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Title: Material Response under Extreme Loading Conditions

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# **Material Response under Extreme Loading Conditions**

**George T. (Rusty) Gray III**  
**Materials Science and Technology Division**  
**Los Alamos National Laboratory**

While the field of shock-wave physics has provided significant insights into many of the processes related to wave propagation in materials, the exact operative micromechanisms of defect generation occurring during the shock and thereafter those controlling defect storage and damage evolution remain incompletely understood and poorly modeled. Attainment of a truly predictive capability to enable accurate simulations of dynamic impact, shock, and high-rate loading phenomena applications *requires* a linked experimental, modeling, and validation research program. In this talk an overview of the microstructural mechanisms affecting the strength of materials at high pressure and strain rates as well as the processes controlling damage evolution during shock loading will be reviewed. Examples from materials science as well as astrophysics illustrating how shock physics is important are presented. I will discuss the rationale why shock physics is important to the NNSA and therefore to the Stockpile Science Academic Alliance (SSAA). I shall finally discuss the challenges and opportunities for the development of physically-based models of shock-wave effects on materials and present some exciting challenge topics in shock physics.

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# Material Response under Extreme Loading Conditions

**George T. (Rusty) Gray III**

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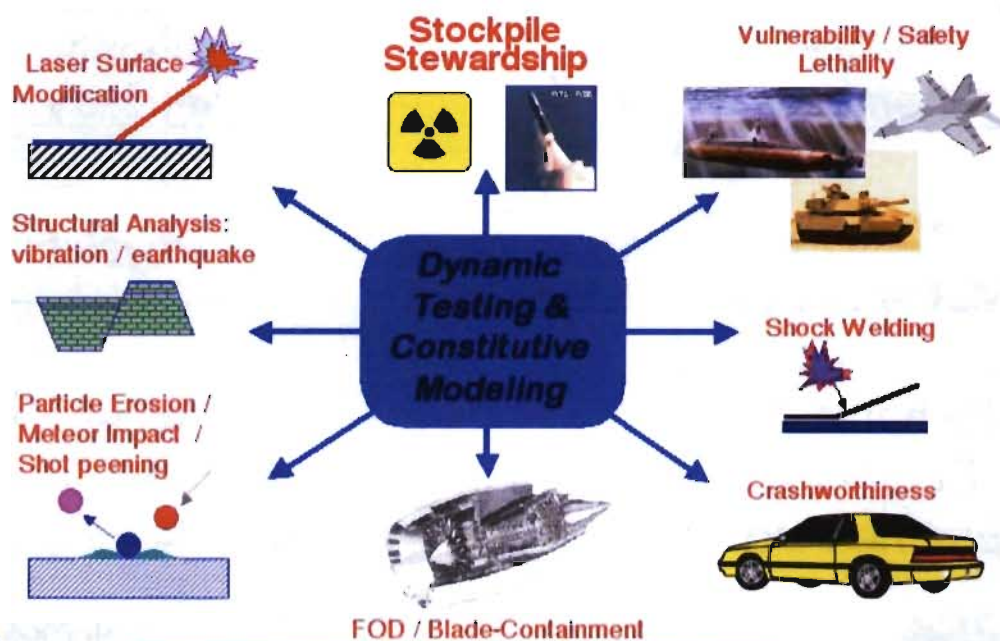
E. Cerreta, N.K. Bourne, R. Olson, P. Rigg

