SAND2015-10717C

Exceptional service in the national interest

Sandia National Laboratories

STAR
Shock Thermodynamics Applied Research

Dynamic Integrated Compression Experimental Facility

Pulsed Power Sciences
Harnessing Extreme Environments

Pulsed Power Sciences: High Energy Density Physics

Scott Alexander
Bill Reinhart

Academic Alliance Materials Workshop: December 9-10, Georgia Tech

U.S. DEPARTMENT OF ENERGY   NNSA National Nuclear Security Administration

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Unclassified Unlimited Release (UUR):

Sandia National Laboratories Material Science Center

- The Nation's Stockpile Stewardship Program as well as other National Security Programs demand that experimental results be detailed in pertinent models to predict/model those results
- Sandia National Laboratories is one of a few institutions in the world with a major high pressure/high temperature condensed matter physics program
- Sandia has an institutional triad (STAR, DICE, Z) that can cover the full pressure range (few kbars to Mbar) for material property studies
  - Z Facility: Pulsed Power
    - Flyer plate experiments (Shock Hugoniot)
    - Ramp (Isentrope), Shock Ramp (Off-Hugoniot states)
  - STAR Facility (Gas and Propellant driven launchers)
    - Shock, quasi-isentropic, flyer plate experiments
      - Hugoniot and Off-Hugoniot, Ballistic Studies, Fracture Fragmentation
  - DICE Facility: Gas Gun and Small Pulsed Power Machine (VELOCE)
    - Technique and diagnostic development

Shock Thermodynamics Applied Research

Dynamic Integrated Compression Experimental Facility

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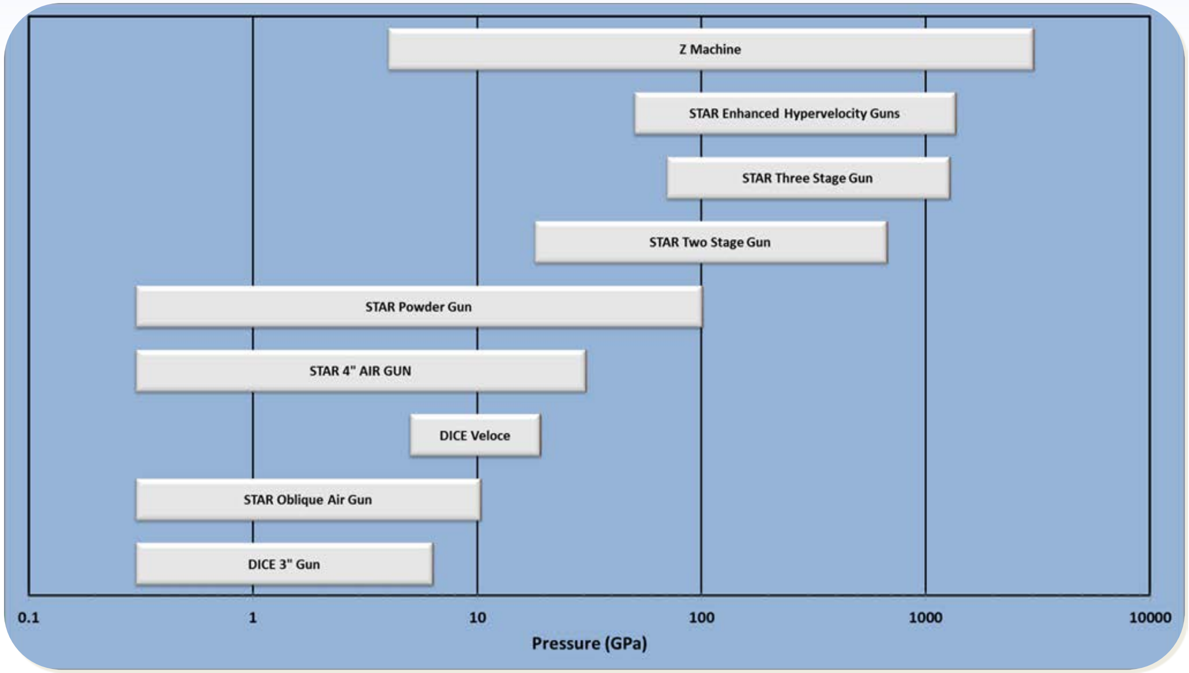
Dynamic Material Properties are Important to National Security Initiatives



- **National Security Initiatives: Stockpile Stewardship, Life Extension Programs, Science Programs, Defense, etc…**
  - **High-fidelity tabular EOS required for Hydrodynamic Simulations**
- **Z Machine, STAR and DICE provide launcher and pulsed power platforms providing equation of state, code validation,**
  - **both shock and isentropic compression experiments**

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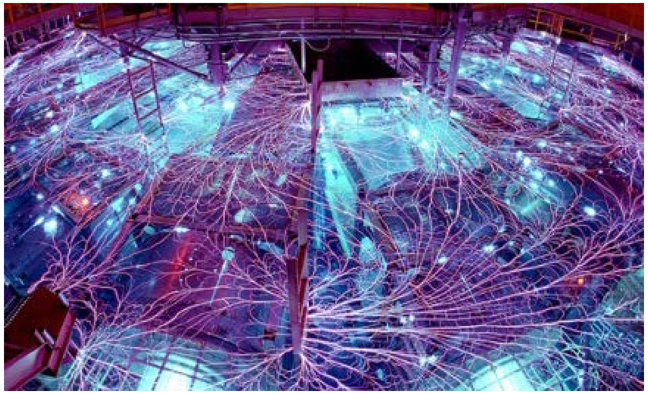
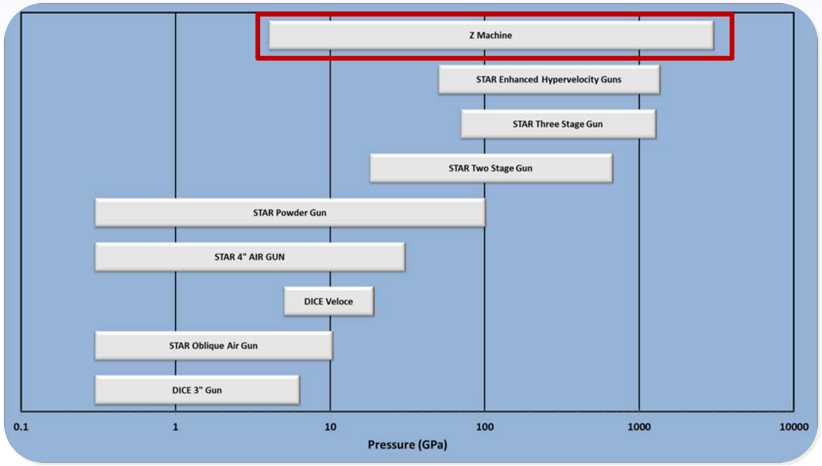
Dynamic Material Properties are Important to National Security Initiatives

Z compresses electrical energy in both space and time . . .

