Dynamic Material Properties
Experiments Using Pulsed Magnetic Compression

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  – Ta samples and equation of state
Outline

• Pulsed Compression on the Z Accelerator

• High-Stress Isentropic compression measurements
  – Tantalum

• High-Pressure Hugoniot measurements
  – Quartz

• Melting of Diamond in the Multi-Mbar Regime
Magnetic compression on Z enables access to a large region of the equation of state surface.
The Sandia Z Machine

Marx generator
Laser-triggered gas switch
Insulator stack
Transmitting lines

Experiment

22 MJ stored energy
~25 MA peak current
~200-600 ns rise time
Magnetic compression on Z produces smooth ramp loading to ultra-high pressures

- pulse of electric current through rectangular coaxial electrodes (shorted at one end) induces magnetic field
- $J \times B$ magnetic force transferred to electrode material

$P = \frac{B^2}{2\mu_0}$

$J \cdot E$

plasma – gas – liquid – solid
Fully self-consistent, 2-D MHD simulations required to accurately predict experimental load performance.

10 mm wide stripline

$t = 3050$ ns
Success requires integration of theoretical, computational, and experimental capabilities.

- Tentative sample EOS & Load Design
- Magnetic Field $B(t)$ in AK Gap Behind Sample
- Load Current $I_{LOAD}(t)$ Including 2D/3D Effects
- MITL Current $I_{MITL}(t)$ Including Losses
- Machine Settings
- Actual Shot

- 1-D Alegra MHD with Dakota optimization
- 2-D Alegra MHD, strip-line approximate method
- Need accurate time-dependent loss model!
- Bertha circuit model

- MITL Current Data
- Quasi-Isentrope
- Velocity Data
- Unfold analysis

QMD
Two platforms have been developed for accurate equation of state studies – both major advances

Isentropic Compression Experiments (ICE)*

Magnetically driven Isentropic Compression Experiments (ICE) to provide measurement of continuous compression curves to ~4 Mbar - previously unavailable at Mbar pressures

* Developed with LLNL

Magnetically launched flyer plates

Magnetically driven flyer plates for shock Hugoniot experiments at velocities to > 40 km/s - exceeds gas gun velocities by > 5X and pressures by > 10X with comparable accuracy
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Ramp compression provides a measure of the stress-density response of a material to peak stress.

- requires simple right-going waves
- compression is usually quasi-isentropic due to dissipative phenomena (plastic work, viscosity, thermal conduction, etc.)

Conservation equations:

\[ d\sigma_x = \rho_0 c_L du \]

\[ \frac{d\rho}{\rho^2} = \frac{du}{\rho_0 c_L} \]

Hugoniot

Isentrope

\[ c_L(u) = \Delta x_L / \Delta t \]

\[ x_L = 0.8 \text{ mm} \]

\[ x_L = 1.2 \text{ mm} \]
High-stress ICE experiments place stringent demands on wave profile measurements

Very high Lagrangian sound speeds at high stress result in small transit times – this places stringent demands on timing accuracy.

~100 ps timing accuracy required to obtain ~1% accuracy in density.

Simulated Free-Surface Data
Al (3700) to 600 GPa

Thicknes Difference $\Delta x = 300 \, \mu m$
The rapid increase in sound speed requires pulse shaping to delay shock formation.

\[ x_L = \frac{c^2}{dc/dt} \]

**Pulse shaping delays intersection of loading characteristics.**

**Early formation of shock at**

**Effective loading histories**

**Snapshots from 1-D simulations**

**Shot Z864** standard pulse

**Shot Z1190** shaped pulse

0 0.5 1.0 1.5 2.0

0 100 200

0 200

0 200

0 0.8 mm 1.8 mm

Lagrangian position (mm)

Longitudinal stress (GPa)

Time (ns)
This process was followed to design an ICE experiment on Ta to 400 GPa.