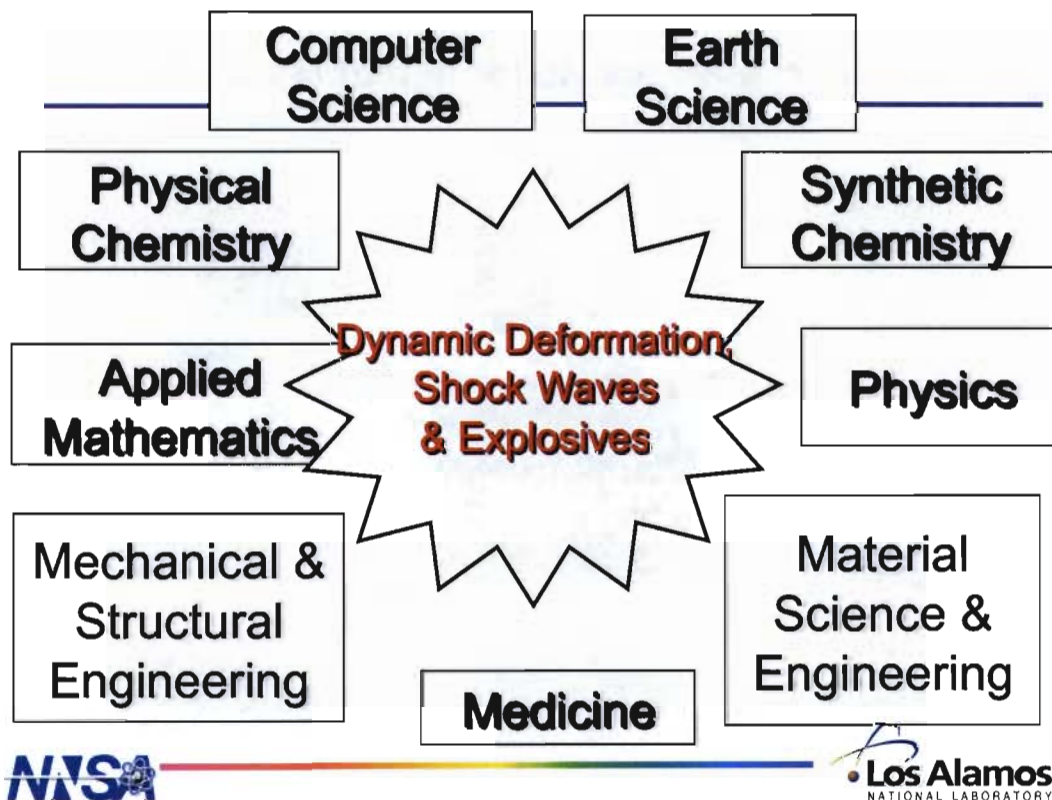
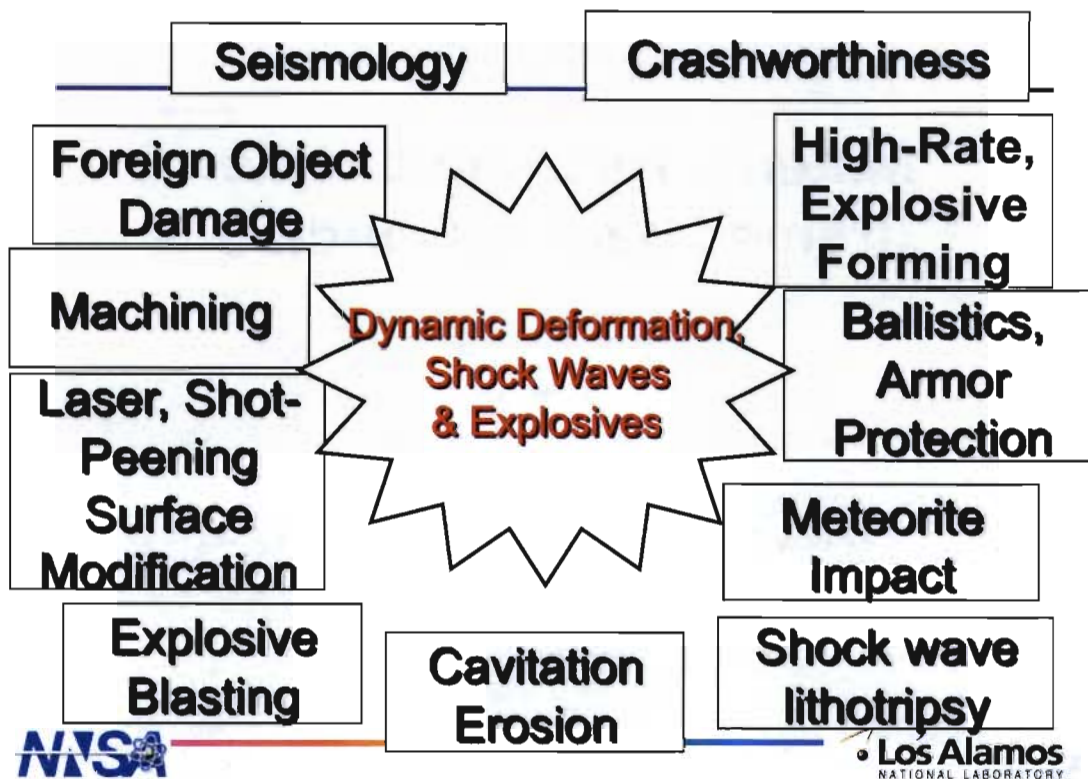
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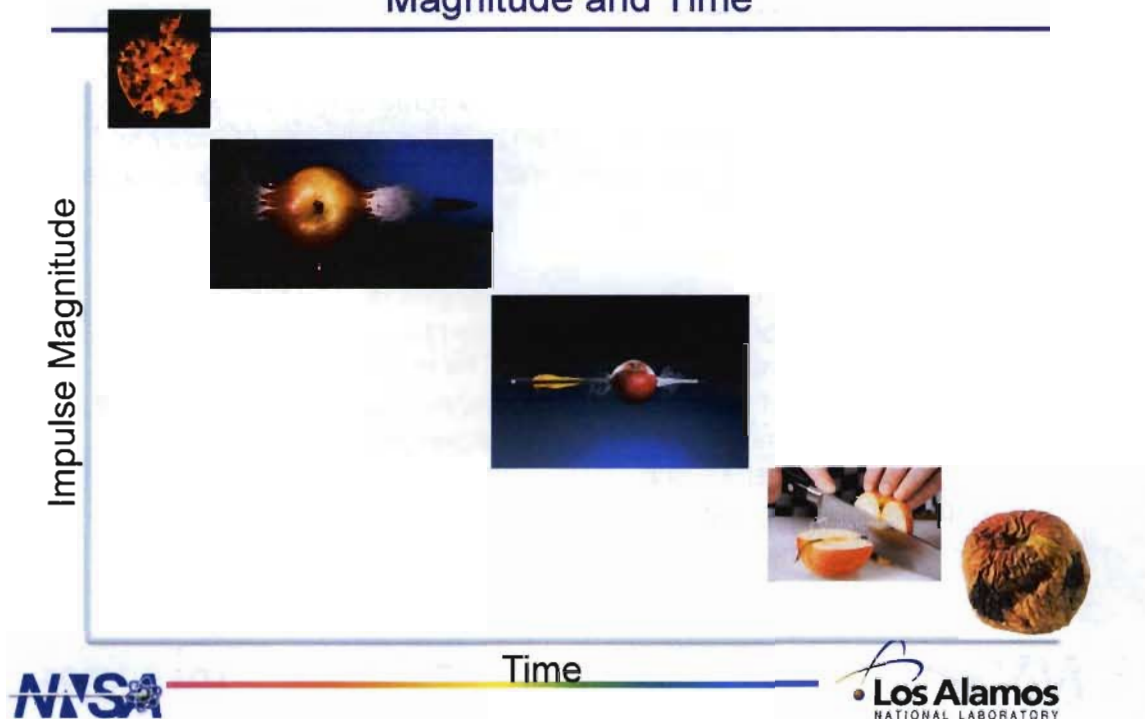
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## Dynamic & Shock Response of Materials

