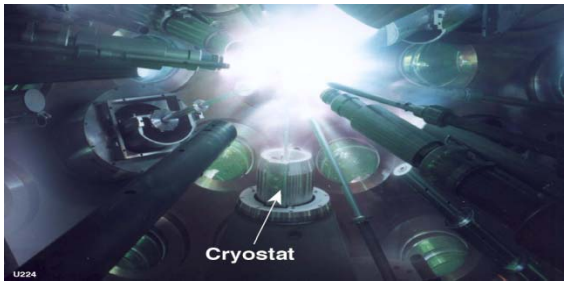
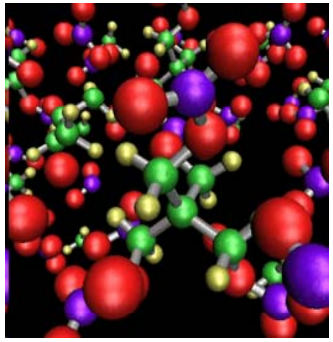
Materials under extreme conditions

Kathleen Alexander
Los Alamos National Laboratory





Stewardship Science Graduate Fellowship
Annual Conference

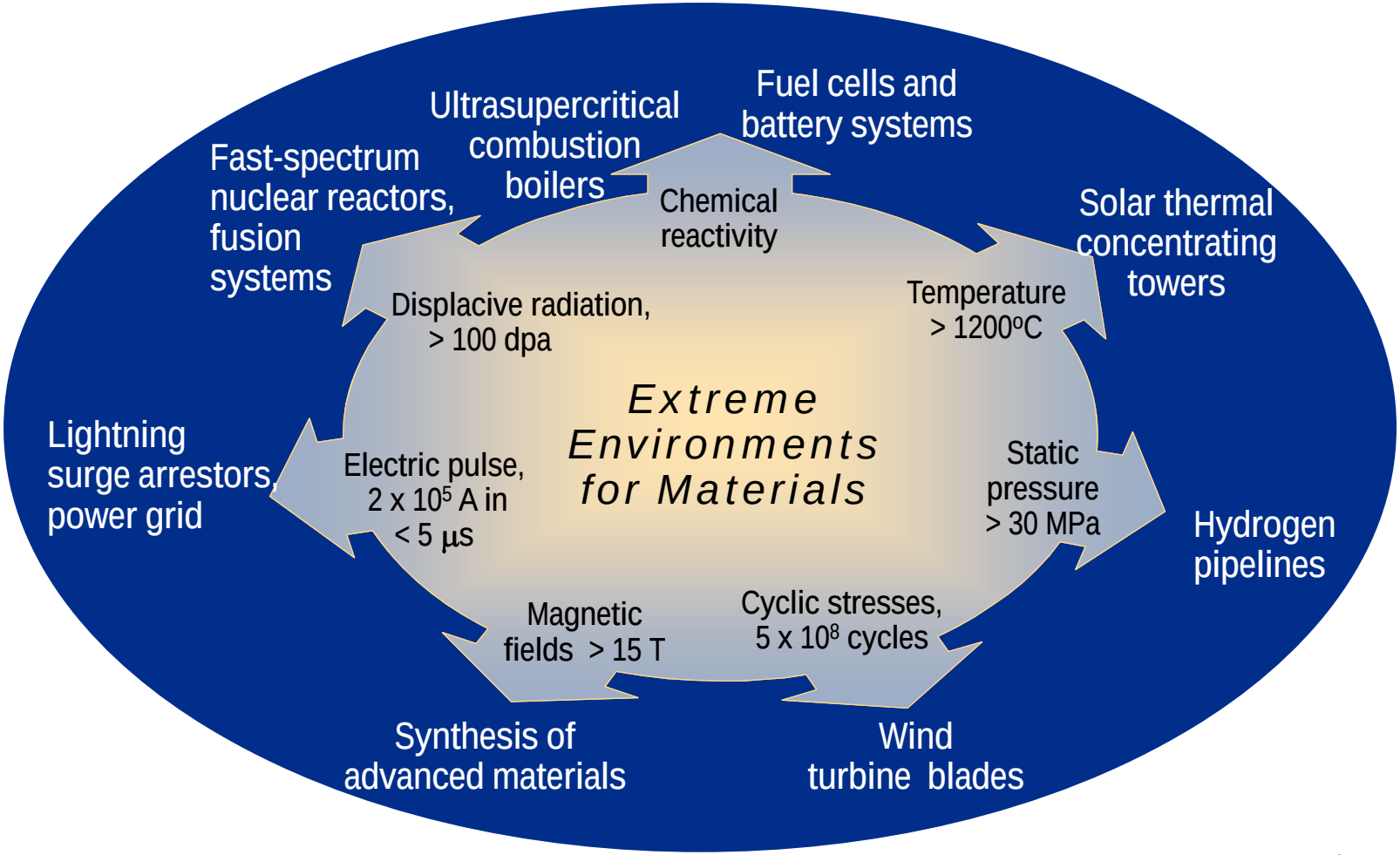
June 22, 2010
Washington, DC

Materials Science

- Crosses many disciplines
  - Physics, engineering, chemistry, biology, statistics ….
- Spans from atomistic to continuum
  - Each requires theory, experiments and simulation at state-of-the art
- Spans basic → applied
  - Pure science: basic science studies
  - Intermediate: application (mission)-driven basic science
  - Applications : what is the right material to use to build ____?
- Spans traditional → hot topics
  - Foundry fabrication to nanoscience
- Required by many (all)
  - Too often the lament of materials scientists is: "Why didn't you come to talk to us before you had a problem? We could have helped prevent it."

Core area in many parts of Department of Energy: Office of Science, NNSA, Energy Efficiency, Nuclear Energy…

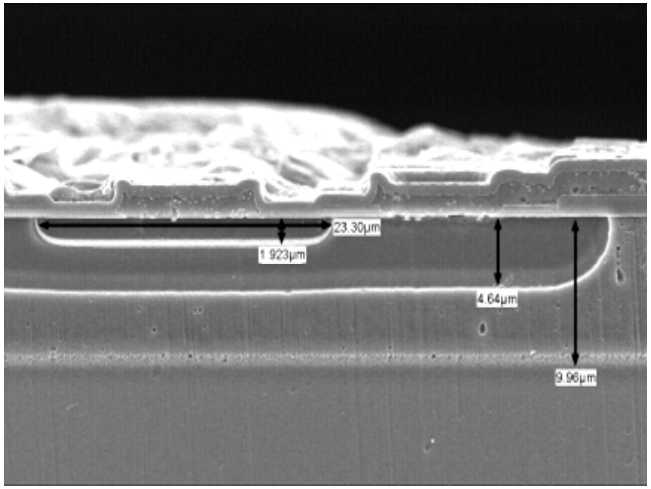
Materials are used in many extreme environments



From: Basic Research Needs Workshop on Materials Under Extreme Environments

June 11-14, 2007

Example: Radiation-hardened electronics
Designing materials for high-performance use in extreme environments



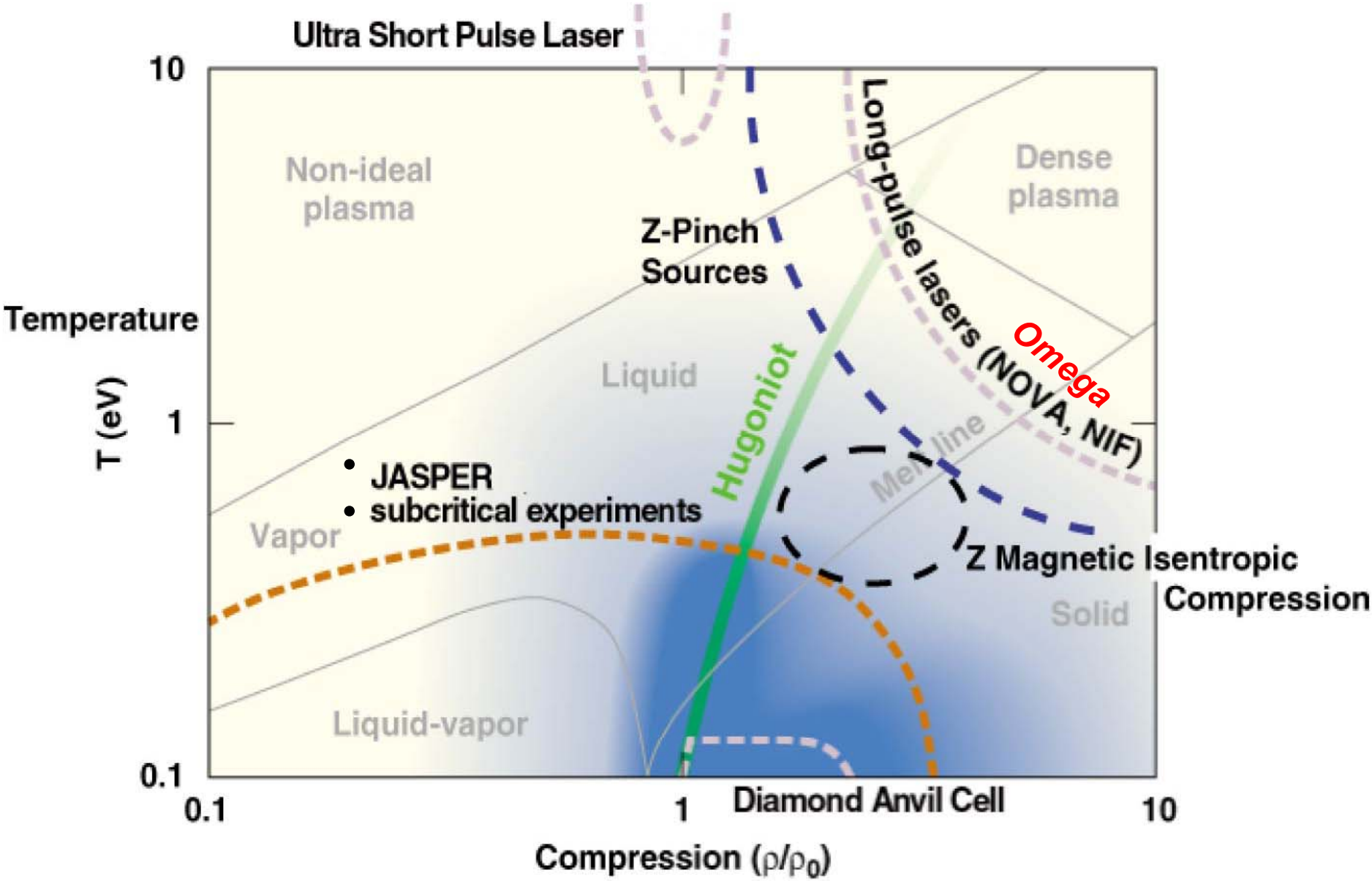
- **Small process changes can significantly enhance the survivability of electronics to radiation**
- **As materials models and process models increase in sophistication, they can be used to optimize material properties**
- **Key applications include:**
  - **Insensitive explosives**
  - **Radiation tolerant materials**
  - **Hydriding-resistant materials**
  - **Reduced weight materials**