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  - Need accurate time-dependent loss model!
- MITL Current $I_{MITL}(t)$ Including Losses
  - Bertha circuit model
- Machine Settings
- Actual Shot
- QMD
- Unfold analysis
- MITL Current Data
- Velocity Data
- Quasi-Isentrope
Desired current is determined through several iterative 1-D and 2-D MHD simulations.
Independently triggerable gas switches provide the variability necessary for pulse shaping.

18 independently triggerable groups of 2 transmission lines.
The Bertha circuit model enables fairly accurate prediction of machine performance.

**Current comparison**

- **Targeted**
- **Unfolded**

**Wave profile comparison**

- Measured (VISAR)
- Simulated (Targeted B-Field)
- Simulated (Unfolded B-Field)

**SHOT Z1841**

- **755 μm Ta**
- **1050 μm Ta**
Data have been obtained which enable extraction of the Ta isentrope to nearly 400 GPa.
The extracted isentrope discriminates between various tabular equations of state for Ta ± 2-3% in density.
We are pursuing a single sample technique to take advantage of the relative large sample thickness.

- Dakota optimization framework drives Alegra 1-D MHD simulations
- \( B(t) \) represented by constrained cubic spline (25-50 points) with time shift and stretch factors
- Objective function is metric of isometry between simulated and experimental velocity history at electrode back surface

MHD simulations:
- High confidence in aluminum EOS and conductivity models
- High spatial resolution (2.5-\( \mu \text{m} \) cells)
Single sample yields isentrope by iterating inverse analysis with simulated “zero-thickness” velocity

1. measure velocity at back faces of sample and opposite electrode
2. use optimization to determine $B(t)$ from electrode measurement
3. use $B(t)$ and first-guess sample EOS (Sesame table + strength) to simulate electrode/sample interface “zero-thickness” velocity
4. perform inverse Lagrangian analysis on simulated “zero-thickness” velocity and measured back-face velocity of sample
5. convert resulting $\sigma_x(\rho)$ curve to full tabular EOS by assuming constant $c_V$ and $\Gamma/V$, equating stress to pressure (strength folded into EOS)
6. use $B(t)$ and new tabular EOS to simulate electrode/sample interface
7. repeat steps 4-6 until material response converges
Outer loop of single-sample approach converges

result changes < 0.015% from 6\textsuperscript{th} to 7\textsuperscript{th} iteration

\begin{center}
\begin{tikzpicture}[scale=0.7]
\begin{axis}[
    title={Z1884-Top (Ta)},
    xlabel={Density (g/cc)},
    ylabel={$\frac{(P_i - P_{i-1})}{P_{i-1}}$},
    legend style={at={(0.5,-0.3)},anchor=north},
    grid=both,
    xmin=15, xmax=30,
    ymin=-0.025, ymax=0.010,
]
    \addplot[blue,mark=none] table[x expr=	hisrowno{0}+1,y={0},col sep=comma]{data.csv};
    \addplot[orange,mark=none] table[x expr=	hisrowno{0}+2,y={0},col sep=comma]{data.csv};
    \addplot[pink,mark=none] table[x expr=	hisrowno{0}+3,y={0},col sep=comma]{data.csv};
    \addplot[green,mark=none] table[x expr=	hisrowno{0}+4,y={0},col sep=comma]{data.csv};
    \addplot[blue,mark=none] table[x expr=	hisrowno{0}+5,y={0},col sep=comma]{data.csv};
    \addplot[orange,mark=none] table[x expr=	hisrowno{0}+6,y={0},col sep=comma]{data.csv};
    \addplot[pink,mark=none] table[x expr=	hisrowno{0}+7,y={0},col sep=comma]{data.csv};

    \legend{Iteration #2, Iteration #3, Iteration #4, Iteration #5, Iteration #6, Iteration #7}
\end{axis}
\end{tikzpicture}
\end{center}
Single-sample measurement of tantalum to 320 GPa decreases uncertainty over two-sample measurement.

