph of the Sandia Z Pulsed Power Facility. The facility is a large industrial complex with several large buildings, including a prominent white building with a flat roof labeled 'Z Building'. There are numerous yellow and blue storage tanks, parking lots with many vehicles, and various smaller structures. The surrounding area is arid and desert-like.

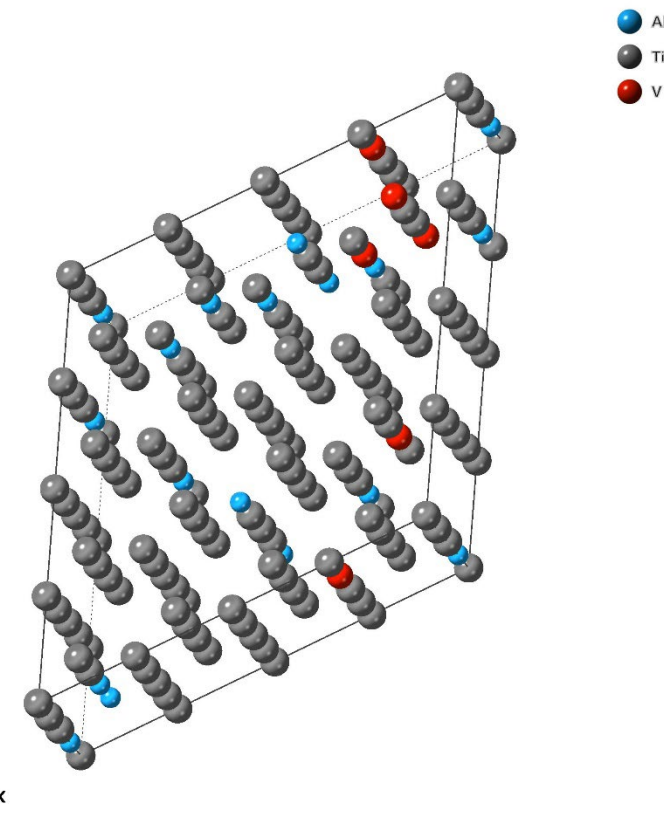


Ti64: DFT calculations of the cold curve & AIMD calculations of the Hugoniot EOS



AIMD - ab initio molecular dynamics simulations:

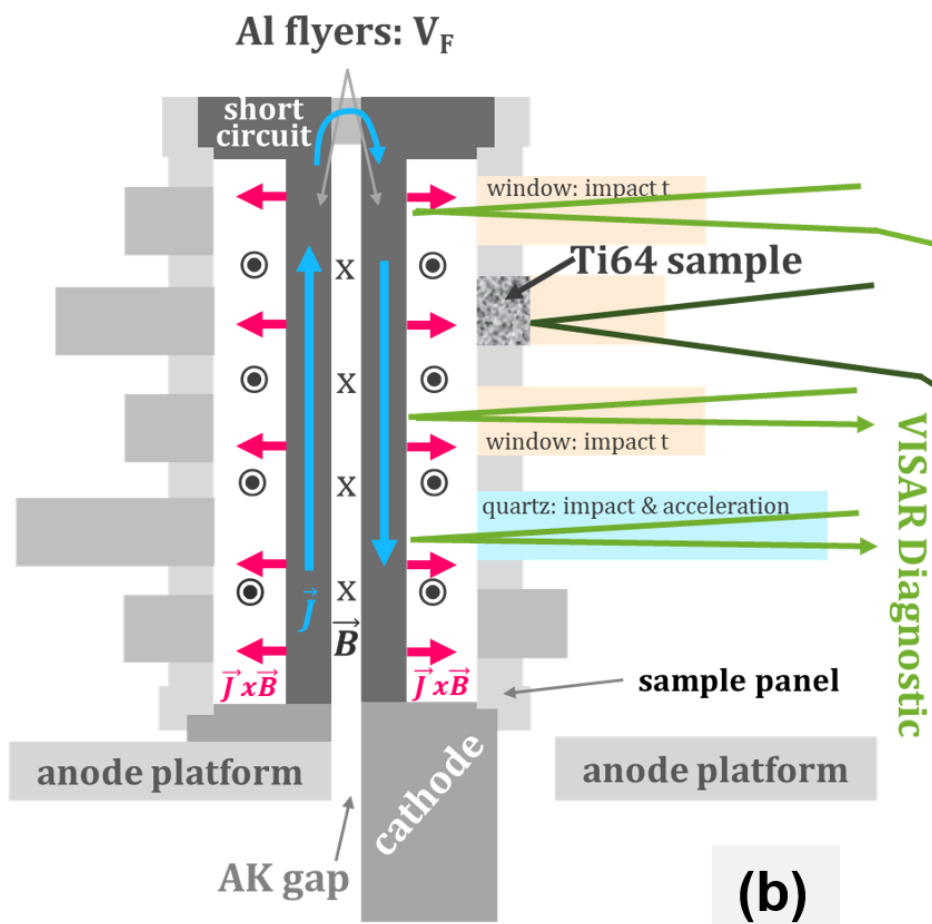
- performed in the canonical (NVT) ensemble with Mermin's generalization of the **Kohn-Sham** equations to finite T
- exchange-correlation energy computed with the parameterization of Perdew, Burke, and Ernzerhof (**PBE**)
- In Kohn-Sham equations, the nuclei were represented by a projector augmented wave (PAW) method. Pseudopotentials contained Al: 3 electrons; Ti: 12 electrons; V: 13 electrons
- The k-point mesh was Monkhorst-Pack [30] $2 \times 2 \times 2$ for a 128 atom hcp cell.
- vanadium 4 wt% and aluminum 6 wt% were rounded to an integer number of 5 and 13 atoms, which were substituted randomly into the titanium lattice using the ATAT code, because DFT is not realistically capable of looking at grain boundary effects.
- only examined the α Ti-64 phase assuming that the contribution to the reference state by β grain boundary would be small.
- good agreement between **DFT** and **SESAME** Hugoniot
- SESAME EOS melt density is consistent with DFT and experiments