NNSA Materials Challenges

- Developing a predictive capability for materials response in extreme conditions
  - Need *materials data at a variety of length scales* under *extreme conditions with relevant drive conditions*
    - ***Materials Data***
      - Discovery data – what is the right phenomenology/physics?
      - Fundamental data - e.g. elastic modulus, constitutive properties …
      - Validation data - did we reproduce nature?
    - ***Extreme Conditions with relevant drive conditions***
      - New tools and facilities push the state-of-the-art (and materials)
  - Need to understand the role of materials processing
- Developing pipeline for the next generation

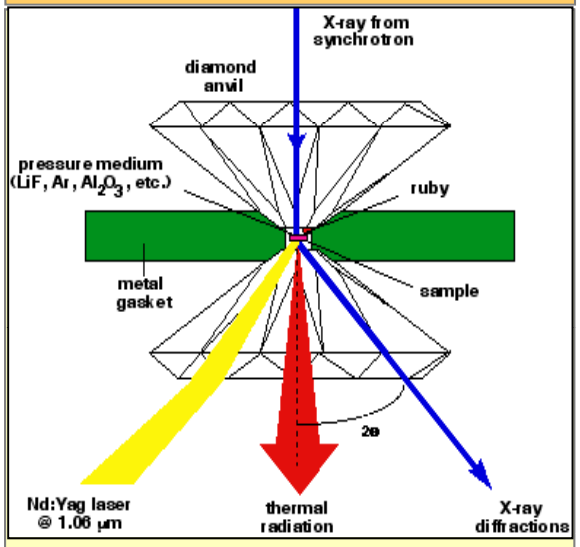
Four key areas: Materials, Nuclear, Hydrodynamics and High Energy Density Physics

Understanding states of matter over a wide range of *temperatures and pressures* is key element of NNSA's mission



The prediction of the properties and response of materials under *high-pressure* conditions is a focus of NNSA research programs

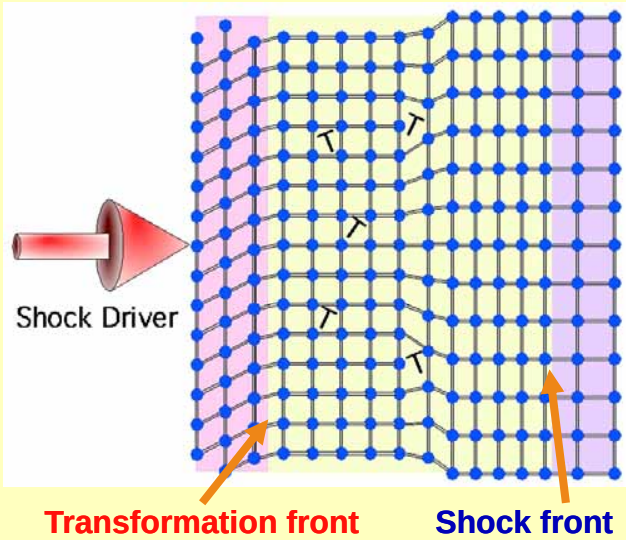
Static high-pressure research



Diamond anvil cell

- **Isotherms**
- **Phase transitions**
- **EOS / melt**
- **Yield strength**
- **Elastic moduli**

Dynamic high-pressure research



- **Ultrafast science of dynamically driven systems — "catching reactions in the act":**
  - **Materials science**
  - **Chemistry**
  - **Biology**

High-performance scientific computing

40 TF platform

- **Multi-scale simulations of materials under extreme dynamic conditions:**
  - **Thermodynamic properties**
  - **Constitutive properties**

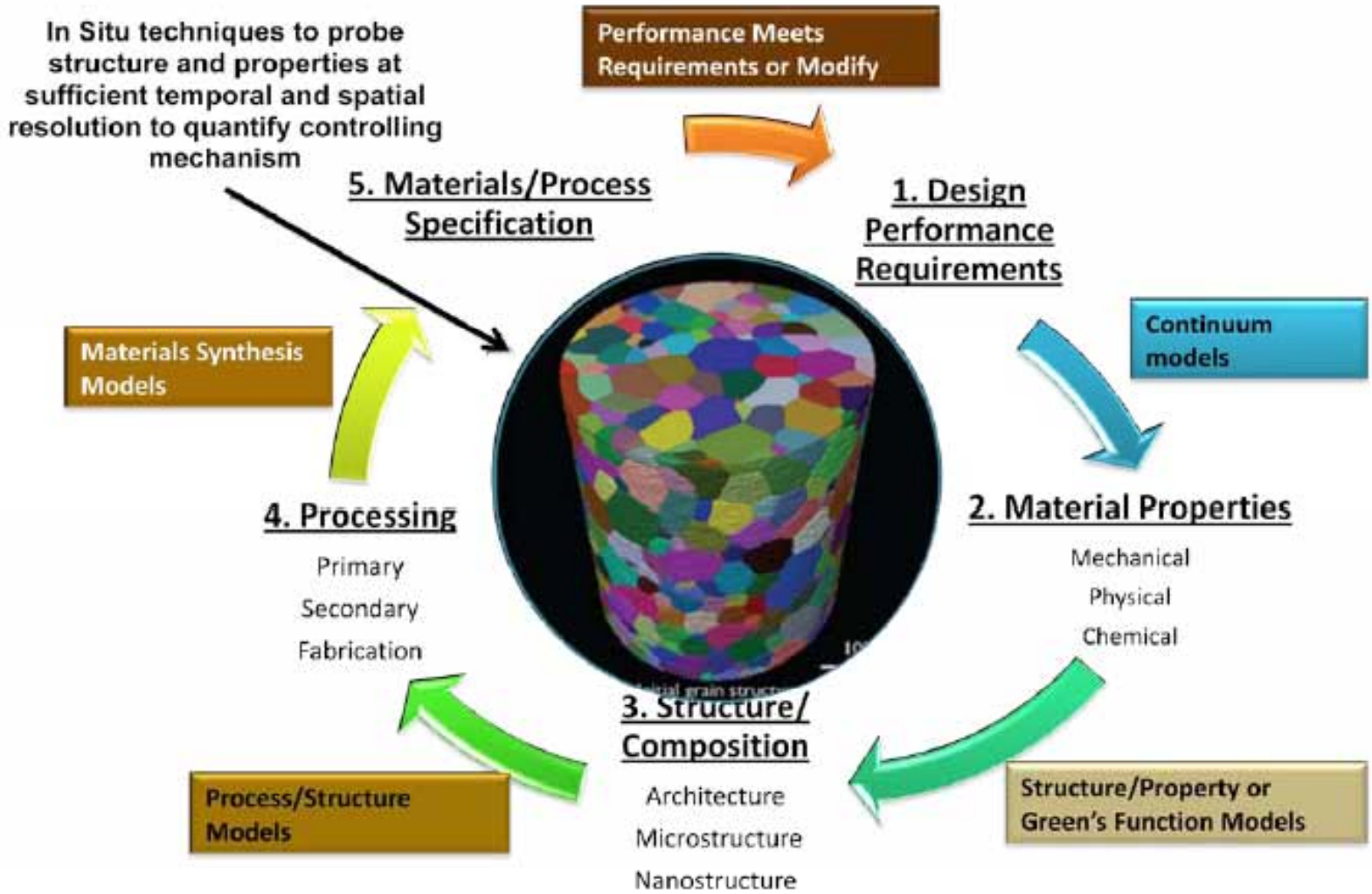
Integration of experimental, theoretical, and computational efforts forms the core approach to executing NNSA's missions

Performing experiments and simulations at the same scale

Operative mechanism for deformation in materials span nine orders-of-magnitude

• Dislocation nucleation	10^{-12} (s)
• Phase Transformation	10^{-12}
• Spallation	10^{-7} to 10^{-9}
• Twin formation	10^{-8}
• Transformation propagation	10^{-7}
• Strain Hardening *3D*	10^{-7}
• Dynamic recovery	10^{-7}
• Damage Evolution (voids / cracks)	10^{-6}
• Dynamic recrystallization	10^{-6}
• Adiabatic shear localization	10^{-5}
• Fracture	10^{-3}

Process-Aware: Linking processing, structure, properties to performance (and specifications)