Graph showing stress or pressure (GPa) vs. density (g/cc) for different samples of tantalum. The graph includes lines for LANL Sesame 90210 (Greeff et al), average Z1491, Z1511, Z1683 (Eggert et al), Z1841-Top (stripline, 2-sample 750/900μm), Z1884-Top (stripline, 1-sample 900μm), and uncertainty bounds.
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• Melting of Diamond in the Multi-Mbar Regime
With proper pulse shape and design the anode can be launched as an effective high-velocity flyer plate.
Quartz has been used as a transparent window enabling multiple flyer velocity measurements.

Typical configuration:

C targets (500, 750, and 1000 μm) (6 mm Φ)

Quartz (or Sapphire) windows (4mm Φ)

Flyer plate

VISAR diagnostics

VISAR provides highly accurate in line flyer plate and quartz shock velocity measurements

Knudson, et al., PRL 103, 225501 (2009)
$U_s - u_p$ Hugoniot for $\alpha$-Quartz

\[ U_s = a + bu_p - cu_p e^{-du_p} \]

Knudson, et al., PRL 103, 225501 (2009)
Pressure – density Hugoniot for $\alpha$-Quartz

Knudson, et al., PRL 103, 225501 (2009)
$U_s$ residuals with respect to the Z-fit indicate dissociative effects extend to much higher pressure.
QMD calculations provide unique insight into the dynamics of the fluid at multi-Mbar pressures.

Differences in Z- and $\Omega$-fits will have a significant impact on quantities inferred from quartz $U_s$.

Knudson, et al., PRL 103, 225501 (2009)
Recently published deuterium data becomes significantly stiffer upon reanalysis.

Errors in density compression, $\eta$, are given by the error in quartz $u_p$ multiplied by the factor $(\eta - 1)$.
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• Melting of Diamond in the Multi-Mbar Regime
Several chemical picture models for diamond

Reflectivity study on Omega suggests complete melt near 1100 GPa

Existing models for diamond exhibit a broad range of predicted melt behavior – melt poorly understood.
Quantum Molecular Dynamics calculations provided estimates for melt and predicted a triple point (TP)
The proposed TP is manifest on the Hugoniot by significant changes in compressibility.
Relatively large flyer plates enabled multiple, redundant measurements increasing accuracy.

C targets (500, 750, and 1000 µm) (6 mm φ)

Quartz (or Sapphire) windows (4mm φ)

Diamond experimental configuration

Flyer plate

VISAR diagnostics

The Z platform provided extremely accurate measurements of the diamond Hugoniot

Flyer velocities

- Multiple samples and diagnostics allowed for redundant measurements for increased accuracy
- Transparency of the diamond samples allowed for in-line measurement of impact velocity and shock transit time
- Impact velocity and shock speed measurement provides tight constraint on the inferred particle velocity and density

This accuracy allowed for quantitative comparison with QMD predictions and evidence of the TP.
Both the three and four piece fits indicate significant changes in slope at ~9.1 and ~10.85 km/s.

Both suggest the onset of melt just below ~700 GPa.

The three piece linear fit would suggest completion of melt below 900 GPa
  - ~200 GPa below the saturation in reflectivity.

The four piece fit is consistent with Bradley, et al. and suggest a TP at ~860 GPa.
The breakpoints of the four segment fit are in excellent agreement with those predicted by QMD.

The slope of each segment is also in excellent agreement with the slopes predicted by QMD.

This level of agreement provides validation:
- Strongly suggests the presence of a higher pressure solid phase of carbon above ~860 GPa.
- Magnetic ramp compression is enabling new regions of a material’s phase diagram to be explored under dynamic compression

- Obtaining unprecedented accuracy in the multi-Mbar pressure regime both on and off-Hugoniot

- Future direction will be to couple advanced capabilities to ramp compression facilities
  - Pre-heat capability
  - Sample recovery
  - Advanced diagnostics
    - pyrometry
    - x-ray diffraction

Conclusion