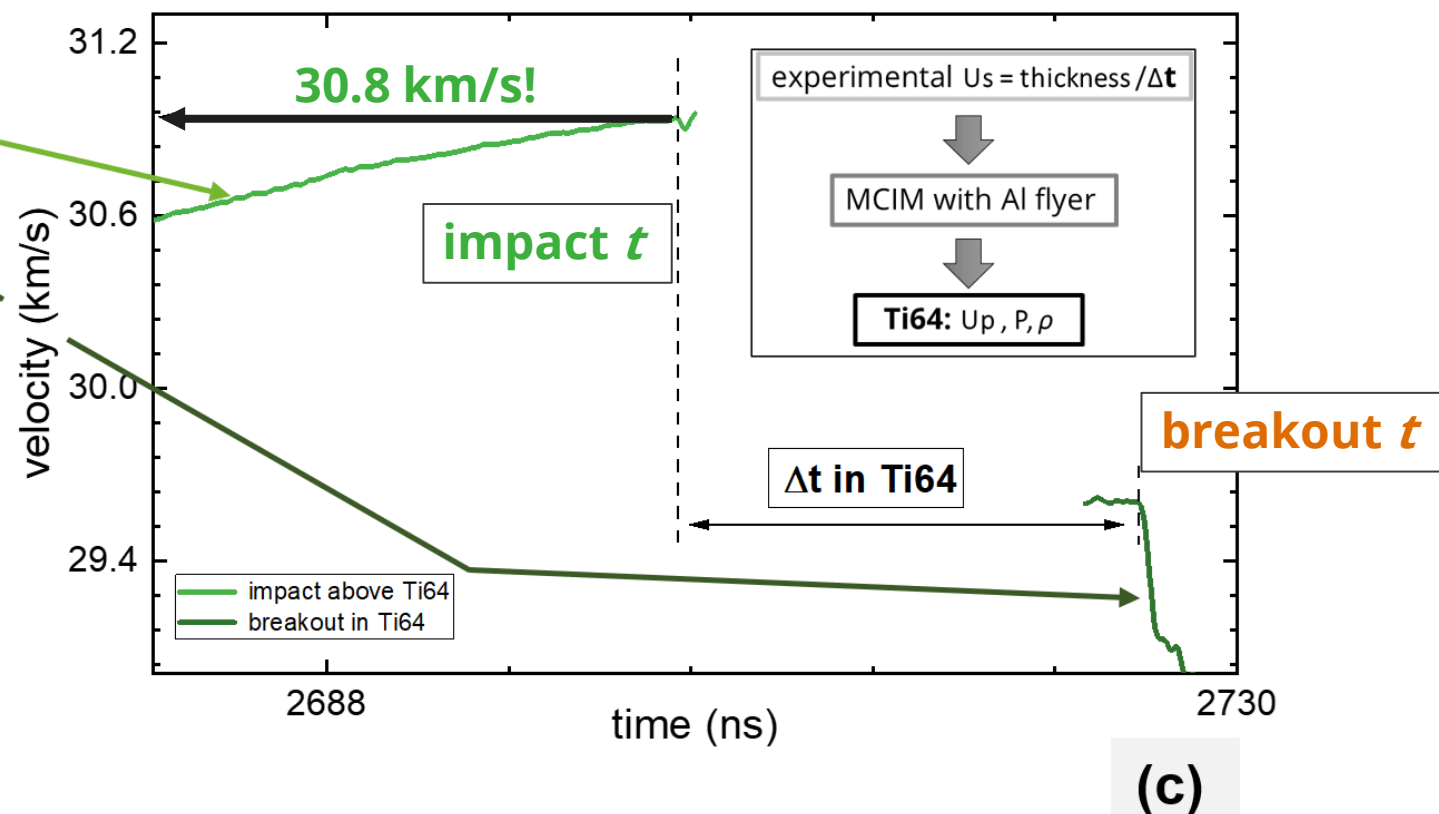
Ti64 alloy: Hugoniot shock experiments on SNL Z Machine