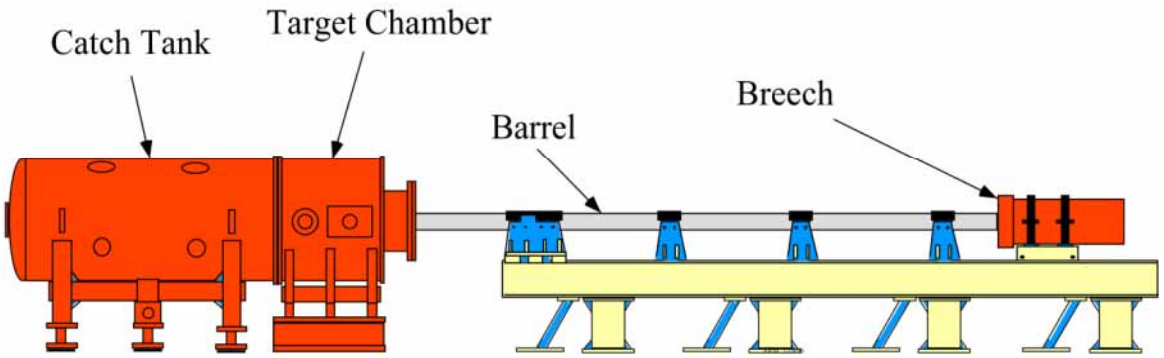


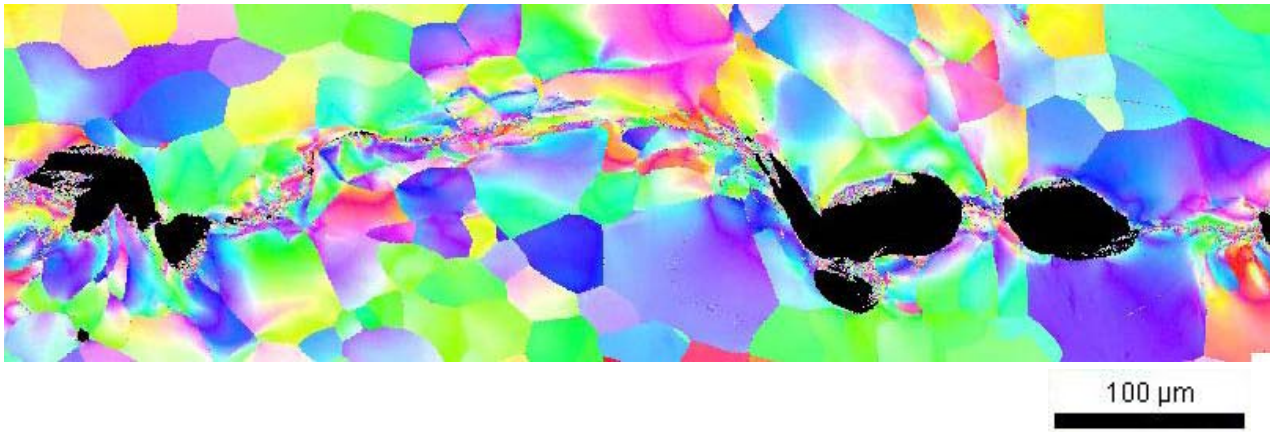
Microstructure image courtesy of E. Lauritsen

“Process-aware” materials sensitivities influence many relevant physics models

- EOS – Influence of material chemistry
- Strength – material pedigree, manufacture and processing, shock hardening
- Instability Growth
- Damage Evolution – microstructure
- Fracture & Fragmentation
- …..

Understanding interactions of defects with microstructure is important



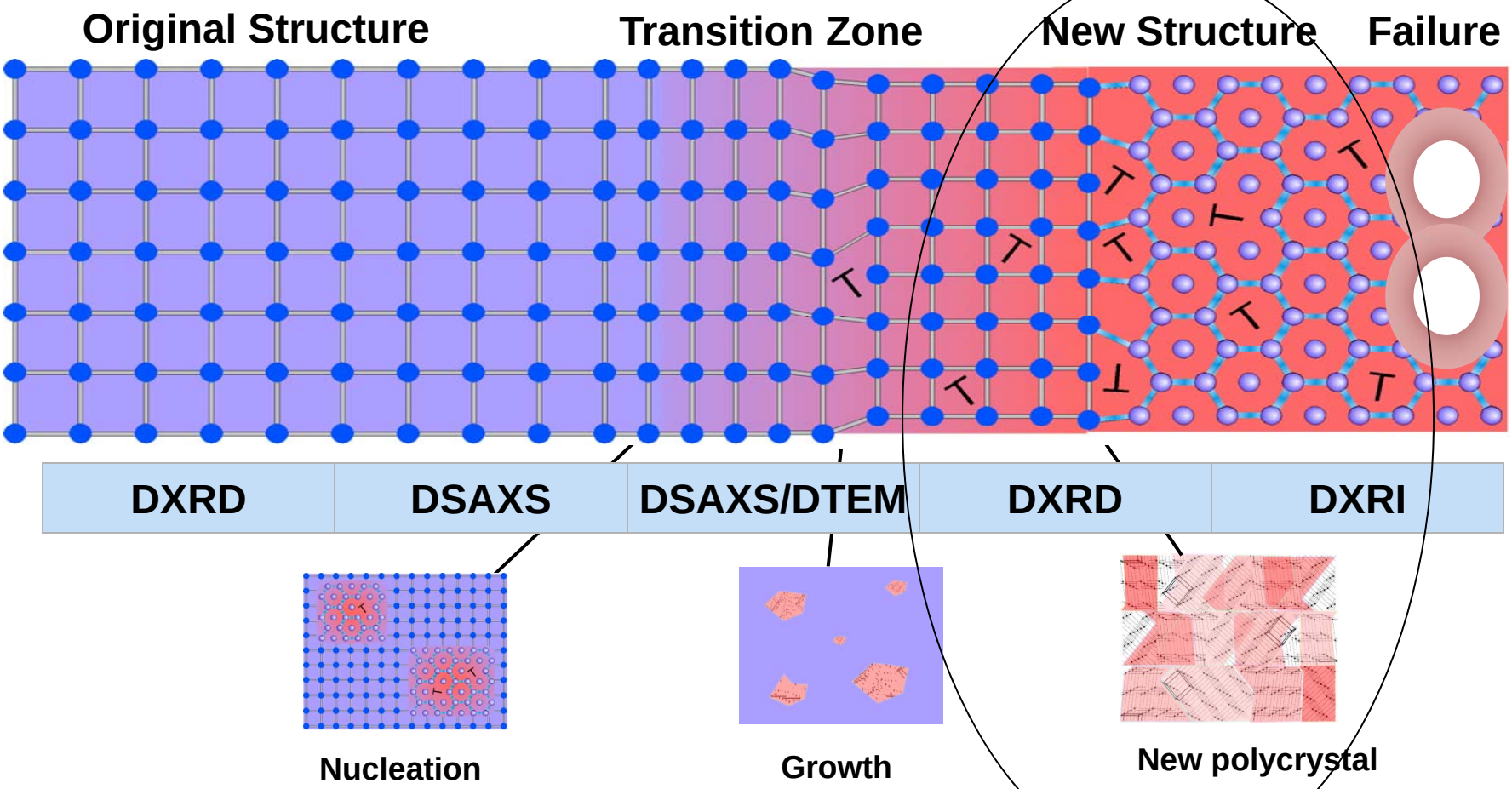


Recovered target

New soft capture system developed to study damage evolution under shock conditions

Dennis-Koller & Cerreta, LANL

Solid-solid phase transformations involve multiple length and time scales: Electron and x-ray probes provide key diagnostic tools



Understanding the response under various drive conditions is critical –

Area of interest

DXRD: Dynamical x-ray diffraction / DSAXS: Dynamical small-angle x-ray scattering
DXRI: Dynamical x-ray imaging / DTEM: Dynamical transmission electron microscopy

NNSA requires a suite of complementary materials science capabilities

- Metallography, thermodynamic and physical property characterization
  - Including hazardous materials
  - How do materials' properties change as a function of process, time, environment?
- Mechanical properties
  - Elastic moduli, strength, …
  - Static and dynamic response (DAC, Gas guns, Hopkinson bar, …)
- Intermediate scale facilities
- Large scale facilities (NIF, DARHT, Z, …)

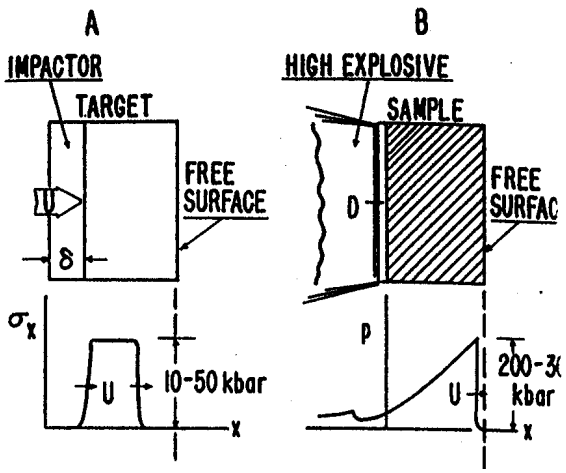
- Theory groups (f-electron physics, etc.)
- Materials modeling
- Code capabilities

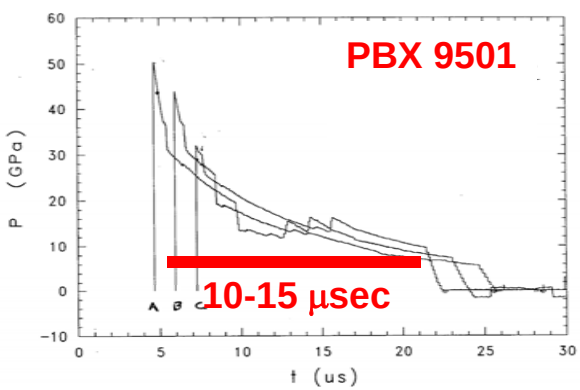
Four key areas: Materials, Nuclear, Hydrodynamics and High Energy Density Physics

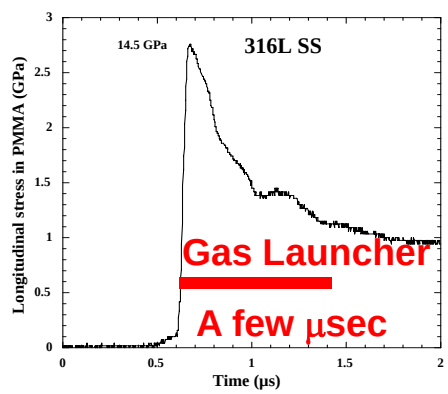
Studying materials responses under different drive conditions is important