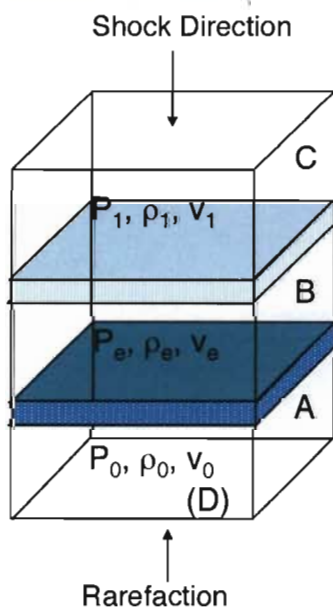




## Operative Mechanisms – A Question of Impulse Magnitude and Time



## What is Unique to Shock Loading?



- Pressure applied for greater than yield strength of material at high strain rate.
- Adjustment of material occurs abruptly at a 2-D shock front, separating undisturbed from the compressed & accelerated portion.
- Microscopic behavior is unlike ordinary deformation.
- In many ways resembles a martensite transformation which occurs at a rapid moving shear interface.

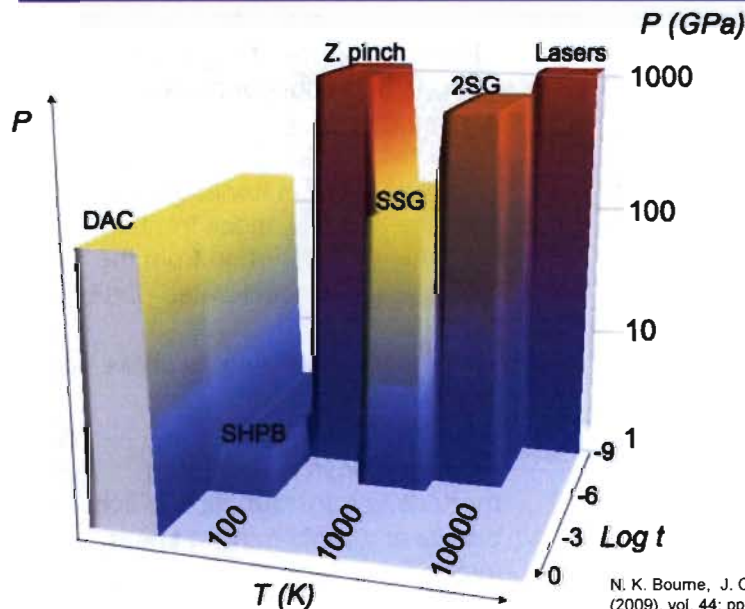


# Why NNSA and SSAA ?

- Increasing fundamental understanding of materials over the broadest range of thermomechanical extreme conditions will fuel enhanced and sustained performance in the materials of today and the design and synthesis of new materials to address a broad range of applications in the future.
- Material response under extreme conditions is of importance to the US defense enterprise (conventional and nuclear deterrence) since the protection and defense of national interests requires an understanding of the dynamic mechanical and physical behavior of materials as it underpins the structural performance critical to the response of materials subjected to high-strain-rate, impact, and/or explosive loading regimes.