2-sided symmetric stripline config. 25-40 km/s

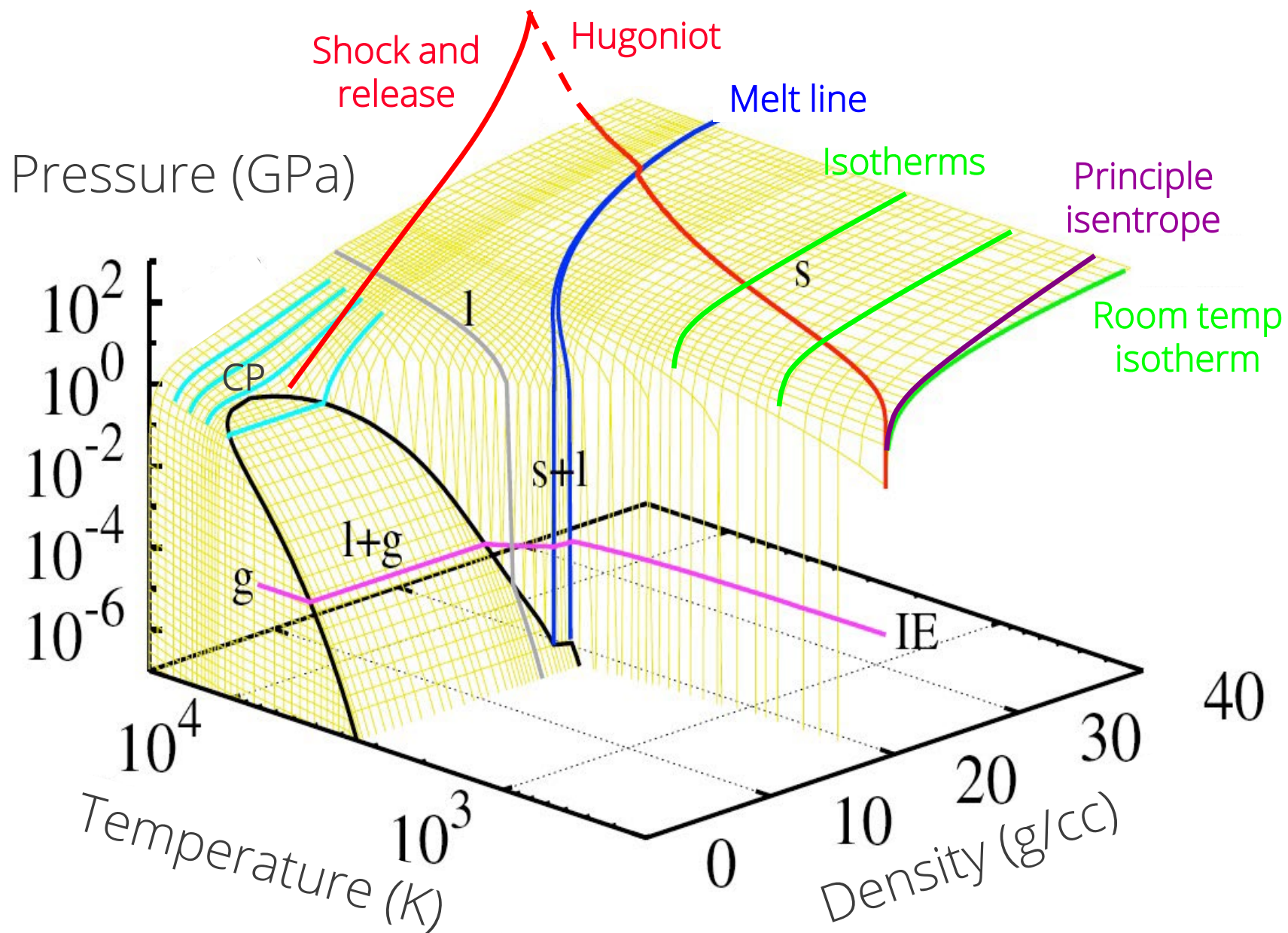


(b)

key diagnostic: VISAR (532nm)



(c)

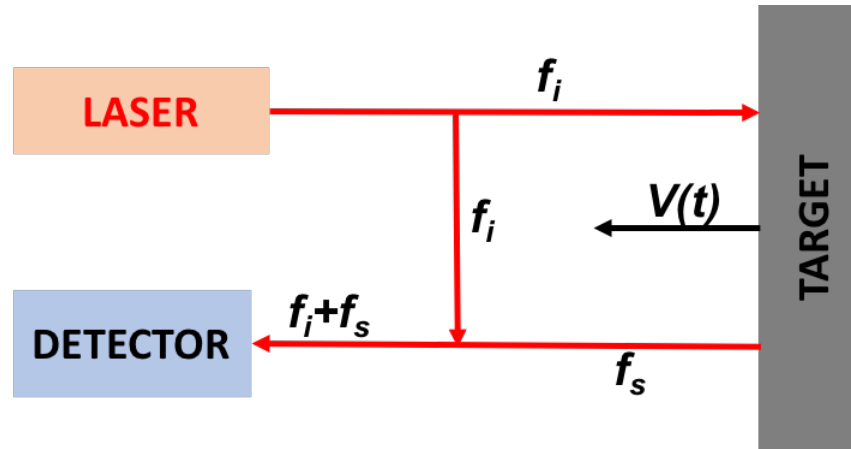