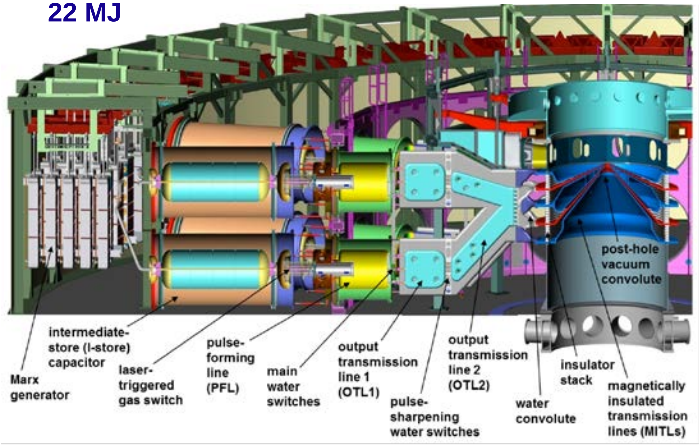




20 TW
22 MJ

80 TW
8 MJ

Charge for 3 minutes to reach 85 kV

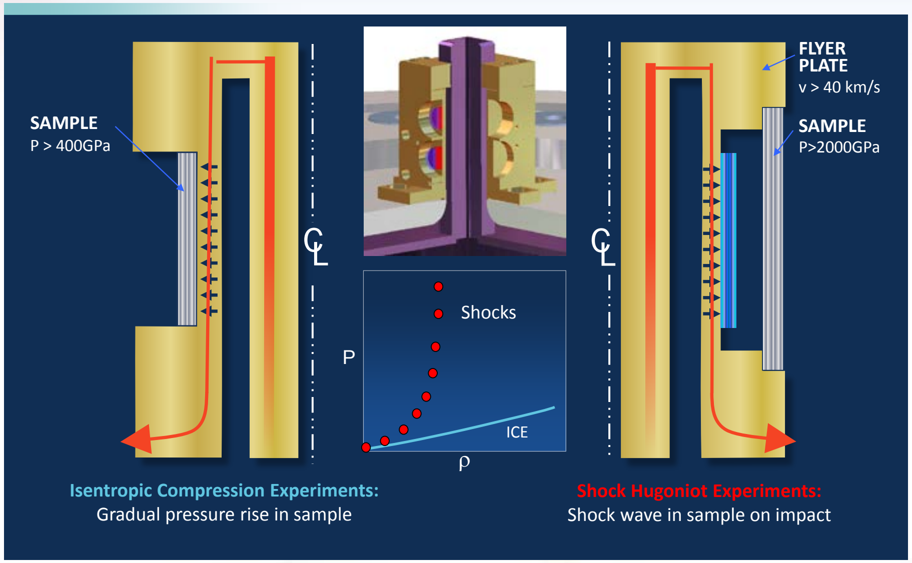


330 TWs & 2.5 MJ of x-ray output in a few ns

Use magnetic fields to create High Energy Density matter for physics applications

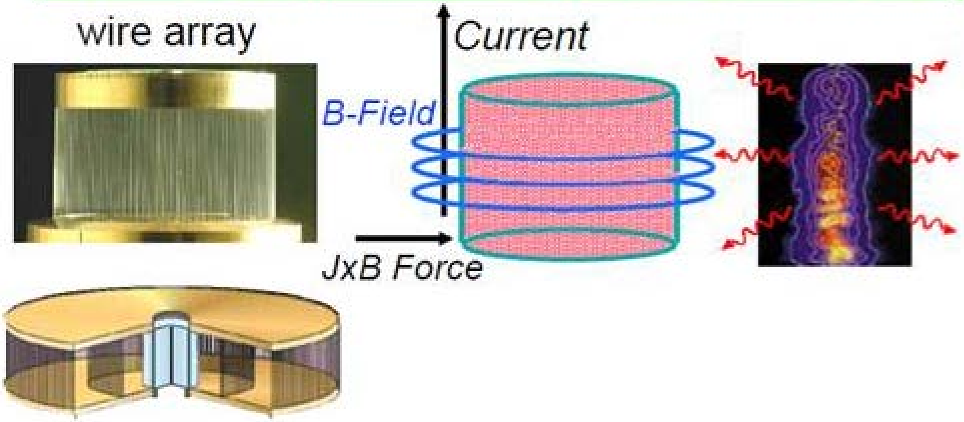
- **Dynamic Material Properties**
- **Z pinch, X-ray Sources, ICF**
- **Magnetically Driven Implosions**

Harnessing the Magnetic Fields on Z

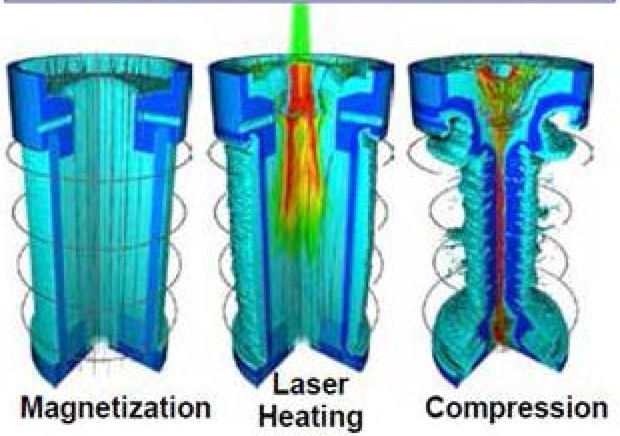


Dynamic Materials Testing

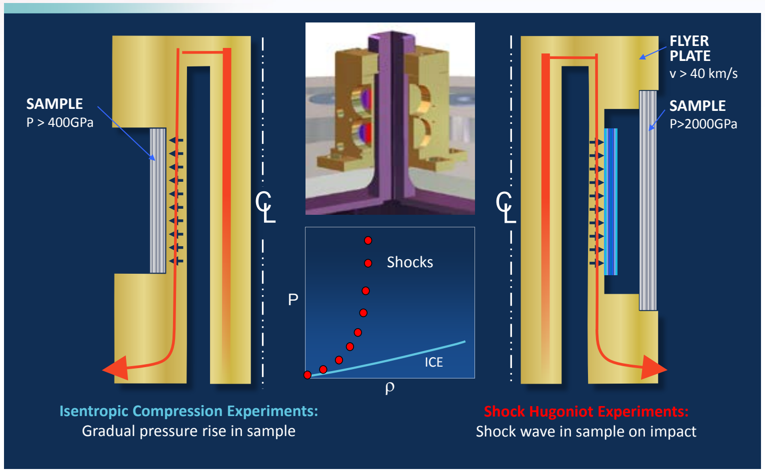
Z-Pinch X-ray Sources (RES, Rad. Physics)



Inertial Confinement Fusion



Isentropic compression and shock wave experiments: map different regions of phase space