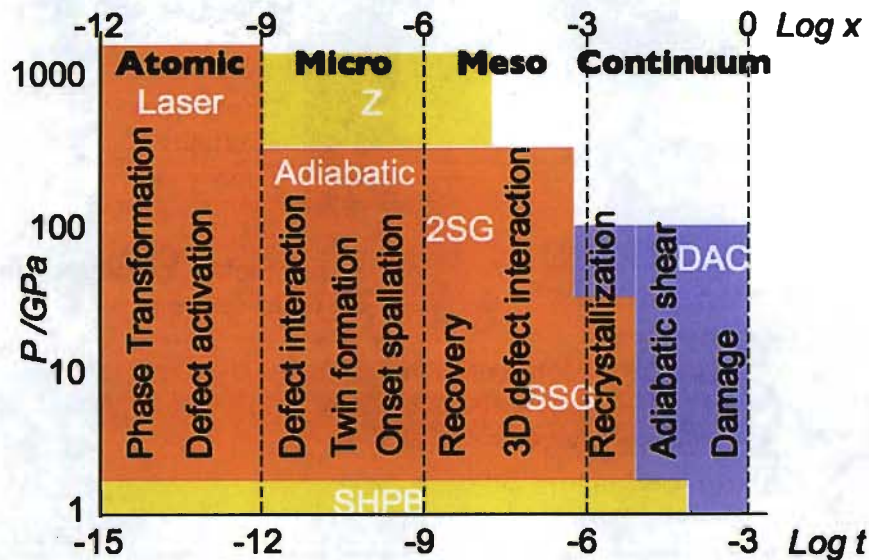
## Facilities – A Question of Operative Loading State Desired, Operative Mechanisms, Kinetics, and the “window” of Observation !



N. K. Bourne, J. C. F. Millett, G. T. Gray III: *J. Mat. Sci.* (2009), vol. 44: pp. 3319-3343. "On the Shock Compression of Polycrystalline Metals"



To study the spectrum of operative mechanisms you  
NEED a range of Facilities

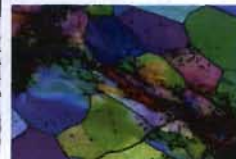
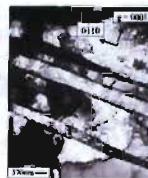


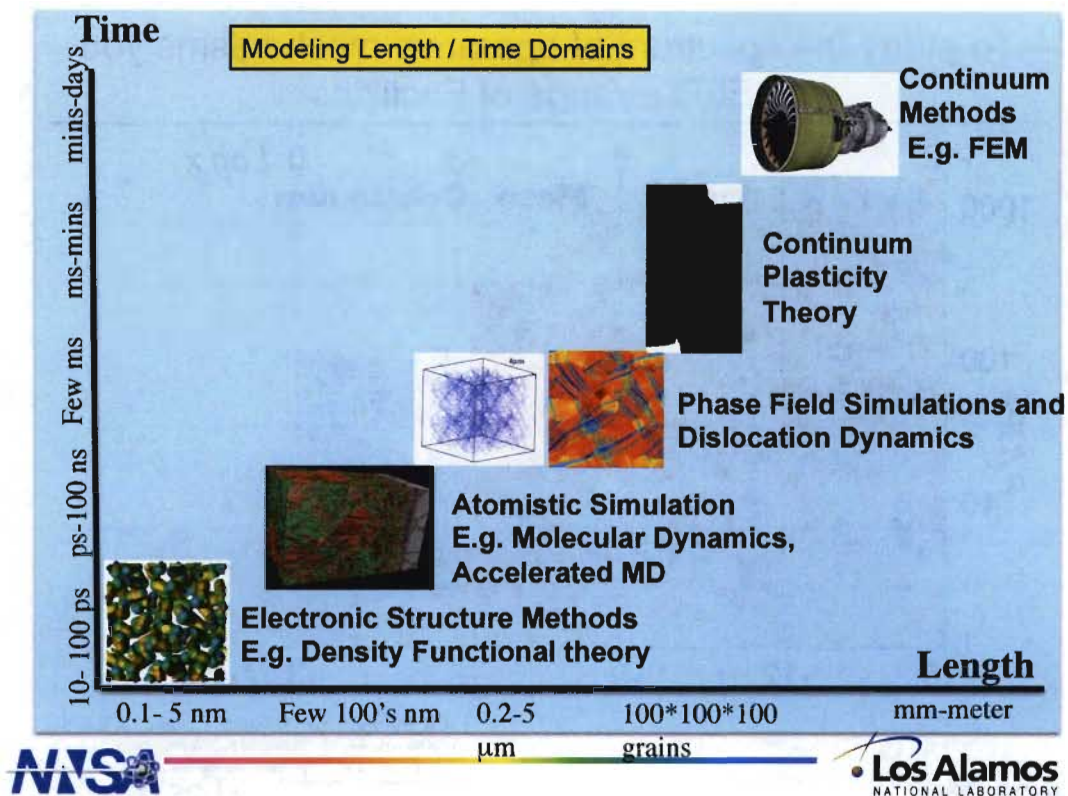
N. K. Bourne, J. C. F. Millett, G. T. Gray III: J. Mat. Sci. (2009), vol. 44; pp. 3319-3343. "On the Shock Compression of Polycrystalline Metals"