Experimental Methods for Shock Compression

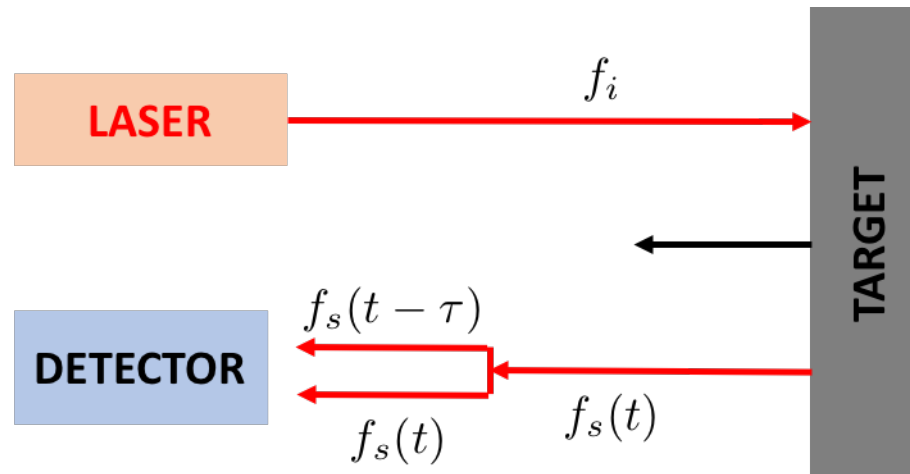


Primary Diagnostics: Velocimetry



Displacement Interferometer (PDV)