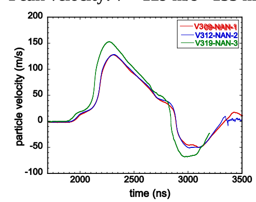


Ramp compression provides "low" temperature high pressure data

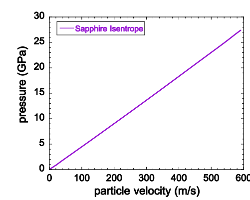
Synthesis of Nanostructured Materials through Magnetic Ramp Compression

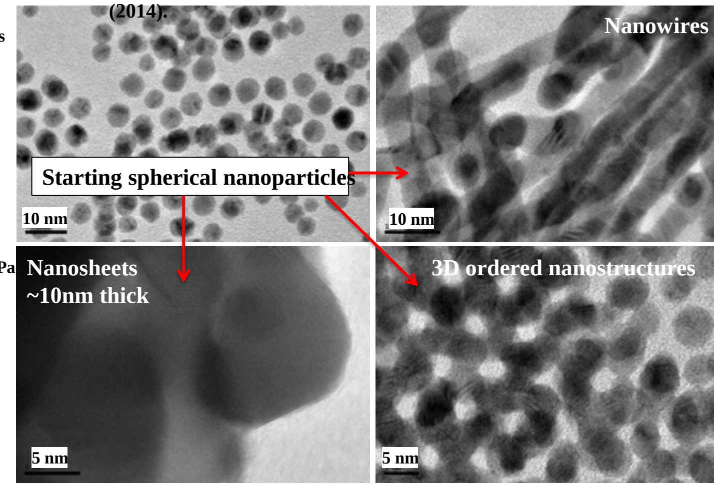
Li, B. *et al. Nature Commun.* 5:4179 doi: 10.1038/ncomms5179 (2014).

Peak velocity: v = 129 m/s - 153 m/s

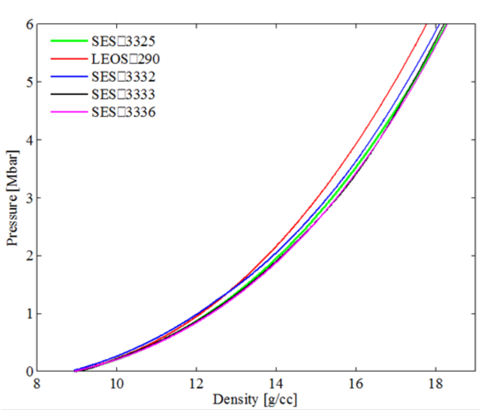


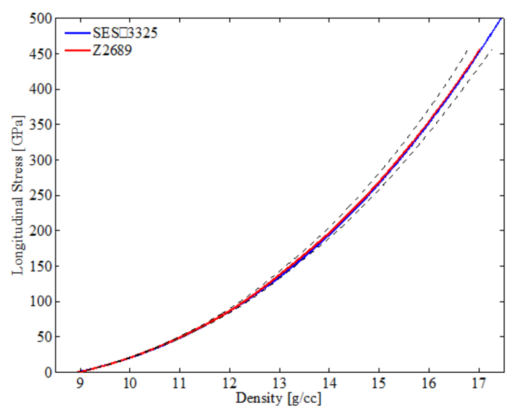
Peak pressure: P = 5.8 GPa - 7.0 GPa





(Contact Hongyou Fan, hfan@sandia.gov, 505-272-7128)



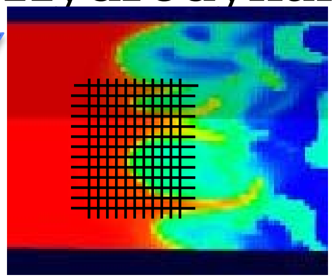


An external mechanical pressure overcomes balanced inter-particle interactions, enables consolidation of ordered nanoparticle arrays to form new one-three dimensional nanostructured architectures.

Material models determine the outcome of radiation and magnetohydrodynamic simulations

The hydrodynamics moves material based on the material properties.

Hydrodynamics

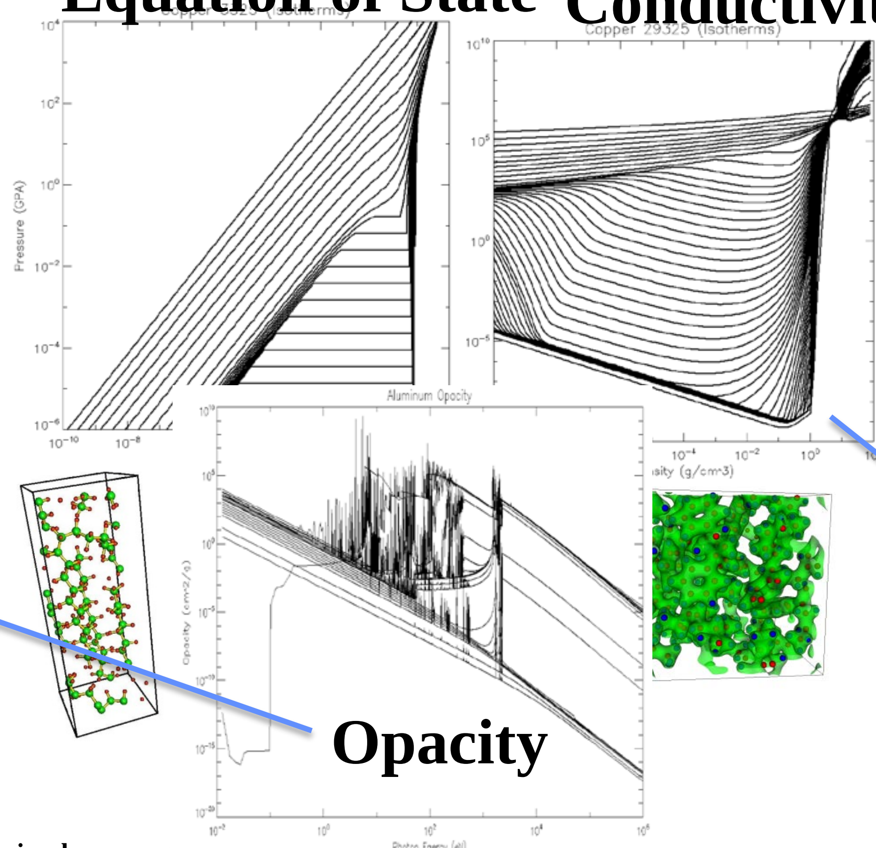


Tom Haill, SNL

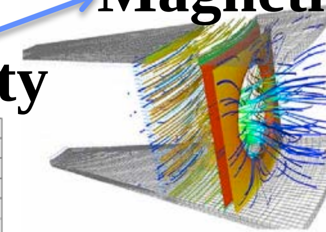
Most simulation codes will tally the total energy in each cell and, based on that energy and the density, compute a new pressure and temperature in preparation for the next hydrodynamic step.