"Linked" multi-length scale physics is needed to build the ties  
between the atomic and engineering application scales

- **Atomic scale**
  - Bond length (nm)
- **Microscale**
  - Dimension of grains (nm)
- **Mesoscale**
  - Dimension of constituent components ( $\mu\text{m}$ )
- **Macroscale**
  - Length scale of the experiment (mm to cm)
- **Engineering System scale (cm -> m)**





Validated physically-based models are needed to support predictive simulations of Material Response to Extreme Loading Conditions

Performance - "Process-Aware" Predictive Capability - f (time-aging, microstructure, etc.)

### Predictive capability

#### Processing

- wrought
- cast
- powder metall.
- plasma-spray
- nano

#### Properties

- Equation-of-state
- mechanical properties
- thermo-physical

#### Chemistry

- alloy content
- phases
- distribution
- impurities (interstitials)

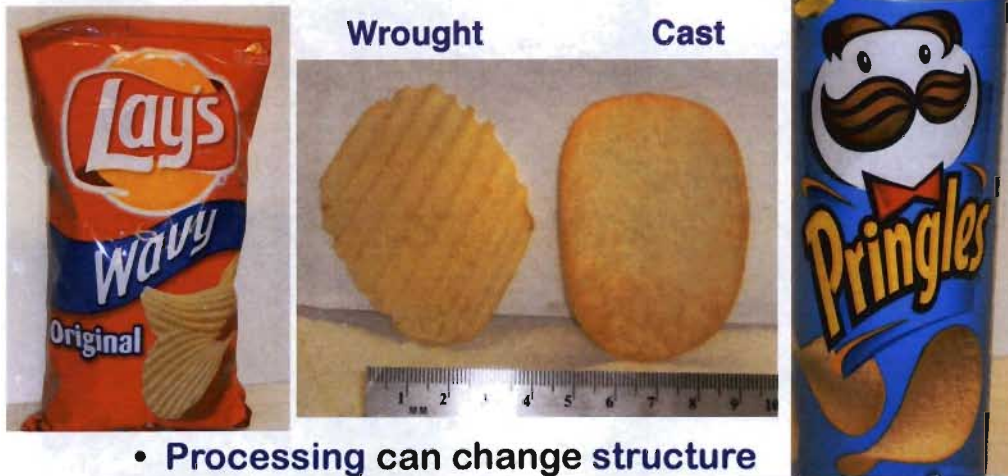
#### Structure

- microstructure (grain size, phases)
- interfaces
- defects (twins, dislocations, voids, growth flaws)
- texture



## Predictive capability of materials requires “process-aware” models

- Properties depend on structure, chemistry



- Processing can change structure

Processing controls structure + chemistry = properties = performance

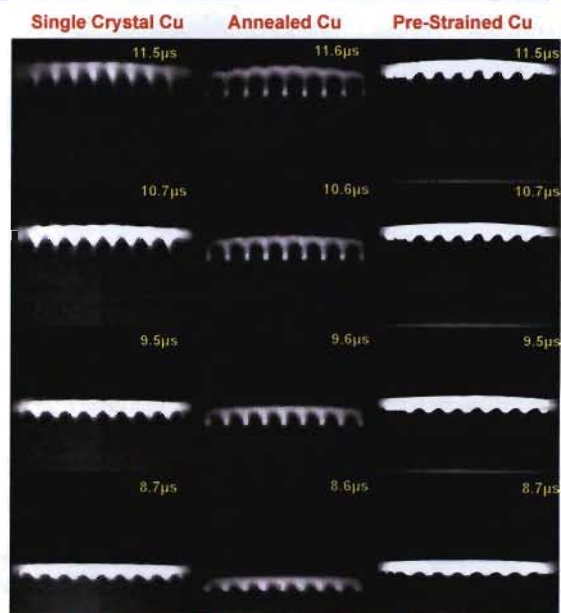


## pRad studies of perturbation growth rates as a function of time demonstrate a strong influence of materials processing