$$B = |f_s - f_i| = \frac{2v}{\lambda_i}$$



Velocity Interferometer (VISAR)

$$v(t) \approx \frac{\lambda_i}{2\tau(1 + \delta)} g(t)$$

No "fringing" at constant velocity

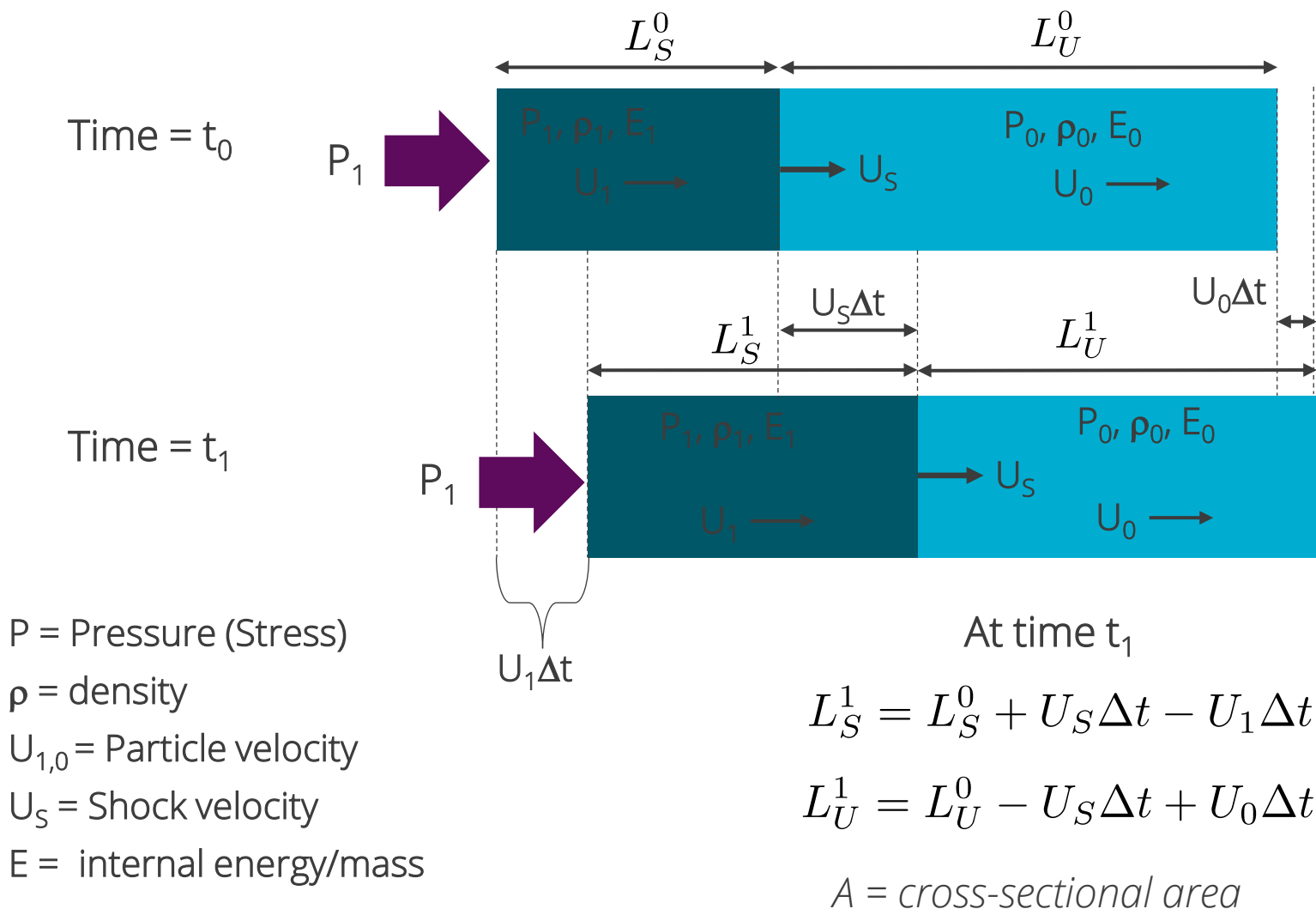
609 m/s
1460 m/s

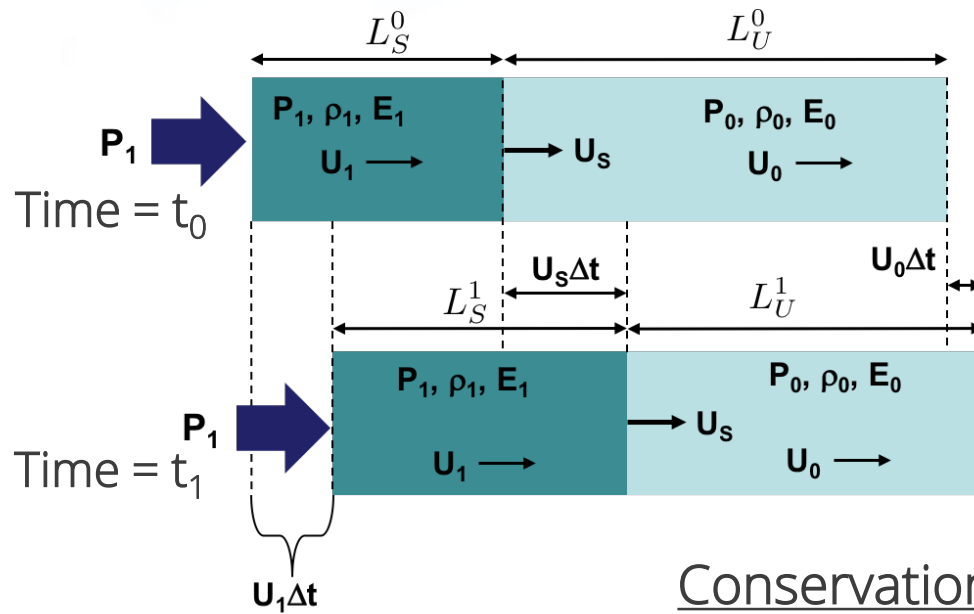
1060 m/s
2290 m/s



Hugoniot: The Equations

The Hugoniot equations are a results of the conservation laws





At time t_1

$$L_S^1 = L_S^0 + U_S \Delta t - U_1 \Delta t$$

$$L_U^1 = L_U^0 - U_S \Delta t + U_0 \Delta t$$