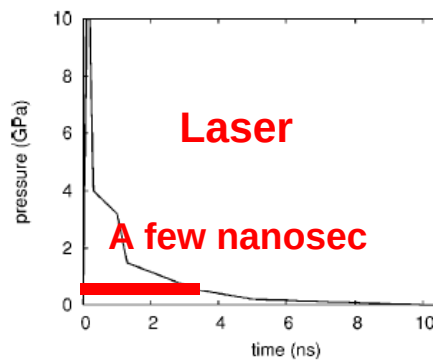
Metals subjected to HE loading have triangular wave shape

- Much of the research on shockwave induced damage (spall, etc) using shock techniques has been done with flat top waves.
- **Time & length scales in experiments are important:**
  - Phase transitions occur in finite times
  - Loading / unloading rates affect processes such as shock hardening & damage evolution
- Gun expts. are of similar timeframe to HE drive
- **Various Techniques can yield a Triangular-Shaped Shockwave Profile (different *time* scales)**









Studying materials responses under different drive conditions is important

The effect of shock wave profile shape on damage in copper

G.T. Gray III[1], L.B. Addessio[1], E. Cerreta[1], C.A. Yablinksy[1], D.D. Koller[2], R.S. Hixson[2], P.A. Rigg[2], J.D. Maestas[2]

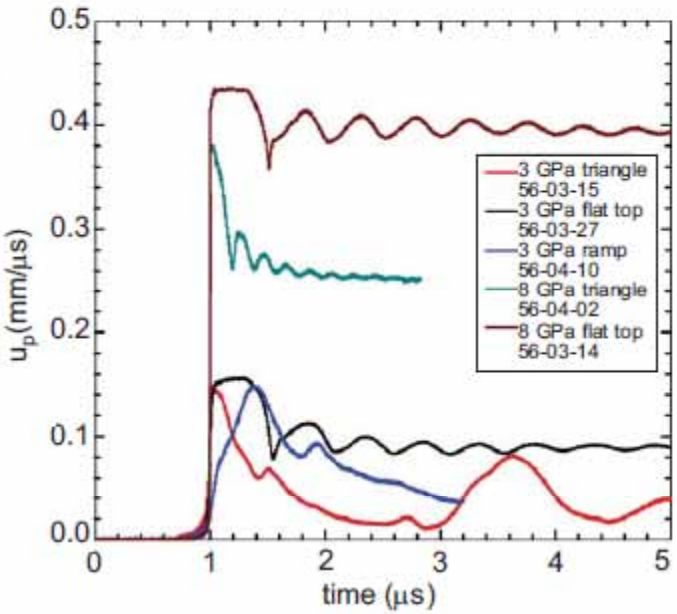


Figure 2. VISAR records for plate impact recovery experiments.

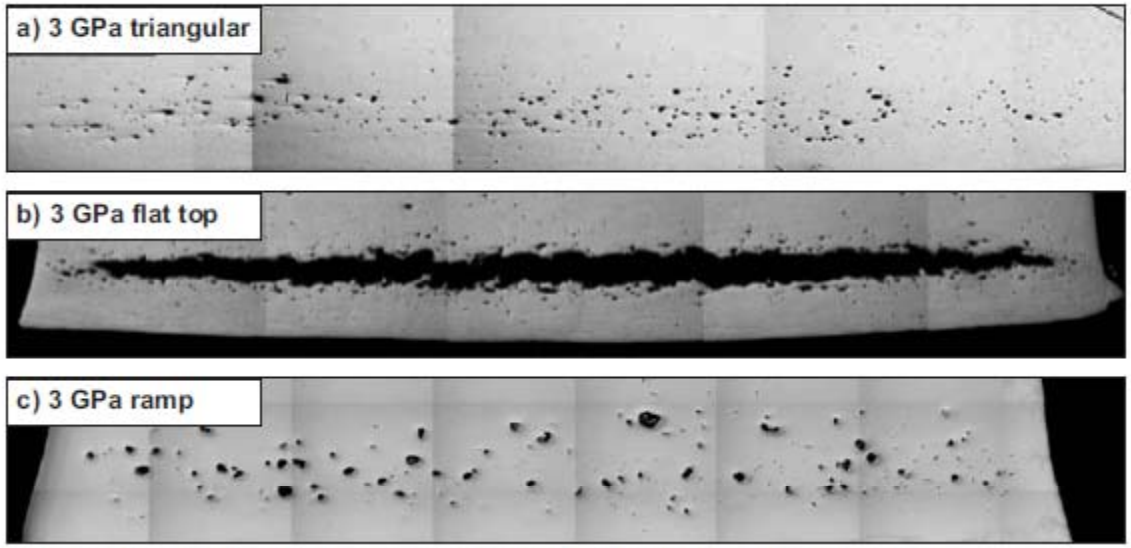
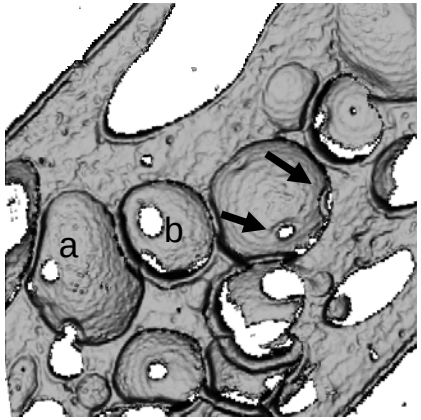


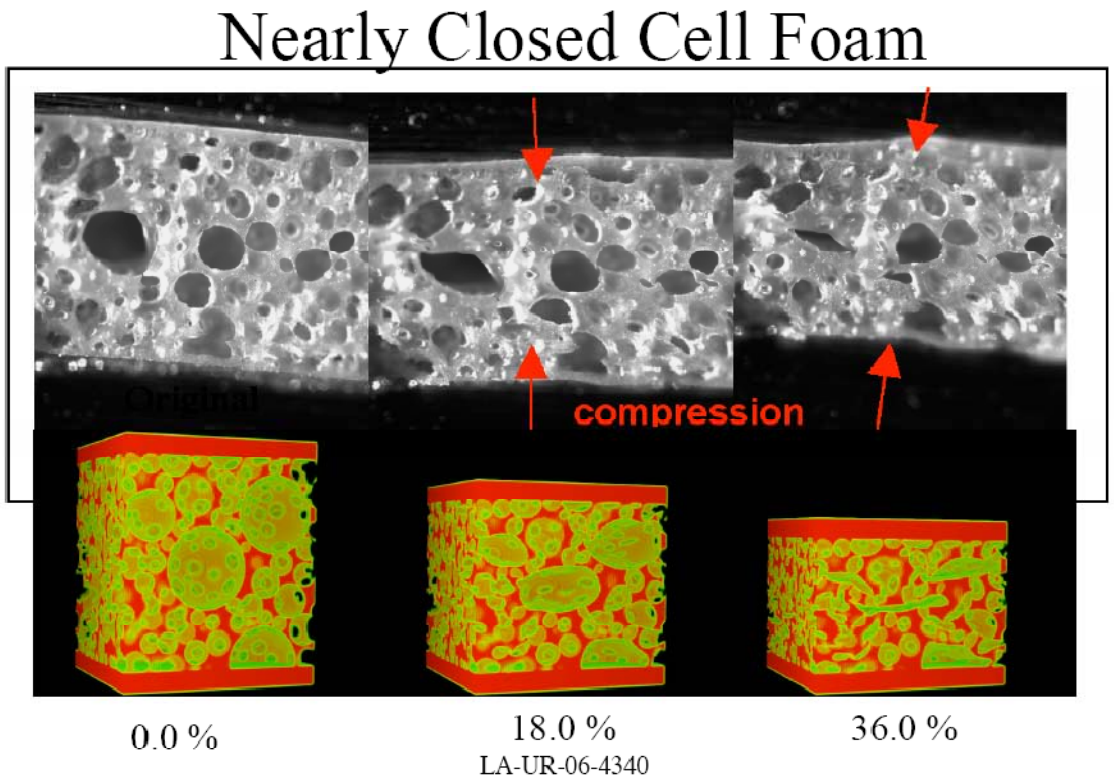
Figure 3. Composite of the optical metallography of the recovered specimens.

NNSA Portfolio includes a wide variety of materials: including polymer and foams

Currently, models do not exist for many materials, or are not based on polymer physics (to capture rate, temperature, pressure, pedigree & composite nature)

We are working to develop constitutive models for low density, closed cell foams by coupling theory with experiment (optical and fluorescence microscopies, x-ray tomography)

