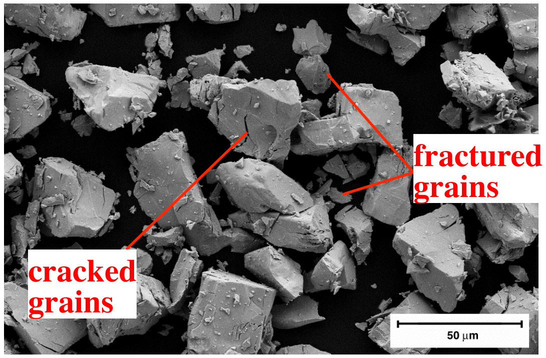
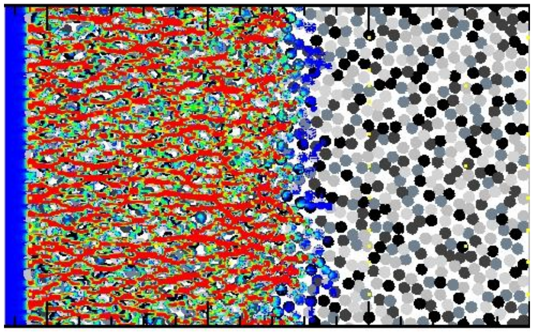
SAND2014-20244PE

# Dynamic Behavior of Granular Materials

Tracy Vogler
Department 8256, Mechanics of Materials
Sandia National Laboratories, Livermore CA

Institute of Shock Physics
Imperial College, London
December 9, 2014



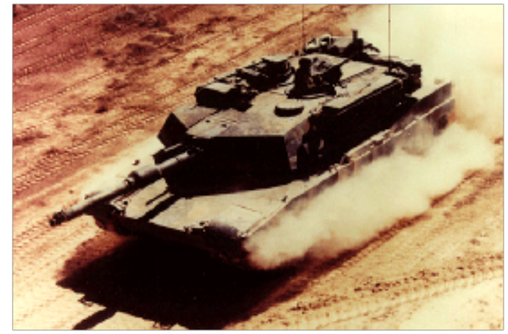



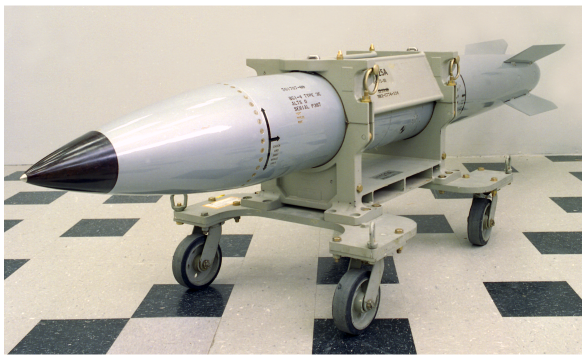
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

- Introduction to Shock and High-Pressure Physics
- Introduction to Granular Materials
- Compaction and Scaling Properties of Waves
- High Pressure EOS – Experiments and DFT Modeling
- The Intermediate Regime – Porosity Enhanced Densification
- Closure and Acknowledgements

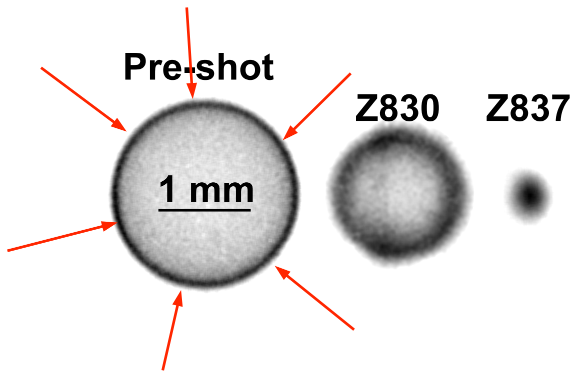
# Why Do We Need To Know the Behavior of Materials Under Extreme Conditions?