$A = \text{cross-sectional area}$

Conservation of Mass

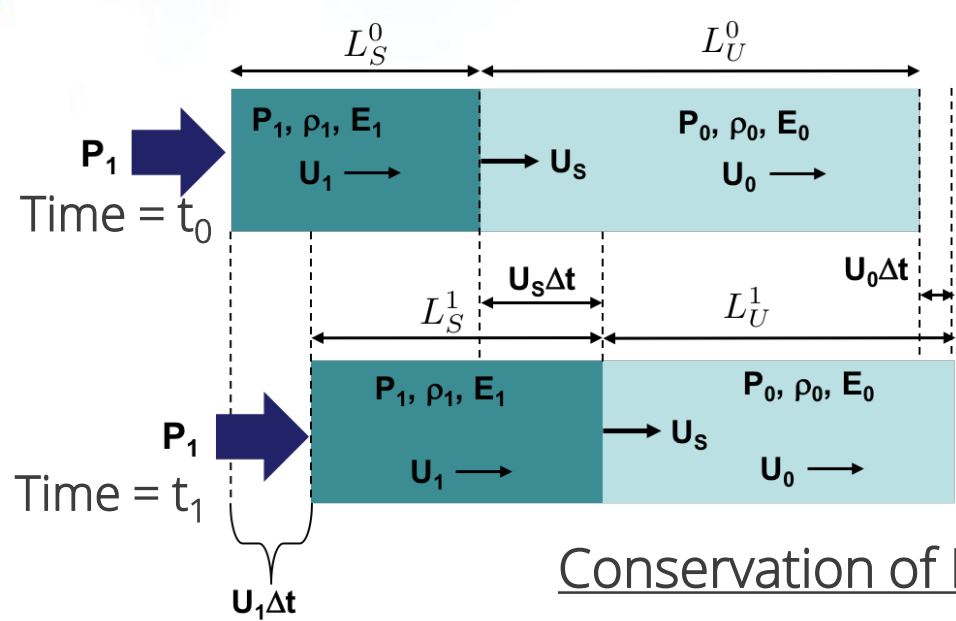
Mass at $t_0 = \text{mass at } t_1$

$$\rho_0 L_S^0 A + \rho_1 L_U^0 A = \rho_0 L_S^1 A + \rho_1 L_U^1 A$$

$$\rho_0 L_S^0 A + \rho_1 L_U^0 A = \rho_0 (L_S^0 + U_S \Delta t - U_1 \Delta t) A + \rho_1 (L_U^0 - U_S \Delta t + U_0 \Delta t) A$$

•
•
•

$$\rho_0 (U_S - U_0) = \rho_1 (U_S - U_1)$$



At time t_1

$$L_S^1 = L_S^0 + U_S \Delta t - U_1 \Delta t$$