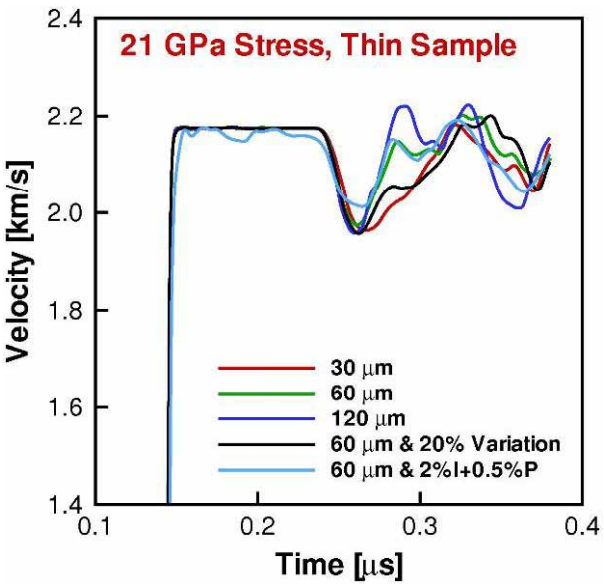




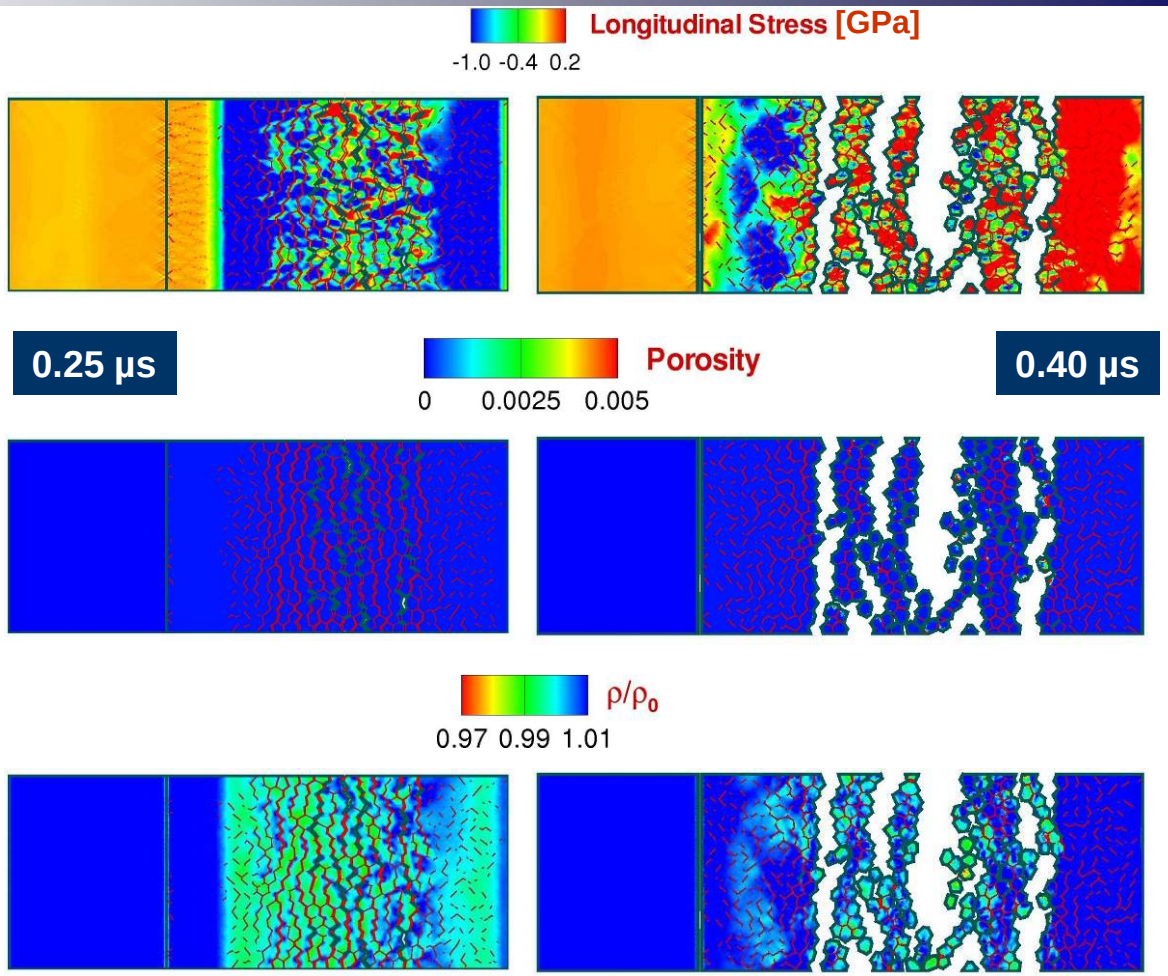
Scott Bardenhagen, Kirk Rector, Dana Dattelbaum LANL

Spall With Mesoscale: Academic Alliances, Institute of Shock Physics, WSU

Pull Back Velocity at 21 GPa Impact Stress



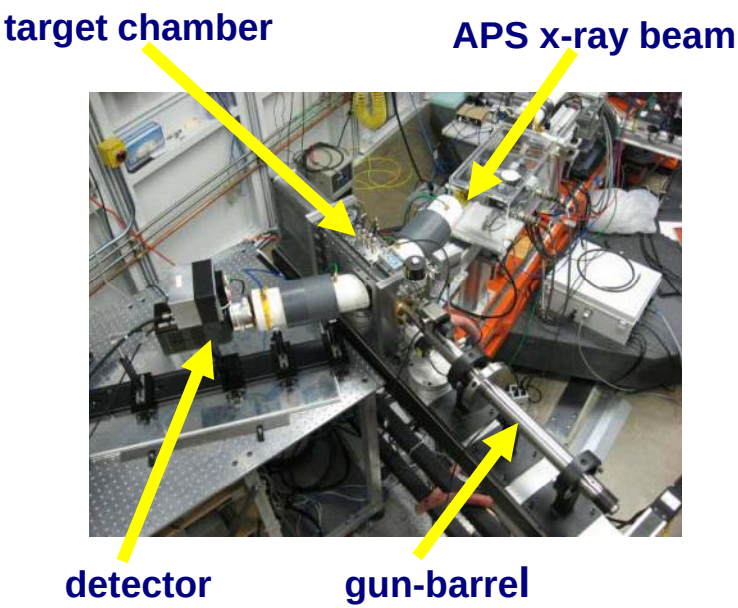
Internal Variables During Spall



- Inhomogeneous spall associated with the velocity structure
- Mesoscale heterogeneities influence velocity profiles

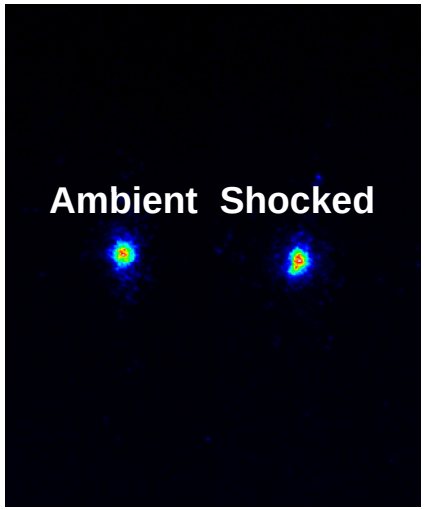
Shock wave x-ray diffraction measurements at the Advanced Photon Source

Dynamic compression experiments at the Advanced Photon Source at Argonne National Laboratory



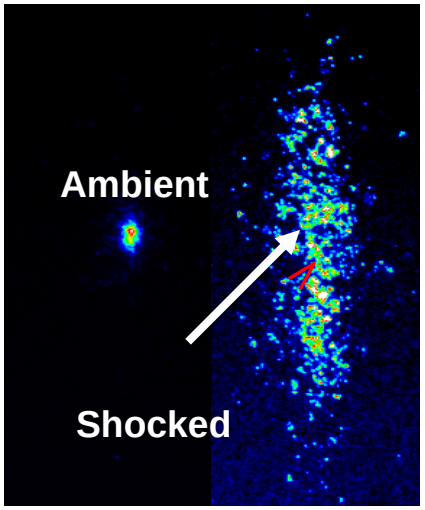
X-ray diffraction peak in shock compressed LiF

LiF(111) elastic



Elastic deformation:
Diffraction peak shifts but does not change shape because shock does not introduce disorder

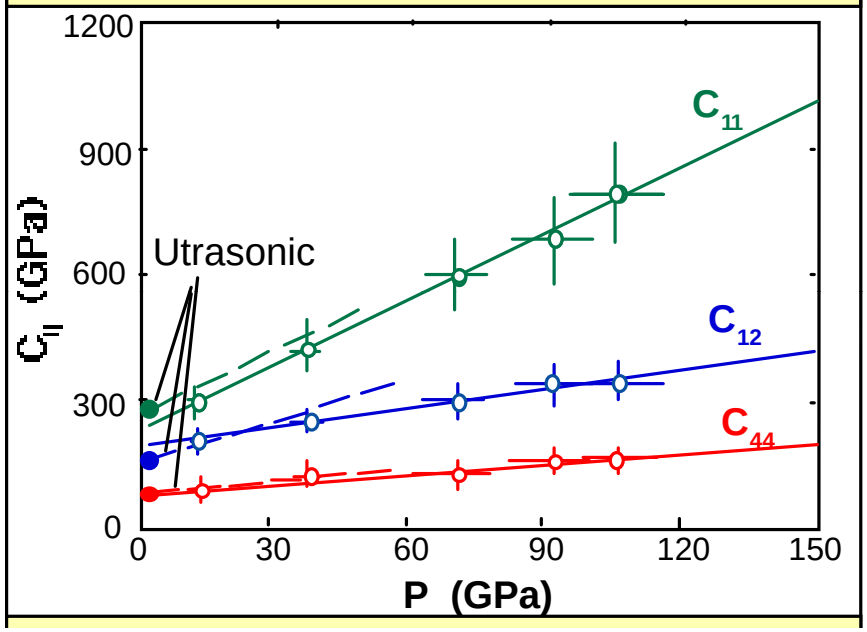
Mg doped LiF(100) plastic



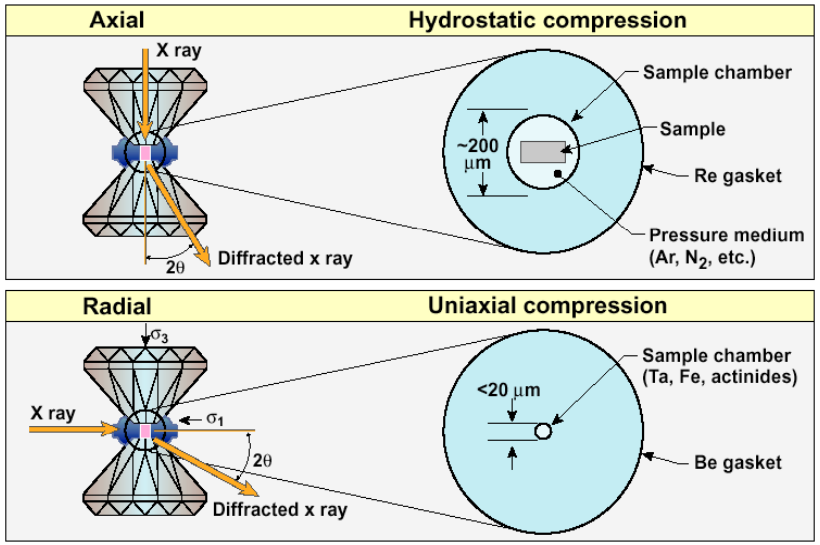
Plastic deformation:
Diffraction peak shifts and change shape (width and height) because shock introduces disorder