Equation of State

Conductivity



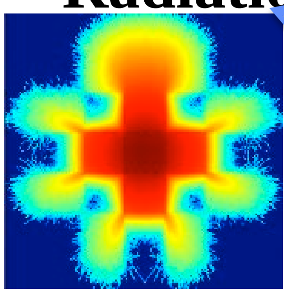
Magnetics



Chris Garasi, SNL

Conductivity determines magnetic field diffusion.

Radiation

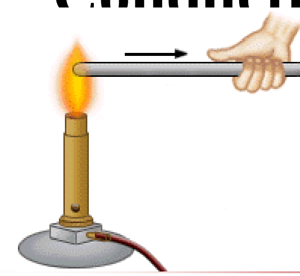


Tom Brunner, LLNL

Opacity

Radiation is a key energy transfer mechanism in some systems

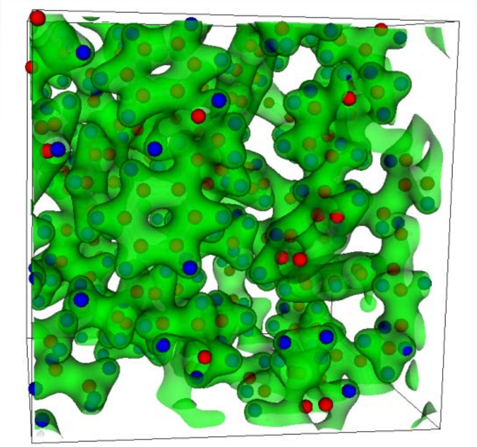
Conduction



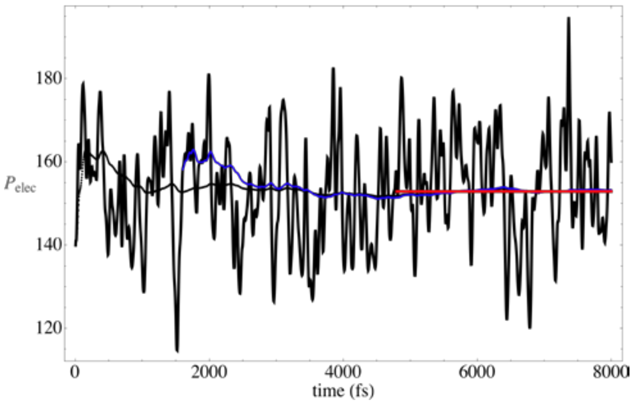
Thermal conduction augments the movement of energy in a simulation.

First-principles thermodynamics based on DFT-MD/QMD has been used extensively to develop material models

- **Warm dense matter**
  - Shock physics and planetary science
  - Traditional plasma models do not work
  - Neither do solid-state approaches (0K models, quasi-harmonic, etc)
- **DFT based finite-temperature MD has proven to be of high fidelity**
  - Electrons in thermal ground state (Mermin DFT)
  - MD simulations yield equilibrium properties
    - Pressure, energy, structure, entropy, and free energy
  - Transport properties (Kubo-Greenwood) from snapshots from the MD runs
    - Diffusivity, electrical- and thermal conductivity, viscosity
  - The approach has many names
    - DFT-MD, CPMD, AIMD, QMD, and FP-MD

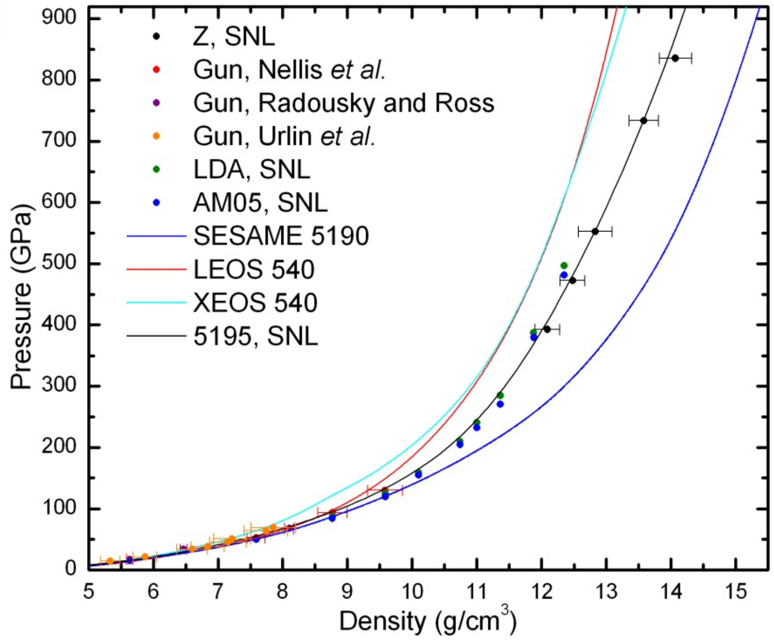


QMD simulation of a GDP polymer – an ablator material for indirect drive fusion



Electronic pressure in an 8 ps QMD simulation

We have seen tremendous scientific impact over the last ten years in combining high-fidelity theory/simulations/experiments



Shock Hugoniot in xenon predicted by DFT/QMD (calculations by Rudy Magyar, experiments by Seth Root: PRL 2010)

This DFT-MD based response of xenon were a true prediction – published before the experiments

- ***Predictive*** **DFT-MD simulations are transforming the design and interpretation of Z experiments**
  - **SCIENCE 322, 822-1825 (2008)**
  - **ICARUS 211, 798 (2011)**
  - **Phys. Rev. Letts.**
    - **2006, 2007, 2008, 2009, 2010, 2011, 2012, 2013, 2015**
  - **SCIENCE 348, 1455 (2015)**
  - **Many articles in PRB, PoP, JAP, JCP, etc.**

We perform multi-scale research – ranging from quantum mechanics to new advanced Magneto Hydrodynamics theory, -algorithms, and –codes.

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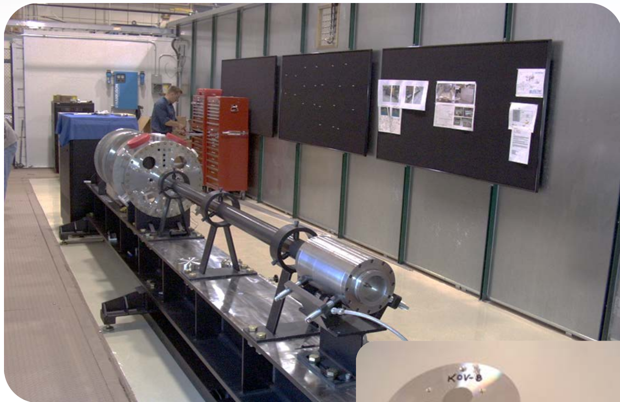
Dynamic Integrated Compression Experimental (DICE) facility