$$L_U^1 = L_U^0 - U_S \Delta t + U_0 \Delta t$$

Conservation of Momentum

A change in momentum must equal the applied impulse

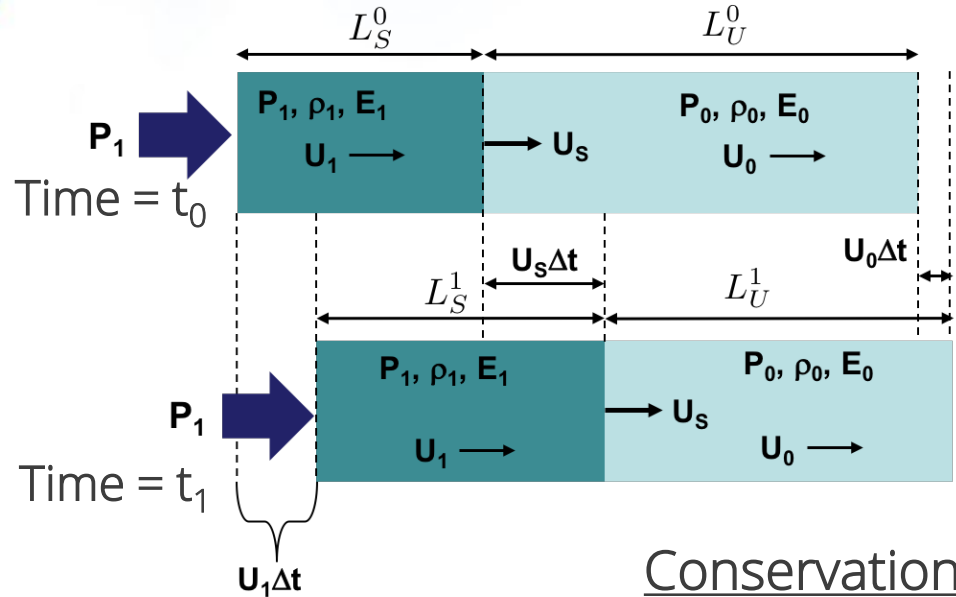
Impulse $F \Delta t = (P_1 - P_0) A \Delta t$

$\Delta(\text{Momentum})$ $\rho_0 L_U^1 A U_0 + \rho_1 L_S^1 A U_1 - \rho_0 L_U^0 A U_0 - \rho_1 L_S^0 A U_1$

$$(P_1 - P_0) A \Delta t = \rho_0 (L_U^0 - U_S \Delta t + U_0 \Delta t) A U_0 + \rho_1 (L_S^0 + U_S \Delta t - U_1 \Delta t) A U_1 - \rho_0 L_U^0 A U_0 - \rho_1 L_S^0 A U_1$$