HPCAT has proven especially useful for high-pressure, high-temperature investigations of metals: EOS, melting, phase diagram, and crystal structure

Elastic constants (C_{ij}) of Ta



- **Constitutive properties and strength data are required for strength models**

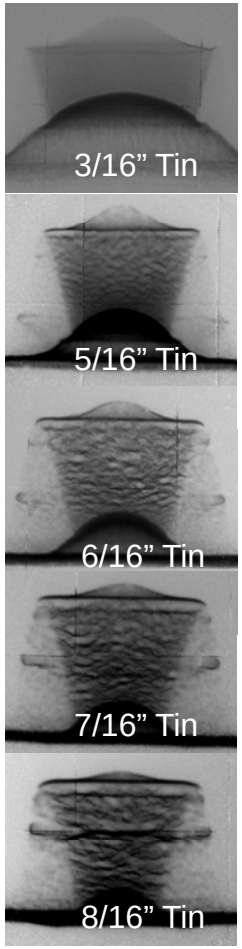


- HPCAT characteristics are **well-matched** to our demand for relevant high-pressure research (c. 2009)
  - 22 journal articles submitted/published in past year
  - 3 PhD students doing thesis research

LANSCE: Proton Radiography is a key capability for developing predictive capabilities for materials

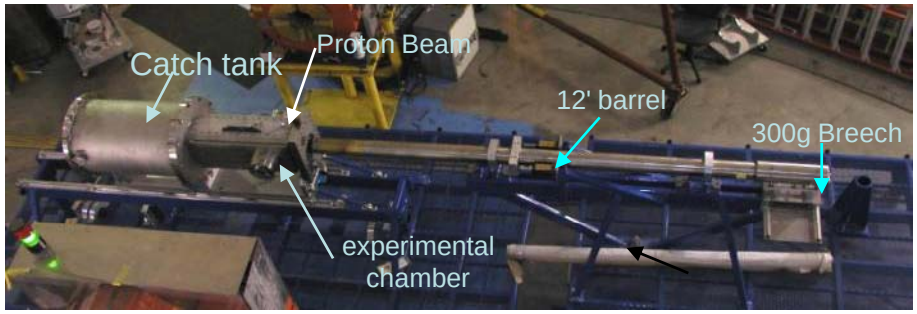
Shock Physics

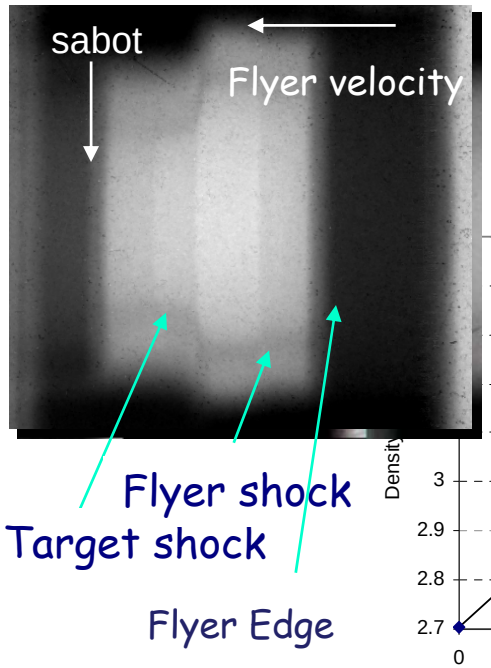
Melt on release in Sn

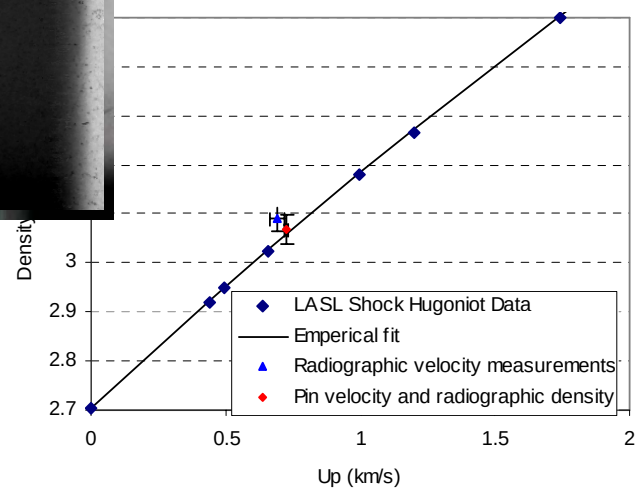


Dynamic Materials Studies

Equation of state measurement with pRad and a powder Gun

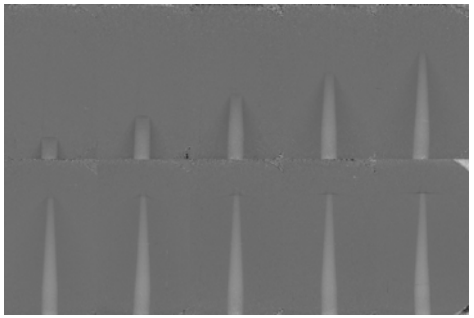


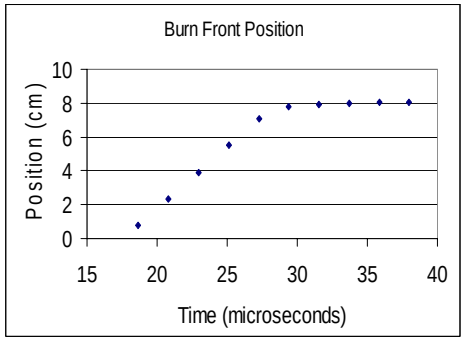




HE Science

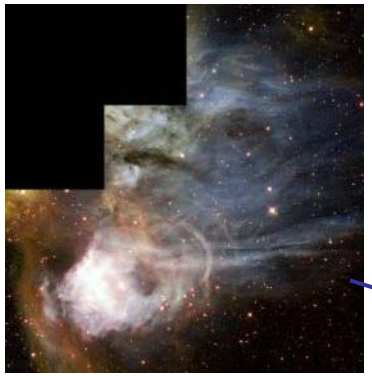
Detonation Failure Studies in PBX-9502



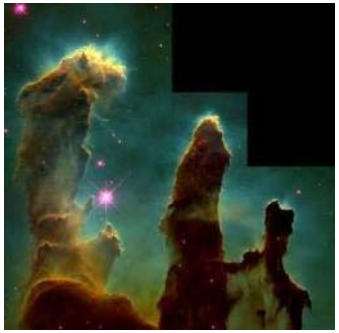


NNSA mission needs have driven the creation of experimental environments to study materials in extremes