- Cu samples tested with identical drive conditions and initial perturbation: (3.0 mm vacuum gap,  $\lambda=2.0$  mm,  $A_0=55$   $\mu\text{m}$ )
  - Annealed Cu: 60  $\mu\text{m}$  average grain size
  - Cold-worked Cu: 30% strain, cross-rolled, deformation twins
  - Single crystal Cu: preferentially activate different crystalline slip systems

**Perturbation growth rate and shape depend strongly on microstructure.**

Cold-rolled Cu Micrograph

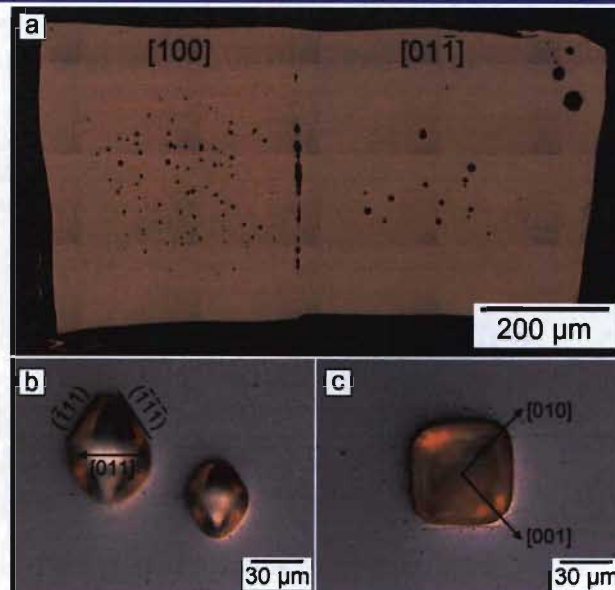
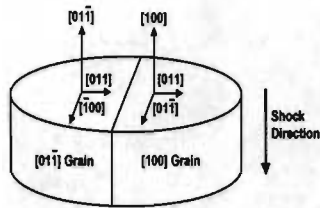


Russ Olson; P-23



Damage models must acknowledge that metals are an assembly of crystals--  
which each deform according to their local state of shear stress

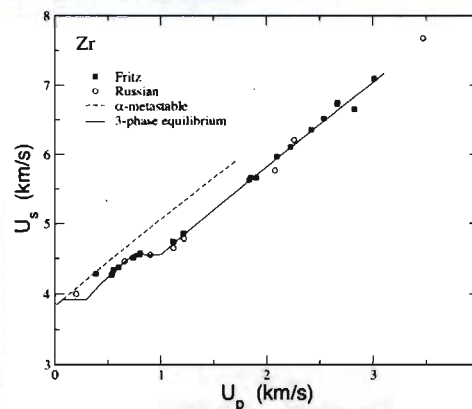
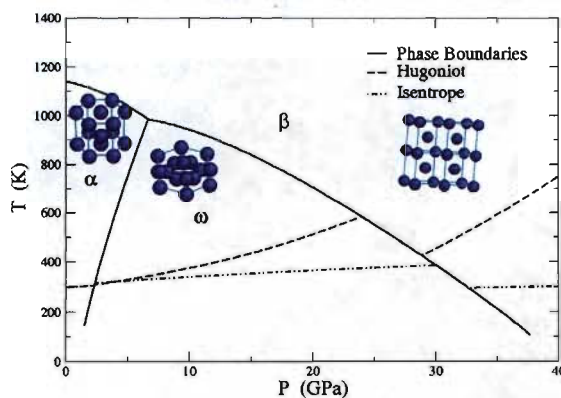
Copper Bi-crystal  
Incipiently Spalled to 2.9  
GPa



Orientation Dependence of Void Formation and Substructure Deformation in a Spalled Copper Bicrystal  
A. G. Perez-Bergquist, E. K. Cerreta, C. P. Trujillo, F. Cao, and G. T. Gray III: Scripta Materialia, (2011)



Zirconium is well suited for investigating solid-solid phase  
transitions under dynamic loading conditions



- Three solid phases exist in Zr in pressure regimes easily accessible through shock and isentropic loading.
- Kinks in legacy  $U_s - U_p$  data indicate that transitions should be observable in shock compression experiments