•
•
•

$$P_1 - P_0 = \rho_0 (U_S - U_0) (U_1 - U_0)$$



At time t_1

$$L_S^1 = L_S^0 + U_S \Delta t - U_1 \Delta t$$

$$L_U^1 = L_U^0 - U_S \Delta t + U_0 \Delta t$$

$$\Delta W = (P_1 A)(U_1 \Delta t) - (P_0 A)(U_0 \Delta t) = E_{Total}(t_1) - E_{Total}(t_0)$$

$$E_{Total}(1) = E_0 \rho_0 L_U^1 A + E_1 \rho_1 L_S^1 A + \frac{1}{2} \rho_1 L_S^1 A U_1^2 + \frac{1}{2} \rho_0 L_U^1 A U_0^2$$

$$E_{Total}(0) = E_0 \rho_0 L_U^0 A + E_1 \rho_1 L_S^0 A + \frac{1}{2} \rho_1 L_S^0 A U_1^2 + \frac{1}{2} \rho_0 L_U^0 A U_0^2$$

⋮

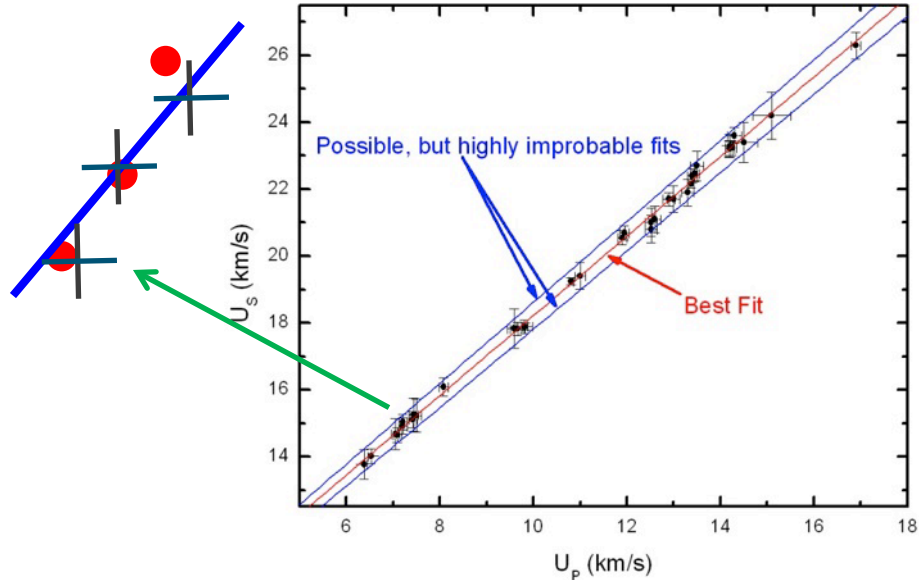
$$V = \frac{1}{\rho}$$

$$E_1 - E_0 = \frac{1}{2} (P_1 + P_0) (V_0 - V_1)$$

Monte Carlo (MC) Impedance Matching

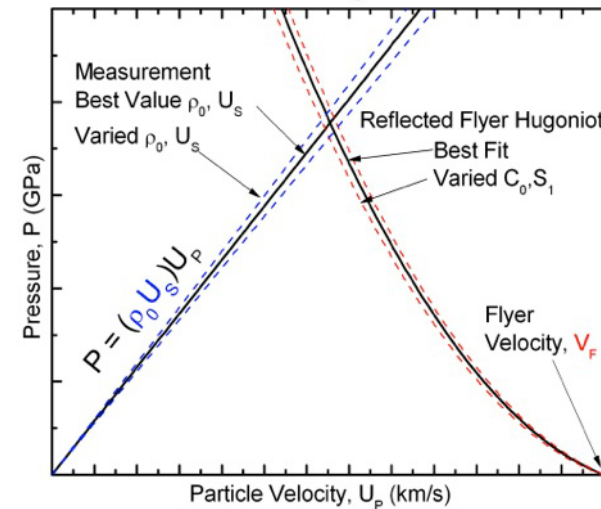
Flyer: Aluminum

- Uncertainty in experimental data (Knudson *et al.*, JAP 2003)
- Vary each U_S - U_P point by an uncorrelated random number with σ = expt. Uncertainty
- Solve for linear fit parameters
- Determine mean, σ , and correlation of fit parameters



Sample

- Vary measured parameters (V_F , U_S , ρ_0) with uncorrelated random numbers, σ = experimental uncertainty
- Vary AI fit parameters using correlated random numbers
- Calculate U_P , P , and ρ
- Determine mean and σ



Monte Carlo technique accounts for all experimental uncertainty and propagates the AI standard's error into the sample or window data.