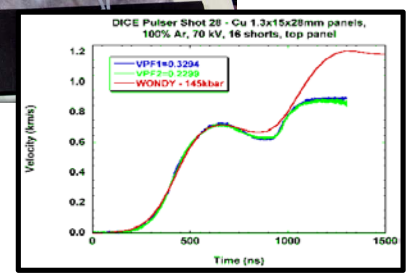


Light Gas Gun

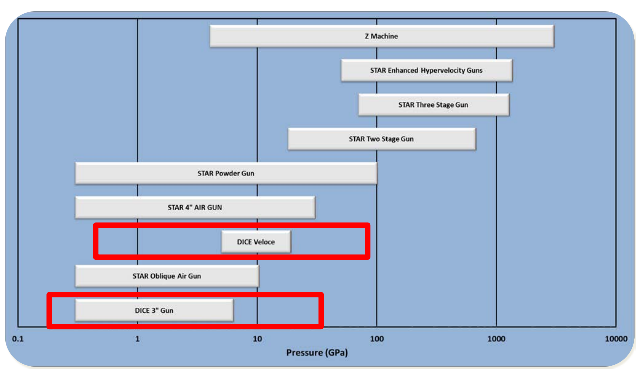
- Compressed gas driven
- 76 mm bore diameter
- 240-540 g projectile mass
- 80-450 m/s impact velocity
- 0.3-6 GPA (60kbar)
- VISAR, PDV
- Heated projectile
- Pre-heat/cooled samples
- Soft sample capture

VELOCE

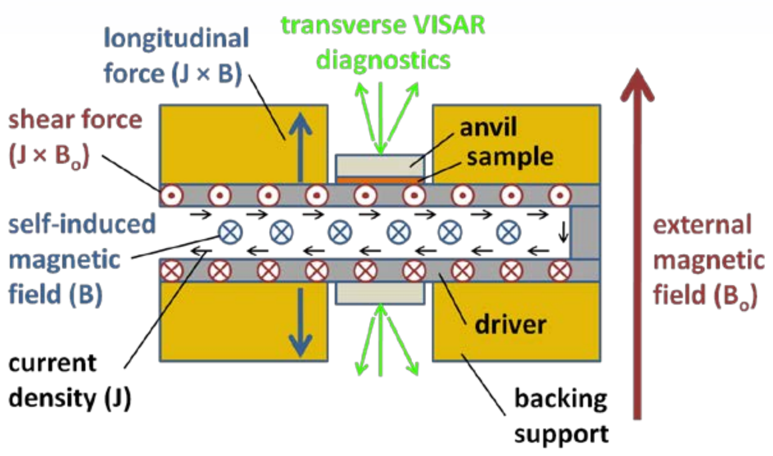
(small pulse power machine)

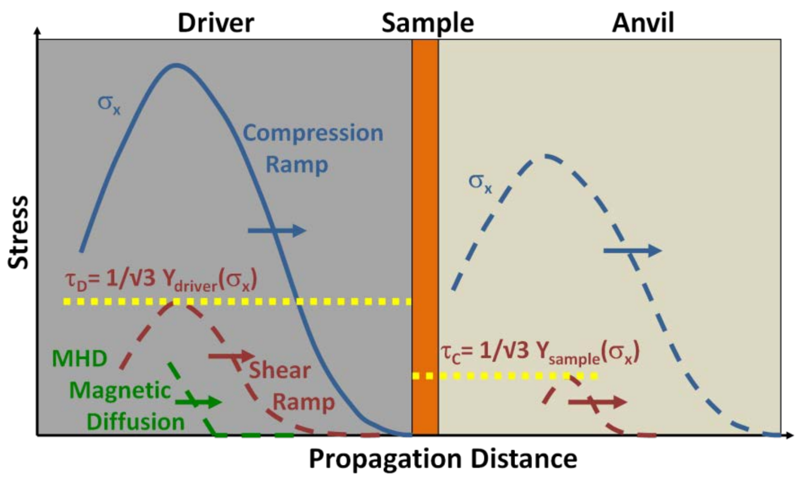


- 10-30 mm panels
- 8-26 mm sample diameter
- 420-540 ns rise times
- 5-14 GPA (140kbar)
- VISAR, PDV
- Sample Pre-Heating, Pre-Cooling
- Soft sample capture



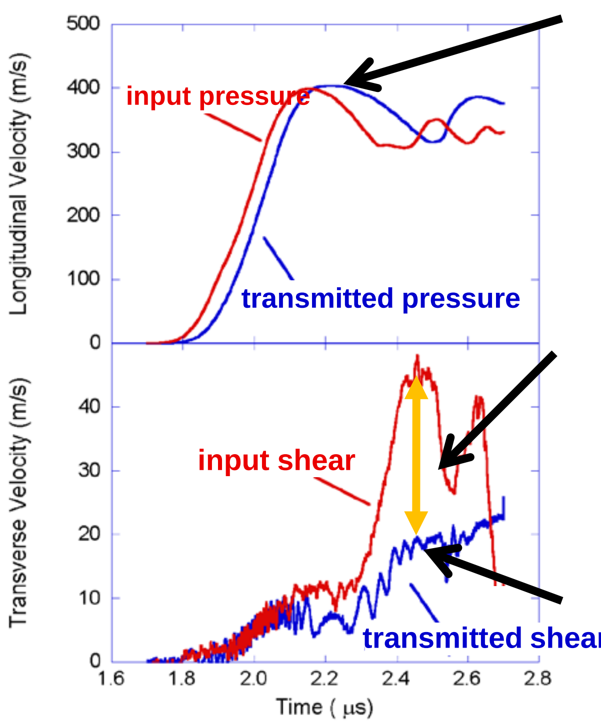
Techniques provide alternative approaches to strength measurement





Magnetically Applied Pressure-Shear (MAPS)

- Secondary applied magnetic field results in shear wave generation during pulsed power driven compression experiments
- Shear wave provides direct probe of strength



Pressure determined from longitudinal velocity

Shear wave magnitude is truncated by sample shear strength

Strength determined from transverse velocity

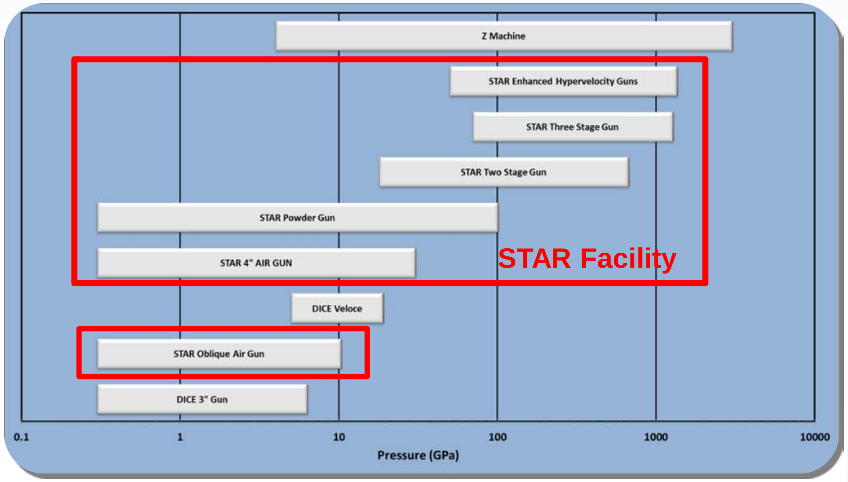
DICE: Future

THOR

- Faster current rise times
  - 200-500 ns
  - Peak current (200 ns): 7 MA
- Pulse shaping through independent, de-coupled switches
- Predicted to generate peak pressures of ~1 Mbar
- Enables a variety of experiments:
  - Soft Materials: Isentropic compression of cerium, lithium
  - Flat Top Pulse: Strength measurements
  - Shock-Ramp: Phase transition properties

Shock Thermodynamic Applied Research (STAR) Facility

The STAR Facility is the most comprehensive Equation of State (EOS) physics research and development facility in the western world testing at pressure regimes unattainable for other similar facilities utilizing laboratory launchers.