P.A. Rigg, C.W. Greeff, M.D. Knudson, G.T. Gray III, and R.S. Hixson:  
J. Appl. Phys., (2009) vol. 106, pp. 123532-1 to 123532-9.  
"Influence of Impurities on the  $\alpha$  to  $\omega$  Phase Transition in Zirconium  
Under Dynamic Loading Conditions"





Quantifying the effects **Process-Aware** variations on mechanisms is **Crucial** if Predictive Capability is to be Achieved



\$ 2.99



> \$ 400



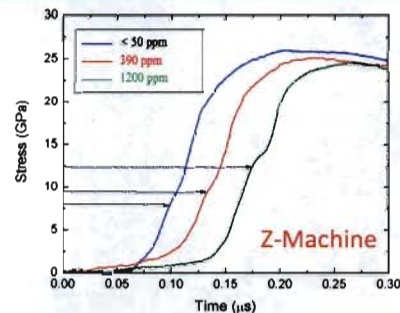
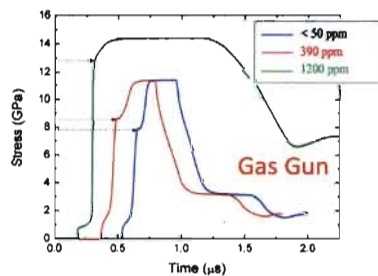
Chemistry /Processing + Aging

Chemistry + Processing = Structure = Properties

While many properties / mechanisms are principally due to structure; MANY are controlled by Impurities & Defects !



The presence of oxygen in Zr dramatically increases the stress at which the  $\alpha - \omega$  phase transition occurs



DAC Results

Zr	$\alpha \rightarrow \omega$ (hydrostatic)	$\alpha \rightarrow \omega$ (non-hydrostatic)	$\omega \rightarrow \beta$
<50 ppm oxygen	6.4	4.6	31.4
390 ppm oxygen	6.9	5.5	34.8
1200 ppm oxygen	11.6	10.8	40.0

- The DAC transition stresses differ from the Gun / Z data
- The transition signature is more pronounced for the isentropically loaded impure sample indicating that strain rate (kinetics) is important.
- Oxygen occupies interstitial sites in the a lattice which inhibits the first step of this process, thus the effective transition stress increases with increased oxygen content.
- No rarefaction shock indicating  $\omega$  phase is retained upon release.

P.A. Rigg, C.W. Greeff, M.D. Knudson, G.T. Gray III, and R.S. Hixson:  
J. Appl. Phys., (2009) vol. 106, pp. 123532-1 to 123532-9  
"Influence of Impurities on the  $\alpha \rightarrow \omega$  Phase Transition in Zirconium Under Dynamic Loading Conditions"

Nenad Velisavljevic, Gary N Chesnut, Lewis L. Stevens and Dana M Dattelbaum; J. Phys. - Condensed Matter, 23, (2011), pp.125402.  
"Effects of interstitial impurities on the high pressure martensitic  $\alpha \rightarrow \omega$  structural transformation and grain growth in zirconium"



## Astrophysics – Impact Response of Materials

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- Craters all over earth: hundreds identified
- Cretaceous/tertiary extinctions
  - Death of the dinosaurs
- Iridium layer
- Produced high-pressure mineral phases
  - Stishovite (high pressure phase of silica)



### Barringer Crater (Meteor Crater)



The object that excavated the crater was a [nickel-iron](#) meteorite about 50 meters (54 yards) across, which impacted the plain at a speed of several kilometers per second.

Modeling initially suggested that the meteorite struck at a speed of up to 20 kilometers per second (45,000 mph), but more recent research suggests the impact was substantially slower, at 12.8 kilometers per second (28,600 mph). It is believed that about half of the impactor's 300,000 metric tons (330,000 short tons) bulk was vaporized during its descent, before it hit the ground.





# Tunguska Event



Eight hundred square miles of remote forest had been ripped asunder. Eighty million trees were on their sides, lying in a radial pattern.

- The **Tunguska Event**, or **Tunguska explosion**, was a powerful explosion that occurred not far from the Podkamennaya (Lower Stony) Tunguska River in what is now Krasnoyarsk Krai in Russia on June 30, 1908.

- Although the cause of the explosion is the subject of debate, it is commonly believed to have been caused by the air burst of a large meteoroid or comet fragment at an altitude of 5–10 kilometers (3.1–6.2 mi) above the Earth's surface.

- Different studies have yielded varying estimates of the object's size, with general agreement that it was a few tens of meters across.