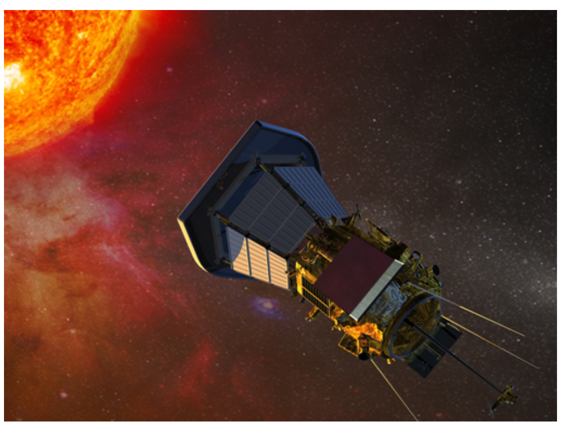
- weapons applications (warheads, armor, etc.)
- explosives behavior and applications



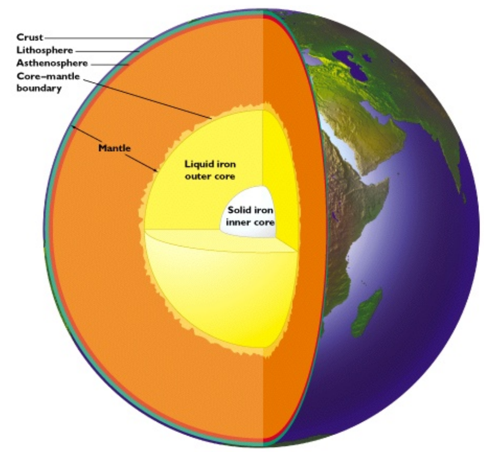


- inertial confinement fusion



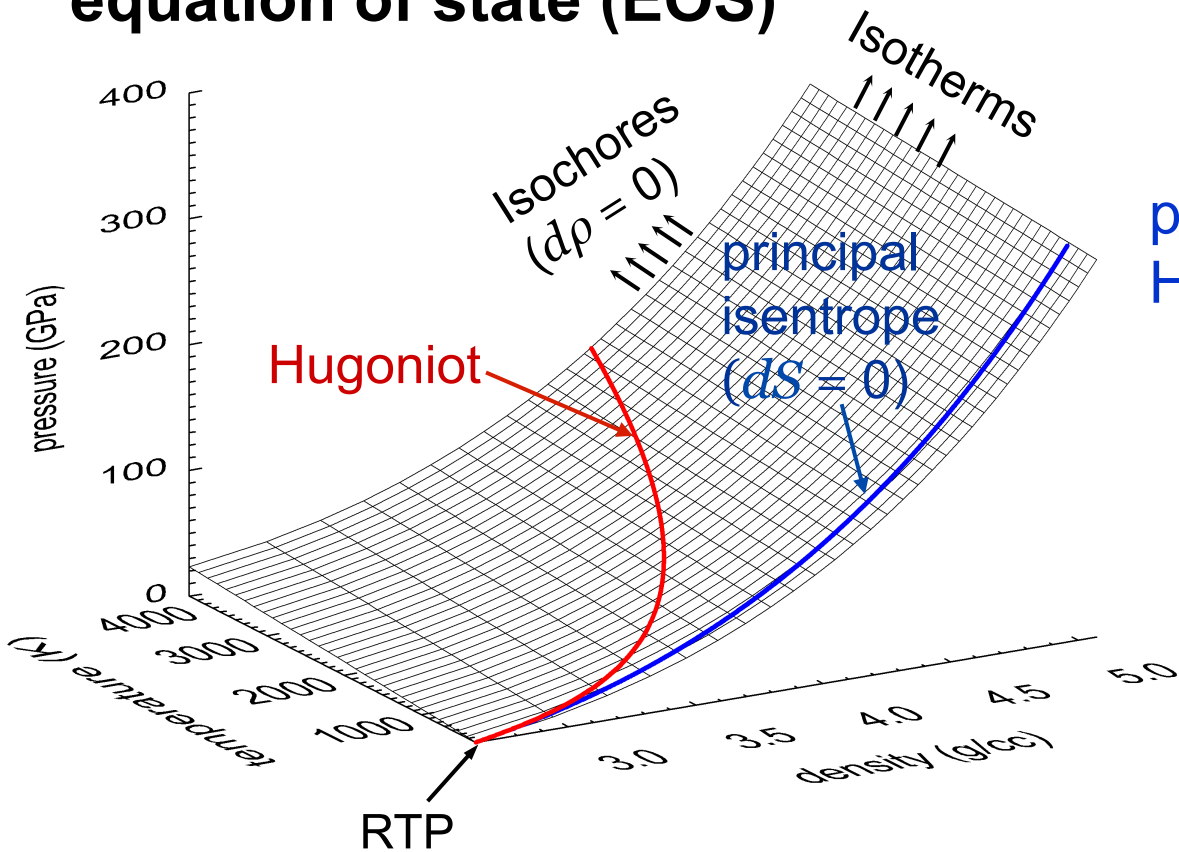
- solar probe
  - 100 μm particles
  - up to 300 km/s velocities
  - $P_{max}$ ~ 100 TPa, $T_{max}$ ~$10^6$ K