Three-stage Gun :
- 1 -19 mm bore diameter
- 7500 - 19000 m/s projectile/particle velocity
- 1300 GPa impact pressure
- 50 g High Explosives (HE)
- Ballistic and EOS applications

Two-stage light gas guns:
- 6 - 30 mm bore diameter
- 800 – 7500 m/s projectile velocity
- 650 GPa impact pressure
- 50 g HE
- EOS/Ballistic/Fragmentation applications

Multiple array of small caliber arms-conventional velocities:
- Ballistic applications

Single stage, smooth bore, powder gun:
- 89 mm bore diameter
- 400 – 2200 m/s projectile velocity
- 100 GPa impact pressure
- 150 g HE (Pre-Heat/Cooling capabilities)

Single stage, smooth bore, compressed light gas gun
- 100 mm bore diameter
- 0.01 – 1000 m/s projectile velocity
- 40 GPa impact pressure
- 50 g HE
- Pre-heat and cooling for targets

Keyed-bore Oblique gun
- Pressure/shear

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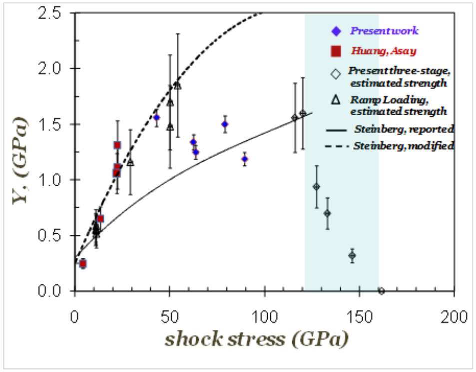
High Pressure Strength

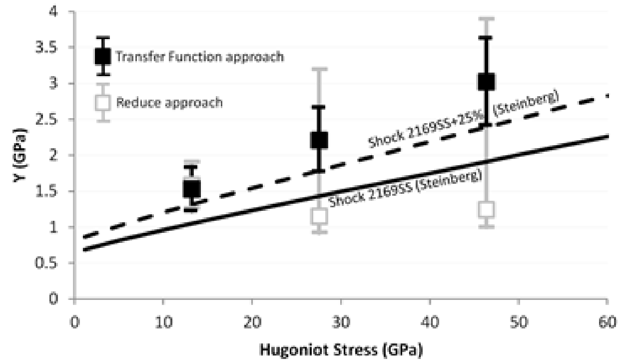
Sandia National Laboratories is world leader in high-pressure strength measurements for multiscale models on variety of materials

- **STAR Facility utilizing explosively welded impactors conducted experiments on the two and three stage light gas gun for investigating flow strength of aluminum**
- **Novel approaches in data analysis for strength measurements**
  - Self-consistent approach for both ramp and shock loading
    - **Aluminum:** Reinhart et. al., J. Dyn. Behav. Mater., V1, 275
    - **Stainless Steel:** Furnish et. al, J. Appl. Phys., 115, 033511
    - **Tantalum:** Brown et. al., J. Appl. Phys., 115, 043530

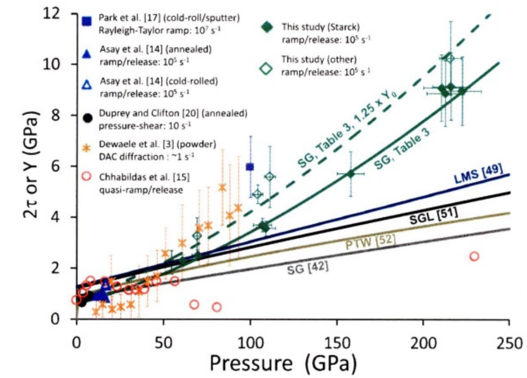
Aluminum: Strength estimates in aluminum can be off by factor of two without proper testing



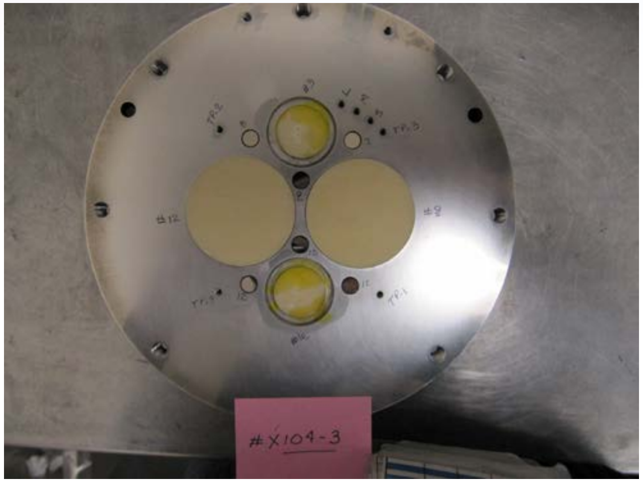
Stainless Steel: strength analysis suggests the flow strength increases with stress from ~1 GPa to ~ 2.5 GPa over the shock stress range



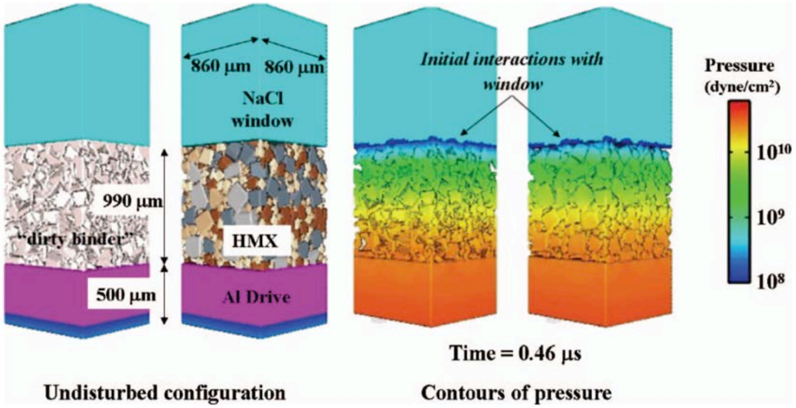
Tantalum: study the strength of material ramp compressed to between 60 and 250GPa