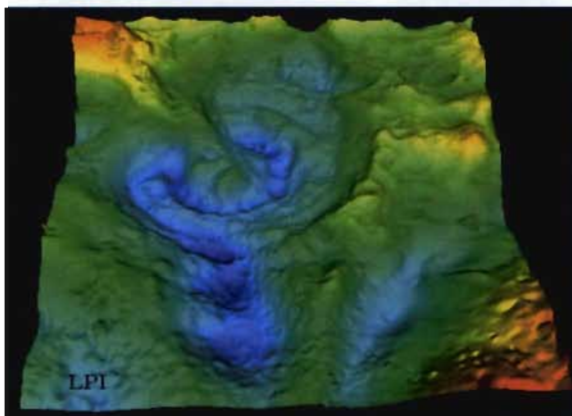
## Planetary Impact on the Earth



## Planetary Impact on the Earth



## Chicxulub crater



The crater is more than 180 km (110 mi) in diameter, making the feature one of the largest confirmed impact structures on the Earth; the impacting body that formed the crater was at least 10 km (6 mi) in diameter.

In March 2010, following extensive analysis of the available evidence covering 20 years' worth of data spanning the fields of palaeontology, geochemistry, climate modeling, geophysics and sedimentology, 41 international experts from 33 institutions reviewed available evidence and concluded that the impact at Chicxulub triggered the mass extinctions during K-T boundary including those of dinosaurs.



# Interplanetary impacts

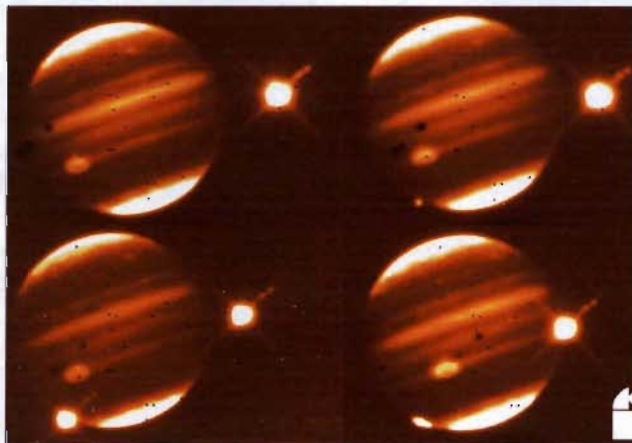
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- Satellites/space probes
  - micrometeorites; 5- 75 km s<sup>-1</sup>
  - Bumper shield designs
- Cratering on all planetary objects
- Shoemaker-Levy comet
- Fragmented into spheres 1-5 km diameter
- 20 impacts at 50 km s<sup>-1</sup>



## Shoemaker-Levy comet

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# Shoemaker-Levy comet

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- 20 ice spheres impacting at  $5 \text{ km s}^{-1}$
- Volume of spheres at 1 km diameter
  - $V = \frac{4}{3} \pi r^3 = 5.23 \times 10^8 \text{ m}^3$
  - $\text{Mass} = V\rho = 5.23 \times 10^{11} \text{ kg}$
- Kinetic energy =  $20 \frac{1}{2} m v^2 = 1.3 \times 10^{22} \text{ J}$
- Largest nuclear blast
  - Russians, equivalent to 58 Mtons
  - Chemical energy = 5 MJ/kg
  - Energy of blast =  $58 \times 10^9 \times 5 \times 10^6 = 2.9 \times 10^{17} \text{ J}$
- Comet impact  $\int 44\,800$  nuclear blasts!



## Challenges facing the Field of Shock Physics

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- The response of materials subjected to extreme environments is central to the stockpile stewardship program tasked with ensuring the safety and reliability of the US strategic deterrence in the absence of full-scale underground testing.
- The scientific and engineering tasks facing NNSA are to nurture and develop predictive modeling capability integrated with small-scale through integrated testing in support of on-going defense system certification and life-extension programs. The development of physics and materials models based on quantifiable physical mechanisms, characterized with inexpensive direct experiments, and validated through comparisons with results of small-scale and integral tests is challenging.
- The study of material response under dynamic extreme loading conditions--particularly experimentally--is taught at only limited select academic institutions with focused programs. As a result, the field often pulls on a diverse set of disciplines for its pipeline. The focus within SSAA on materials under extremes can provide an academic focus for this exciting and challenging area of study.





# Exciting Research Frontiers

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- The field of material response under extreme loading conditions has reached a critical point of truly interdisciplinary study embracing the disciplines of Materials Science, Shock Physics, and Chemistry among others to tackle a new level of mechanistic understanding of the complex phenomena that exist in this regime.

Four examples are:

- **the determination of the thermodynamic properties of materials** defining the structural and electronic changes that occur when materials are subjected to extreme environments ,
- **material strength under loading of differing impulses** varying loading stress, time, and path, stress state, and temperature ,
- **the determination and characterization of dynamic damage evolution**, spall, and dynamic fracture mechanisms in materials, and
- **assessing chemical reactions** within a dynamic environment of interest.