- planetary science (P~360 GPa, T~7000 K)

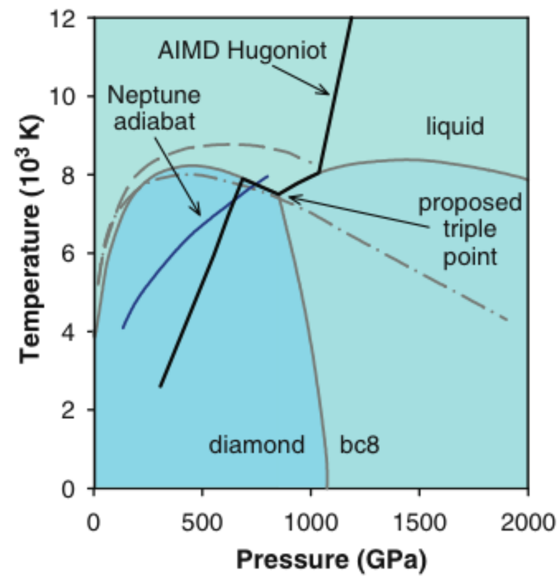
# Material Behavior:
# EOS & Constitutive Aspects

## equation of state (EOS)




one thermodynamic state variable as a function of two others:

pressure $P = P(\rho,T)$
Helmholtz energy $f = f(v,T)$

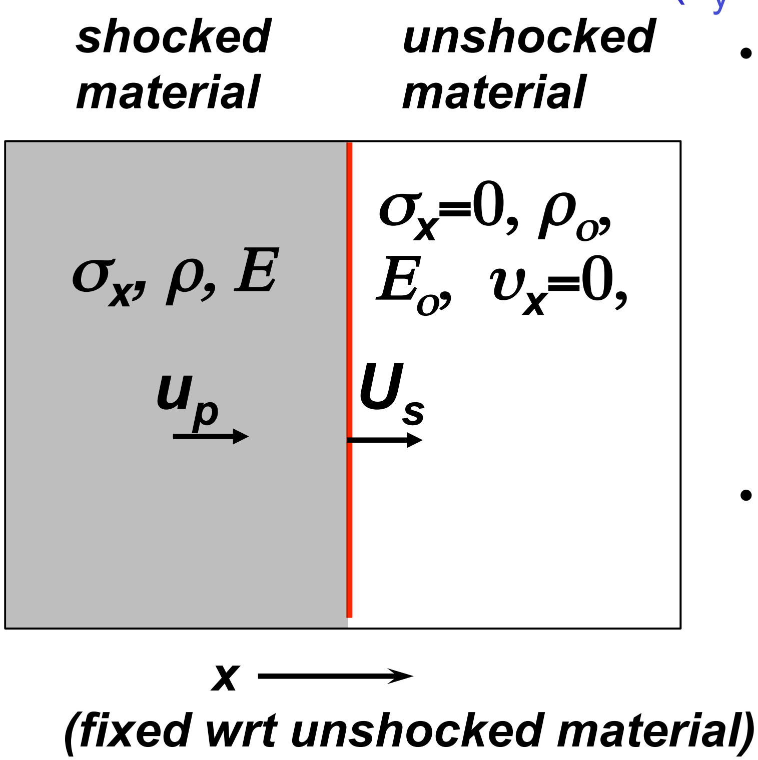



Knudson, M. D., M. P. Desjarlais and D. H. Dolan (2008). "Shock-wave exploration of the high-pressure phases of carbon." *Science* **322**: 1822-1825.

***Also: strength, damage, spall (tensile failure), compaction***

# What is a Shock Wave?

- A "discontinuous" wave that moves at a fixed velocity (if steady)
  - wave front moves at speed $U_s$ *(shock velocity)*
  - shocked material moves at speed $u_p$ *(particle or mass velocity)*
  - uniaxial strain condition ($\varepsilon_y=\varepsilon_z=\varepsilon_{xy}=\varepsilon_{yz}=\varepsilon_{xz}=0$)