Mesoscale Response of Energetic Materials



Propagation test in IMX-104



Mesoscale CTH results for HMX

- Study detonation propagation in explosives
- STAR facility provides controlled environment for testing
- Insensitive munitions require less sensitive explosives
- Provide mesoscale modeling for not only TATB, HMX, and RDX based explosives, but on IHE where RDX is replaced (IMX-101) with other, less sensitive materials.
- Improved results provide greater reliability in hydrocodes

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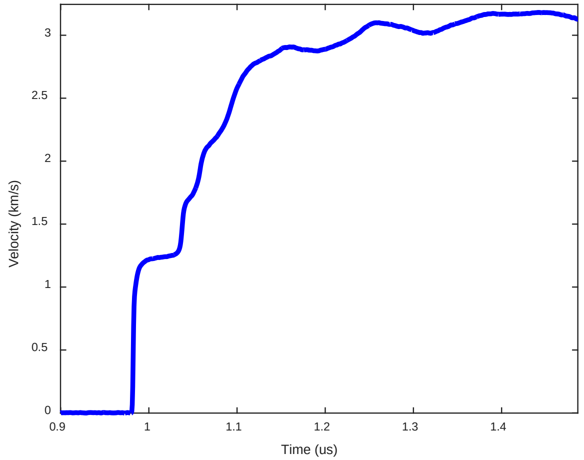
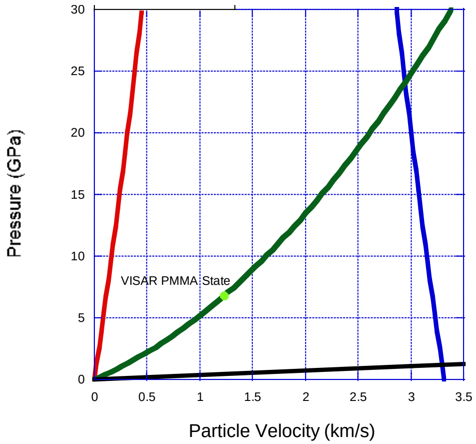
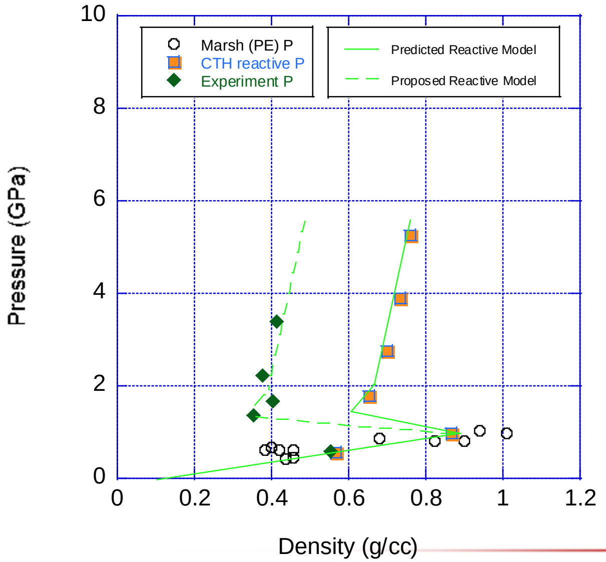
Dynamic response of foam

Shock compression of very low density micro-cellular materials allows entirely new regimes of hot fluid states to be investigated experimentally

- new data is necessary to develop complete equations-of-state including both inert and reactive states of foam.
- The STAR facility implementing new impact conditions to apply necessary pressure states in foam to investigate the reactive regime
    - Tests required to calibrate new models for foam (e.g. reactive decomposition) at higher shock pressures
- significant differences in the response of foam learned from recent experiments at STAR and has been instrumental in implementing improved models.



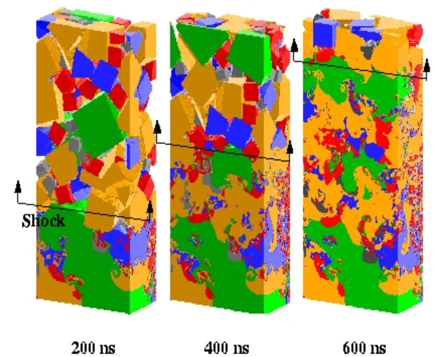


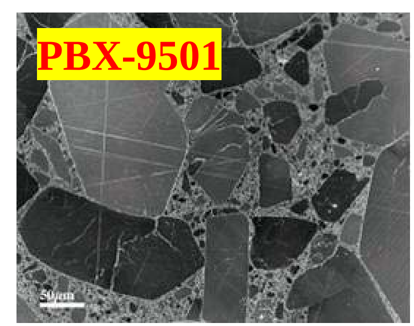


Dynamic Behavior of Heterogeneous Materials and Statistical Phenomena

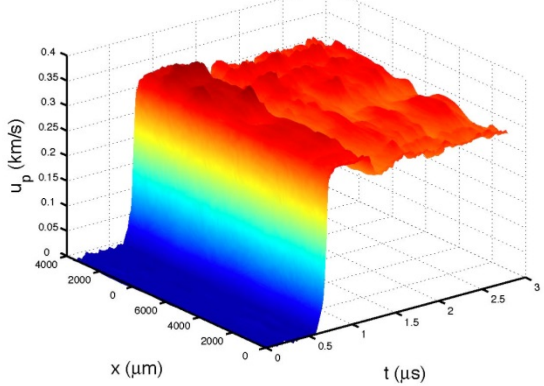
Heterogeneous materials are common, and phenomena at the scale of the heterogeneity control many aspects of behavior but are difficult to resolve with present diagnostics