High Mach Number unstable flows

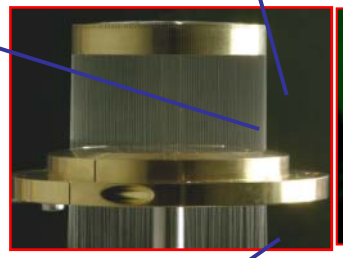


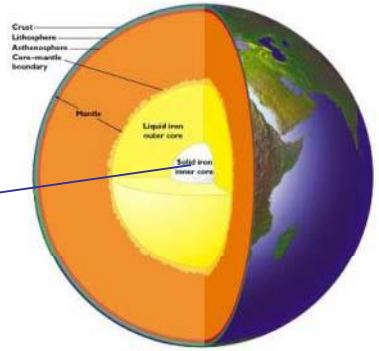
Jets

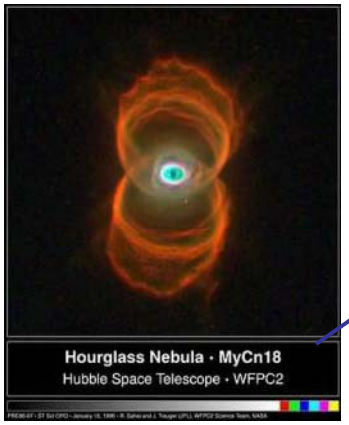


Rayleigh Taylor Instabilities

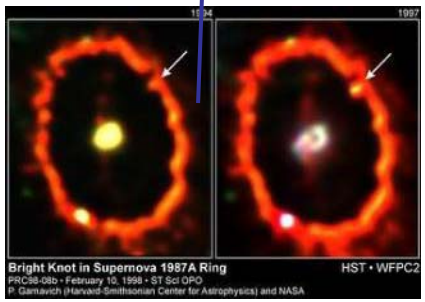
Materials in the Extreme







Mass Outflow

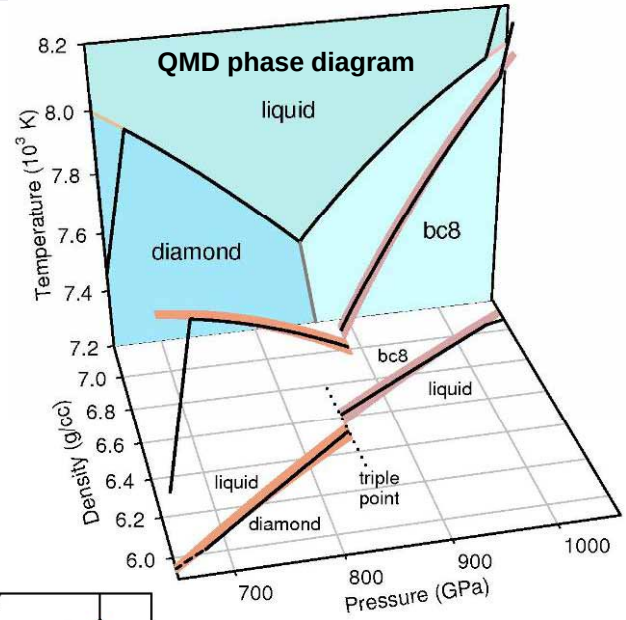


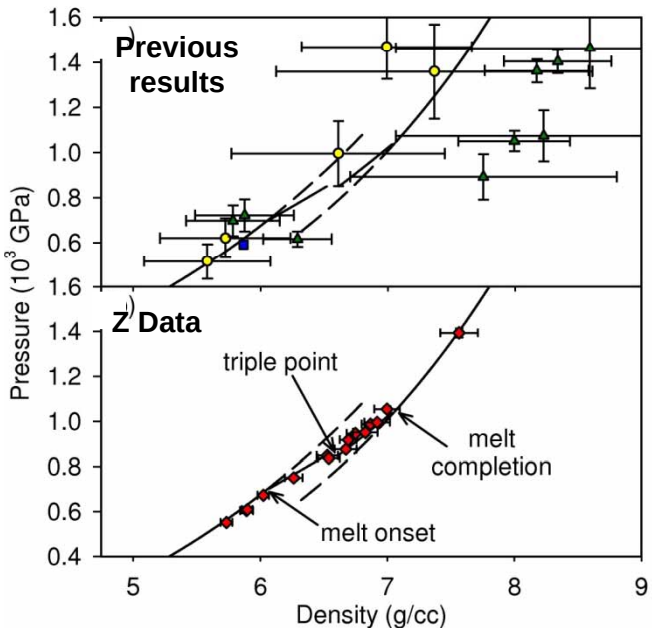
Shocks and radiation transport

MHD, thermo-electric, and "anomalous" heating

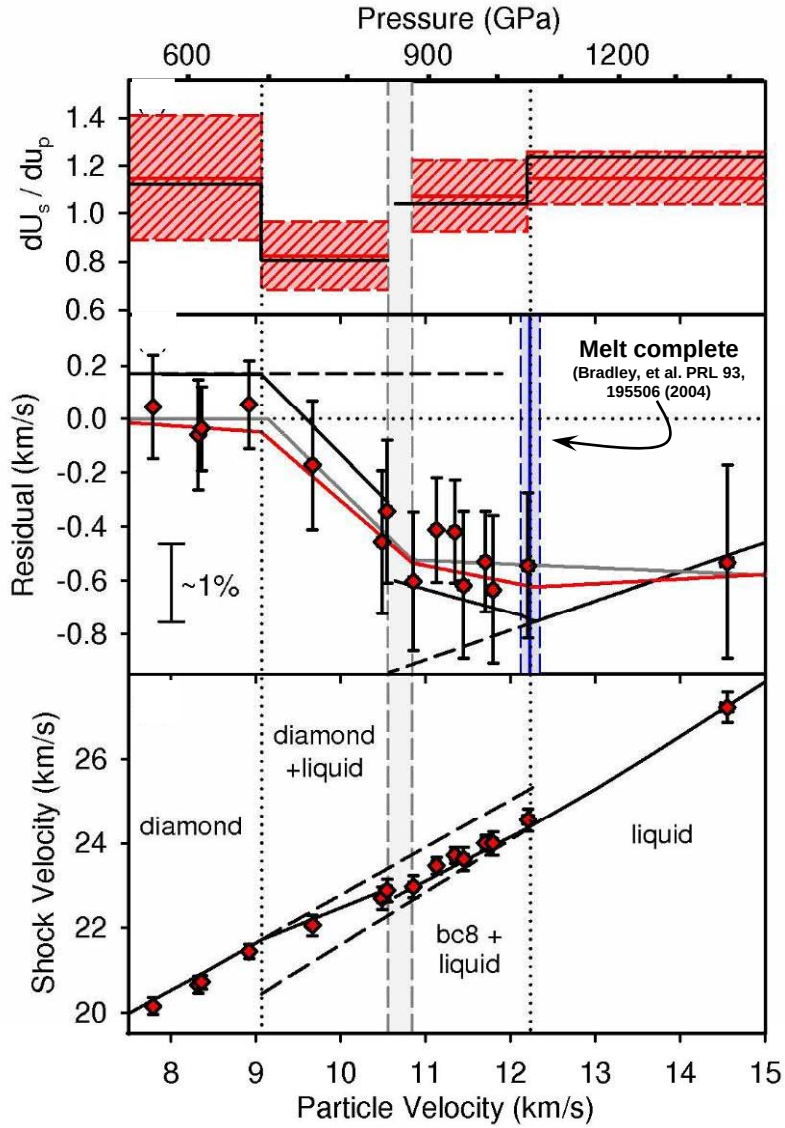
Precision measurements on Z enabled identification of a triple point on the melt curve of carbon

Quantum molecular dynamics (QMD) calculations predicted the existence of a triple point along the coexistence region of the diamond Hugoniot and how the presence of the triple point would be manifest in the shock velocity data.



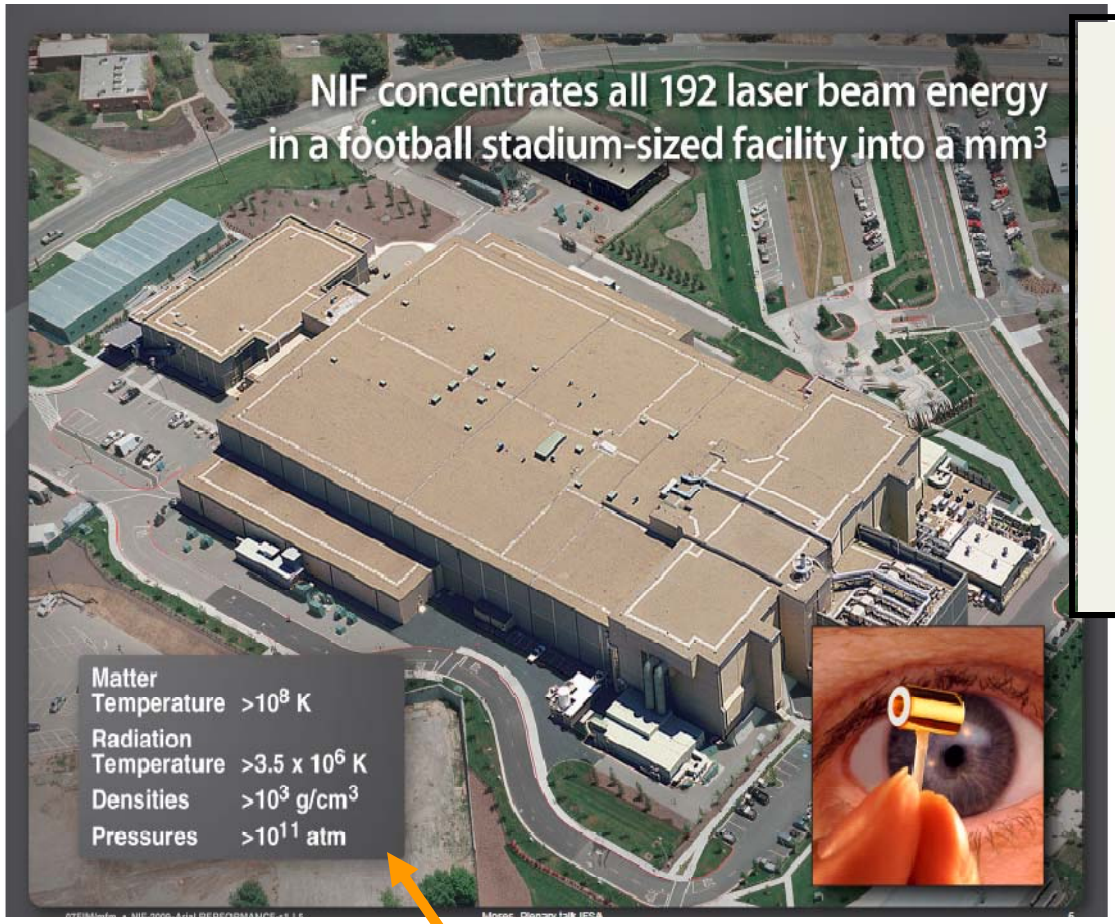


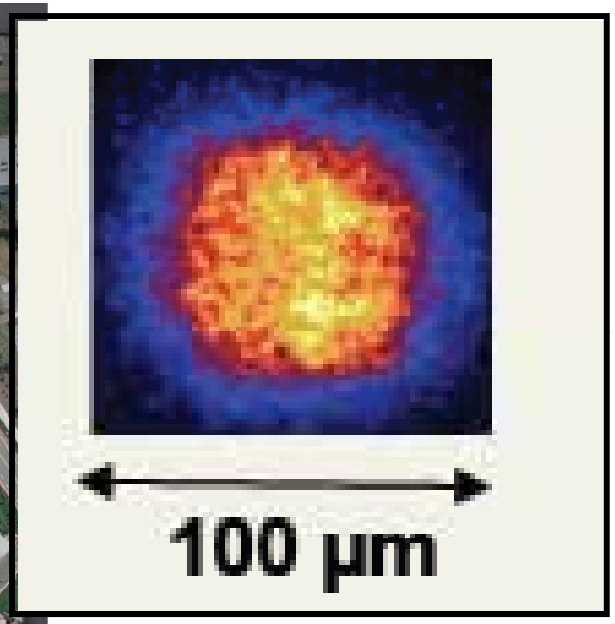
Previous laser-driven shock experiments lacked the precision necessary for quantitative comparison with QMD predictions. The Z results provided an order-of-magnitude improvement in precision and enabled quantitative comparison.



M.D. Knudson, M.P. Desjarlais, D.H. Dolan, *Science* 322, 1822 (2008).