- States ahead and behind shock <u>*assumed*</u> to be in thermodynamic equilibrium
  - well defined temperature in each state
  - described by equilibrium thermodynamics
- Shock compression is adiabatic
  - very fast process (< 1 ns)
  - irreversible (i.e. NOT isentropic)
  - temperature *typically* increases

# Conservation Equations and the Shock Hugoniot

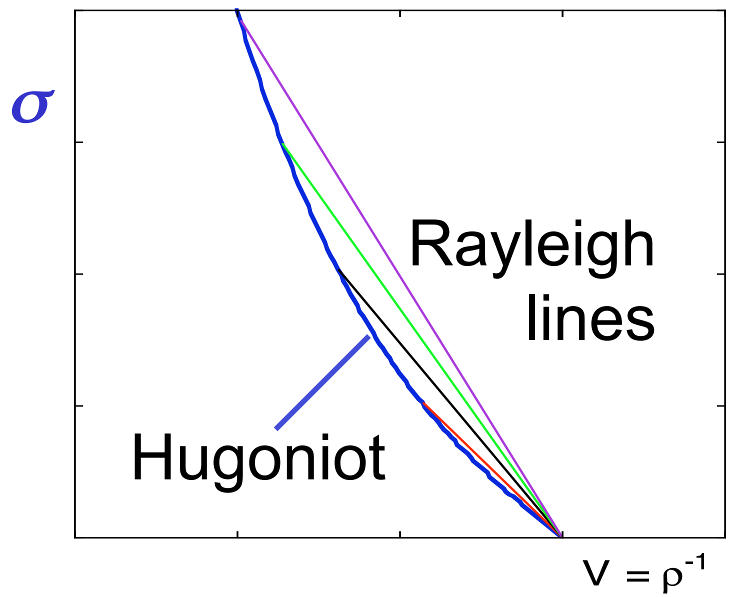
- Five variables: $\sigma_x$, $u_p$, $U_s$, $\rho$, and $E$
- Three conservation relationships (Rankine-Hugoniot jump conditions)
  - By measuring two variables (typically $\sigma_x$, $u_p$, or $U_s$), the other three can be determined

**conservation of**

mass: $\rho_o U_s = \rho (U_s - u_p)$

momentum: $\sigma_x = \rho_o U_s u_p$

energy: $E - E_o = 0.5\sigma_x (V_o - V)$




material loads along the Rayleigh line, so the Hugoniot is a collection of end states, not a material response curve