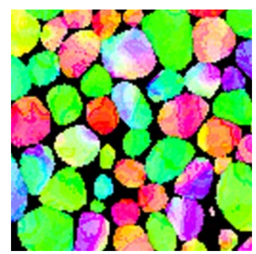
Energetic Materials



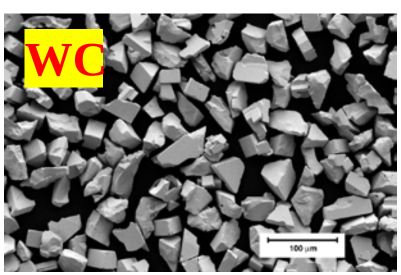


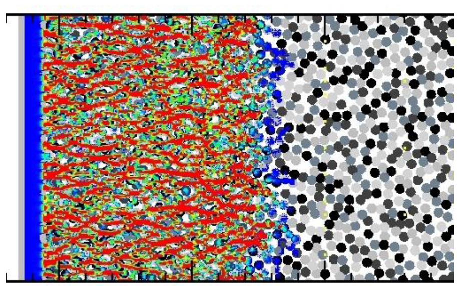
Two-Phase Alloys





Granular Materials

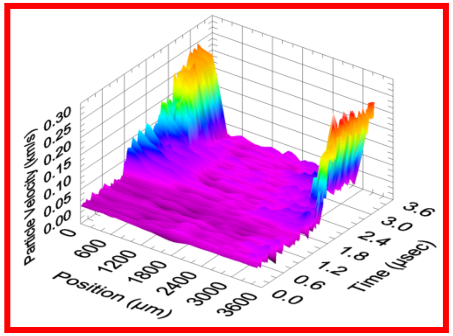


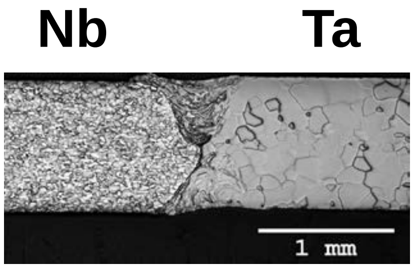


Statistical Aspects of Material Failure and Spatially-Varying Phenomena

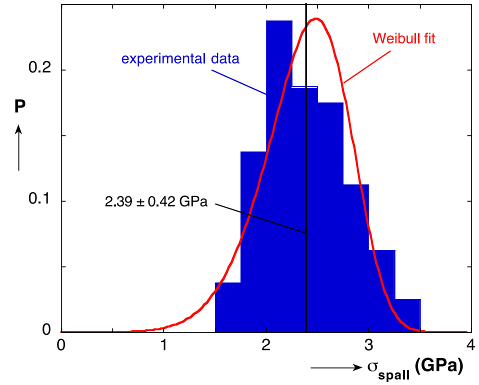
Even in nominally homogeneous materials, failure processes are heterogeneous due to local anisotropies and flaws.

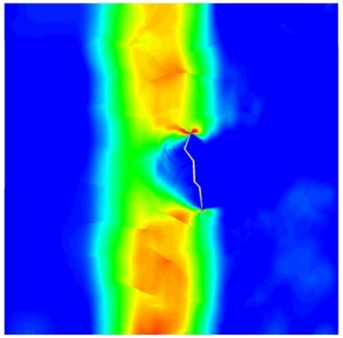
Welds and Material Joining



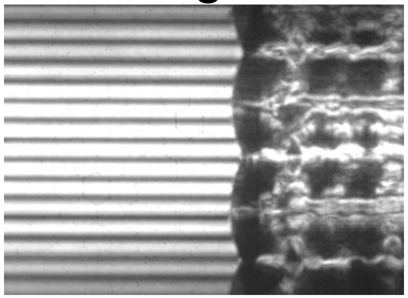


Spall Failure of Brittle Materials



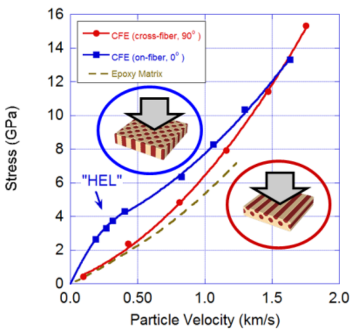


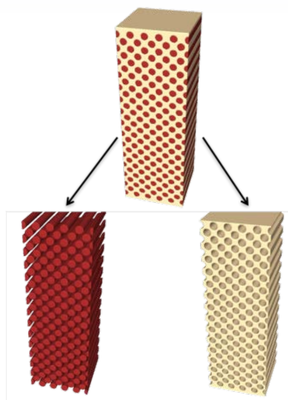
Perturbation Decay Experiments to Probe Strength and Viscosity

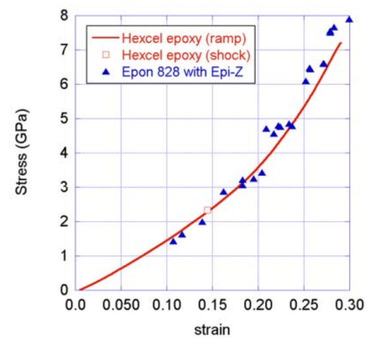


Engineering-scale features such as welds and holes introduce complex behavior, and spatially-resolved information needed in certain experiments

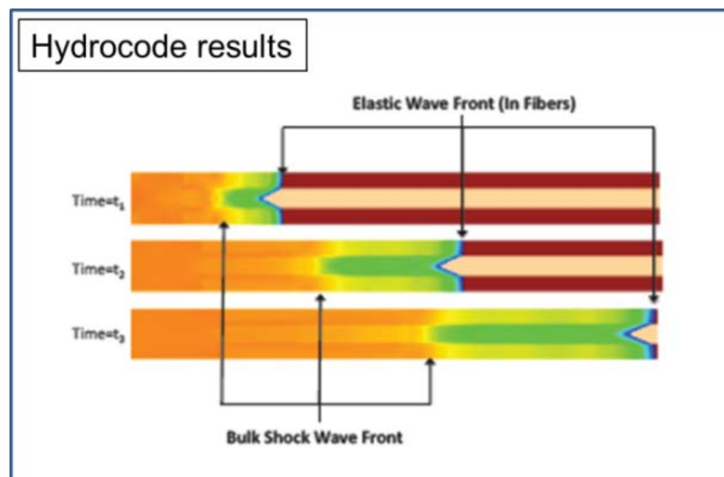
Dynamic Response of Armor Composite Materials







- STAR testing provides vital data used to model anisotropic materials
  - Moving beyond microscale
  - Separate fiber and binder
- Large scale testing was required due to heterogeneity in test materials
- Data is being used by all military branches as well as other DOE labs
  - Direct impact to warfighters



Academic Alliance Workshop: Tentative Agenda February 2016, Sandia National Laboratories, Albuquerque NM

Organizers: Amy Sun, Eliot Fang

Wednesday, February 10th, 2016. 12:00 – 5:30 pm

12:00 - 12:30 pm	Meet, building 960, room 1001
12:30 - 01:00 pm	Welcome Announcements(Sun)
	Introduction (Mattsson, Flicker)
	Review Focus Area(s) (Fang)
01:00 - 03:30 pm	SNL data Science, Materials under Extreme Environments*
	(15 minutes each, 8 talks)
03:30 - 05:30 pm	Tour of the Shock Thermodynamics Applied Research (STAR) Facility

Thursday, February 11th, 2016. 08:00 – 5:30 pm

08:00 - 09:00 am	Meet, Building A97-Announcements
09:00 - 10:00 am	Z Tour (tentative)
10:00 - 10:30 am	Break/Discussions
	Review Focus Area(s) (Fang)
10:30 - 12:00 am	SNL data Science, Multiscale Materials Science*
	(15 minutes each, 6 talks)
12:00 - 01:30 pm	Lunch
01:30 - 03:00 pm	Talks (15 minutes each, 6 talks)
03:00 - 03:30 pm	Break/Discussions
03:00 - 04:00 pm	Talks (Continuation of Multiscale Materials or other topics)
04:00 – 04:45 pm	Discussions: Moderated by Fang, McDowell, Sun
04:45 – 05:00 pm	Recruiting/Business Processes
05:00 - 05:30 pm	Closing – Path Forward (Sun, Fang, All)

*Focus Area I and III

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