NIF is operational and provides new experimental regimes

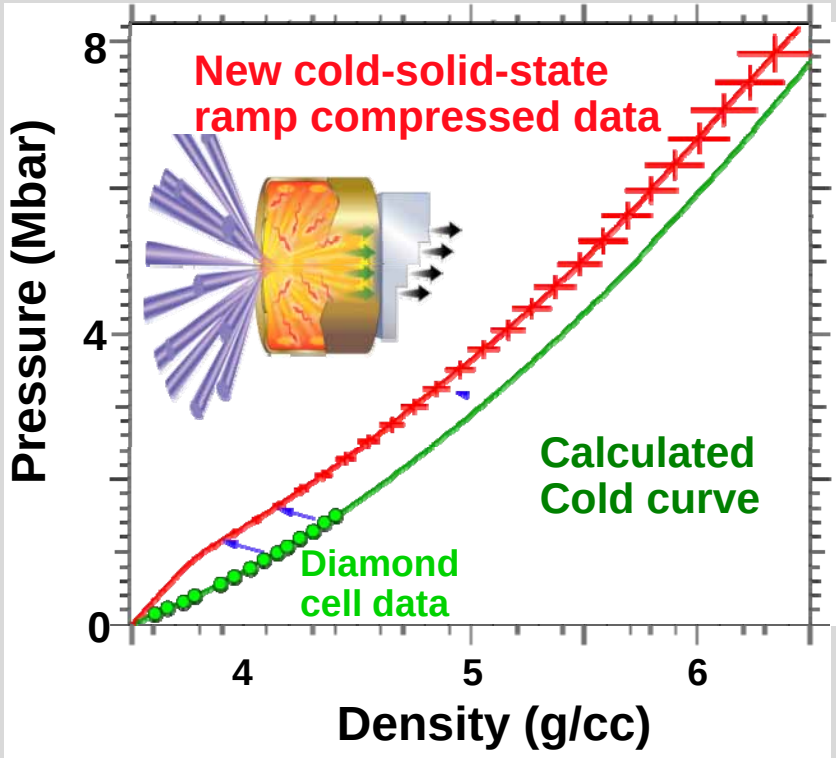




Exciting new opportunities to study materials under extreme conditions

High energy lasers have been used to extend solid state physics to the 10 Mbar regime

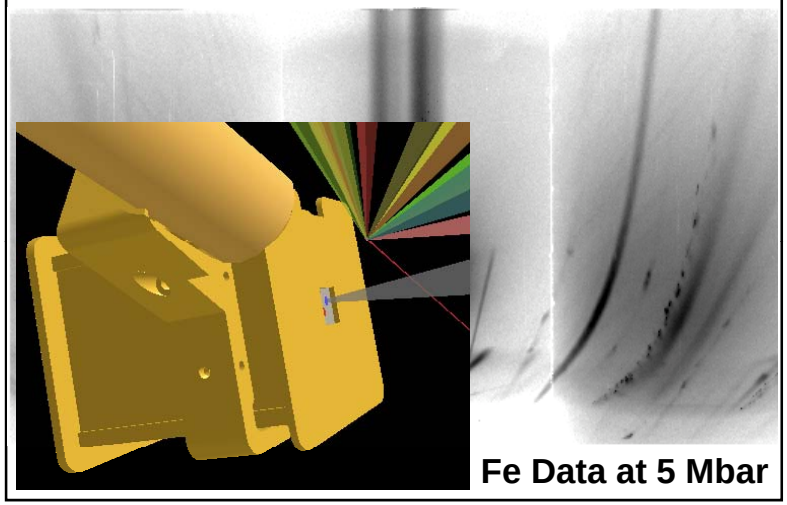
Ramp compression shows diamond is stable and strong to 8Mbar



Bradley et al

NIF designs use the same technique to study solids to many >30 Mbar

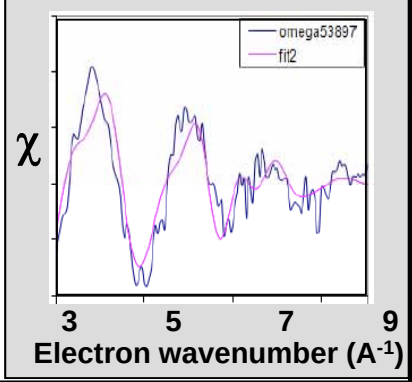
Diffraction for structure & strength =>Fe is HCP to 5 Mbar

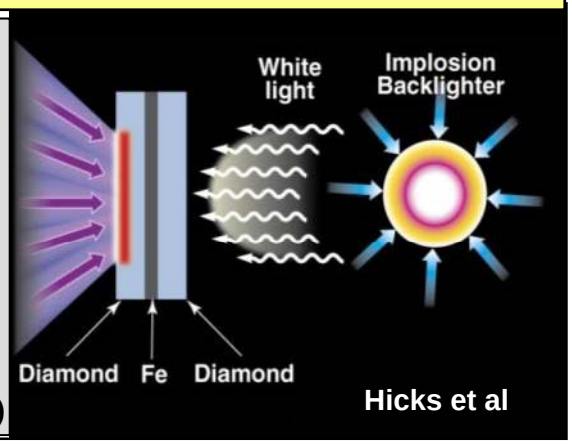


Eggert et al

EXAFS is being used to measure T & structure in Fe to 3 Mbar

Fe data at 3 Mbar

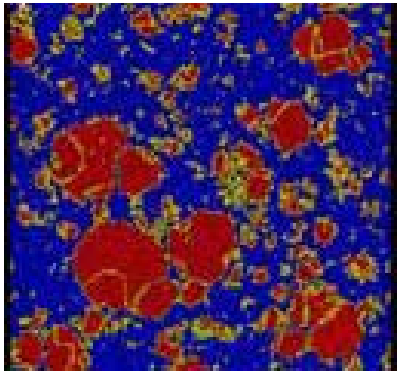




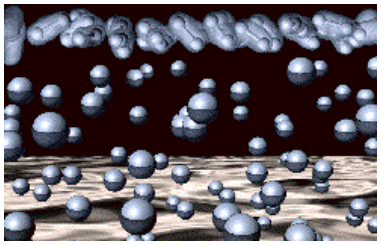
Hicks et al

Widely Acknowledged Accomplishments in Computational (Materials) Science in Support of NNSA Helps Retain Scientific Staff

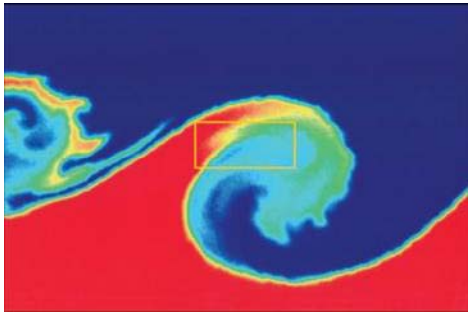
NNSA Mission-inspired Science



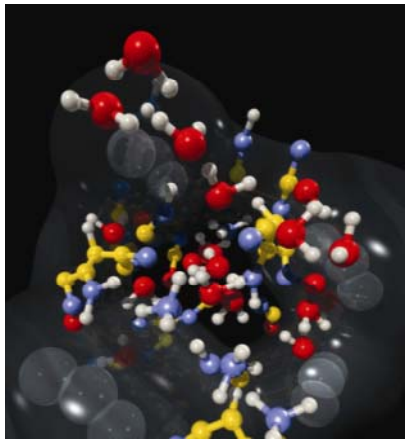
Gordon Bell Prize 2005



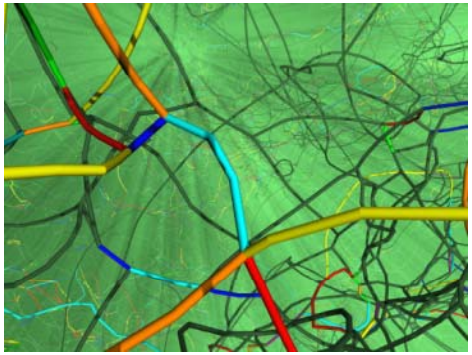
Gordon Bell Prize 2006



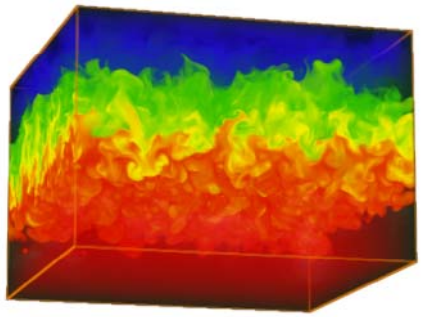
Gordon Bell Prize 2007



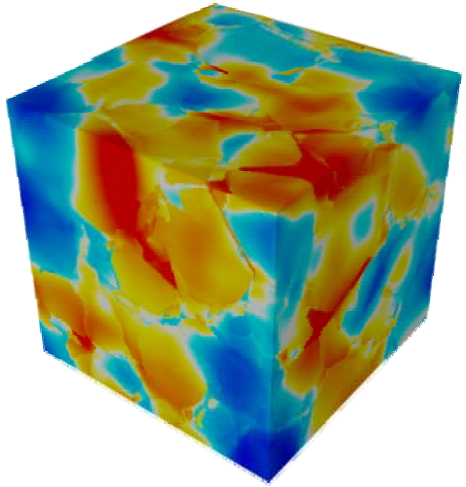
QMD of detonating HE
Nature Physics, 2008



Dislocation Dynamics
Nature, 2006



DNS of R-T instability, 2007



Phase transformation
at the crystal level, 2009

Conclusions

- Materials data in extreme conditions with right drivers is important to NNSA
  - Requires discovery, fundamental *and* validation data on many materials
- Materials response of interest spans many orders-of-magnitude in both length and time-scales
- Multiple probes to examine the material response with appropriate drivers is important
- Need to continue training the next generation

Atomistic to continuum
Theory, experiment and simulation
←----State-of-the-art tools----→