*the Hugoniot is not a complete equation of state (EOS)!*

# Gas Guns to Generate Shock Waves

Single Stage Gun 100mm

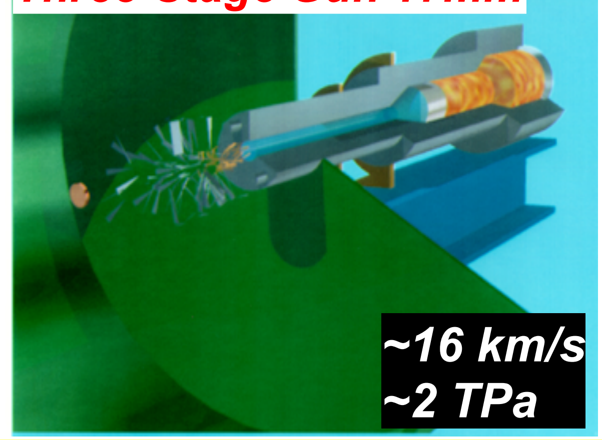

Propellant Gun 89mm


Two-Stage Gun 29mm


## gas guns

- launch thin plates (mm's) at high velocities
- well-posed, repeatable initial conditions
- sample is in uniaxial ***strain***
- used to study material behavior at high pressures and strain rates
- usable in laboratory setting

Three-Stage Gun 17mm

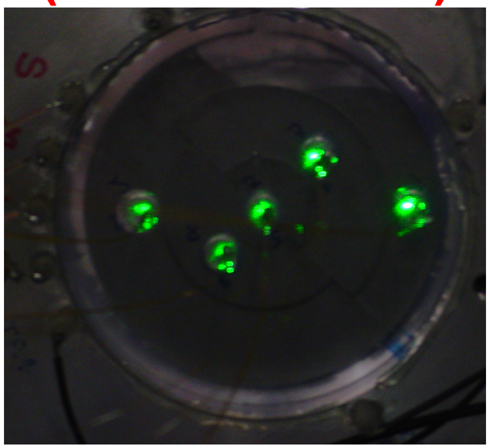



Chhabildas, L. C., Dunn, J. E., Reinhart, W. D., and Miller, J. M. (1993). "An impact technique to accelerate flier plates to velocities over 12 km/s," *Int. J. Impact Eng*. **14**, 121-132.

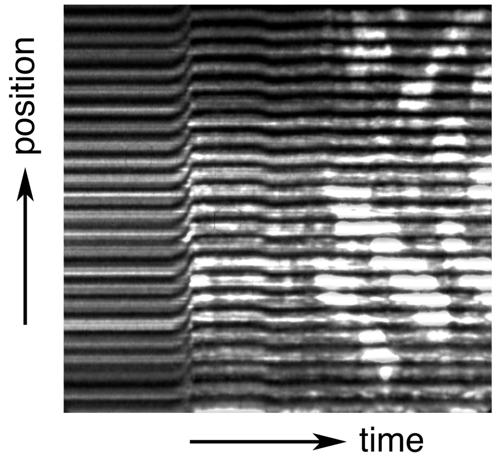
*also: explosives, lasers, magnetic loading (Z)*

# Diagnostics for Dynamic Experiments

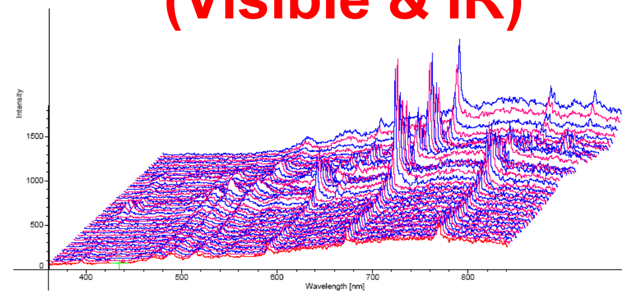
## Velocity Interferometry (VISAR & PDV)



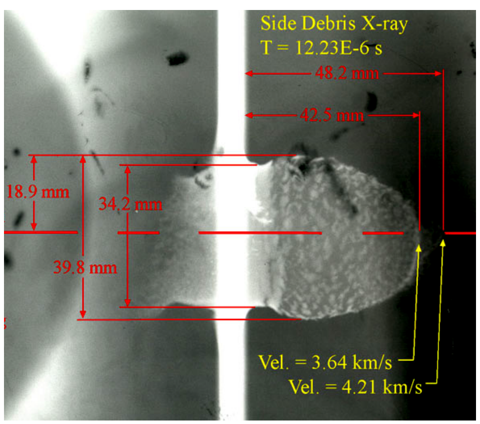
## Line-VISAR



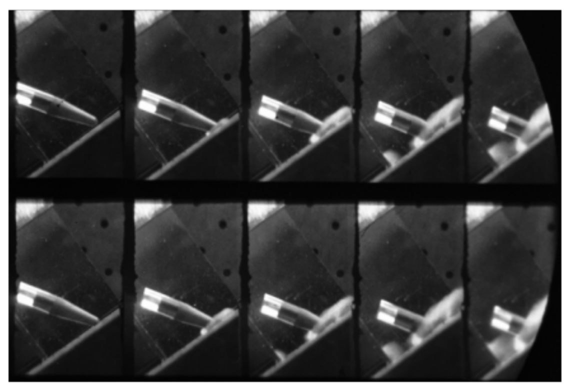

## Time-Resolved Spectroscopy (Visible & IR)



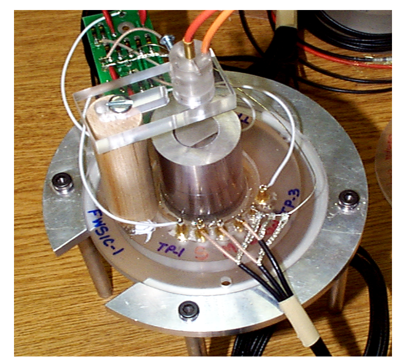

## Flash X-rays




## High-Speed Photography



## Pressure Gauges

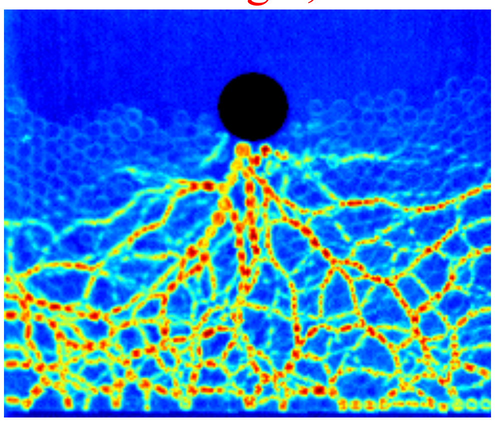


Advanced Diagnostics: pRad, synchrotron (DCS), etc.

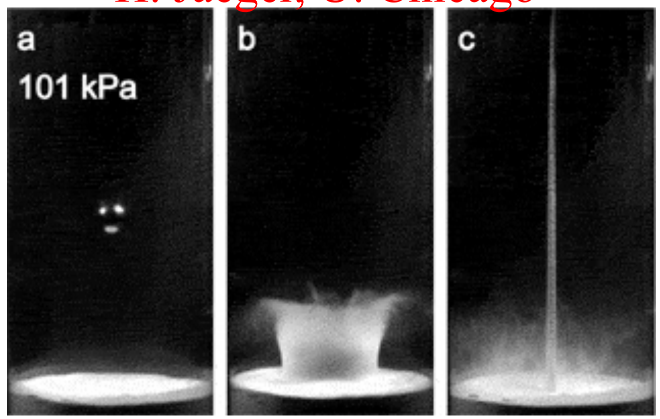
- Introduction to Shock and High-Pressure Physics
- Introduction to Granular Materials
- Compaction and Scaling Properties of Waves
- High Pressure EOS – Experiments and DFT Modeling
- The Intermediate Regime – Porosity Enhanced Densification
- Closure and Acknowledgements

# Background on Dynamic Behavior of Granular Materials

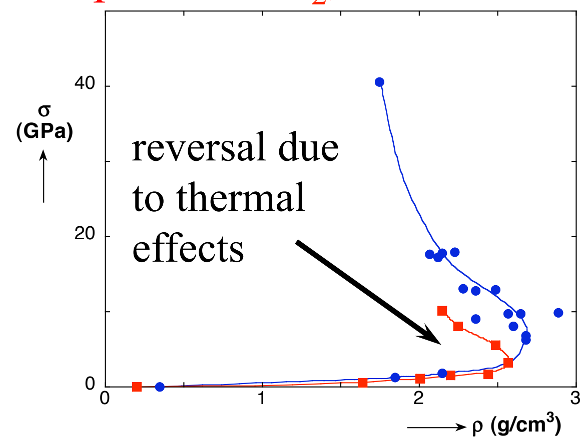
B. Behringer, Duke



H. Jaeger, U. Chicago




porous $SiO_2$, Trunin et al.

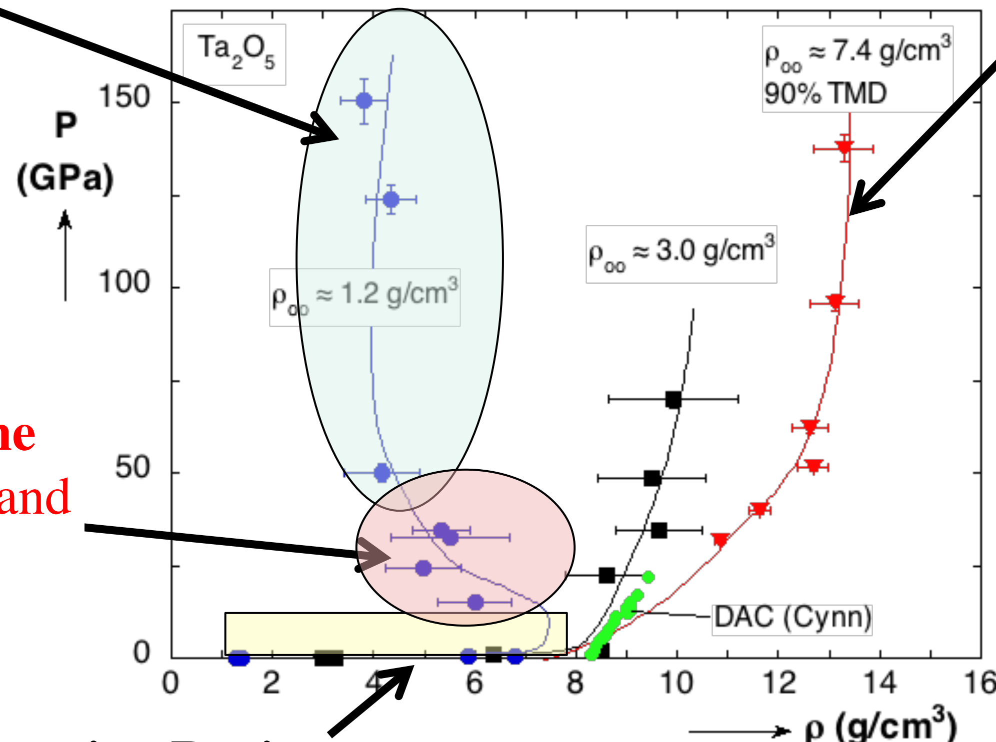



- granular materials display a rich variety of behaviors
- significant experimental and modeling challenges
- extensive quasi-static and low-velocity impact work
- determine thermal behavior through P-V work (Trunin, 2004)
- consolidation studied extensively to optimize loading, etc.
- partial compaction region seldom addressed
- applications: dynamic consolidation, energetic / reactive materials, planetary science, energy/blast absorption, ceramic armor

# Regimes of Behavior for Granular Ceramics

**High Pressure Expanded Regime**
warm dense matter regime, thermal EOS melting, ionization, disassociation, etc.

**Principal Hugoniot**
EOS, strength, phase transformations, melt

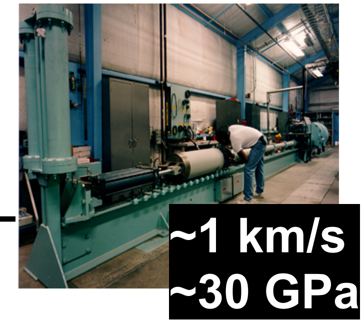


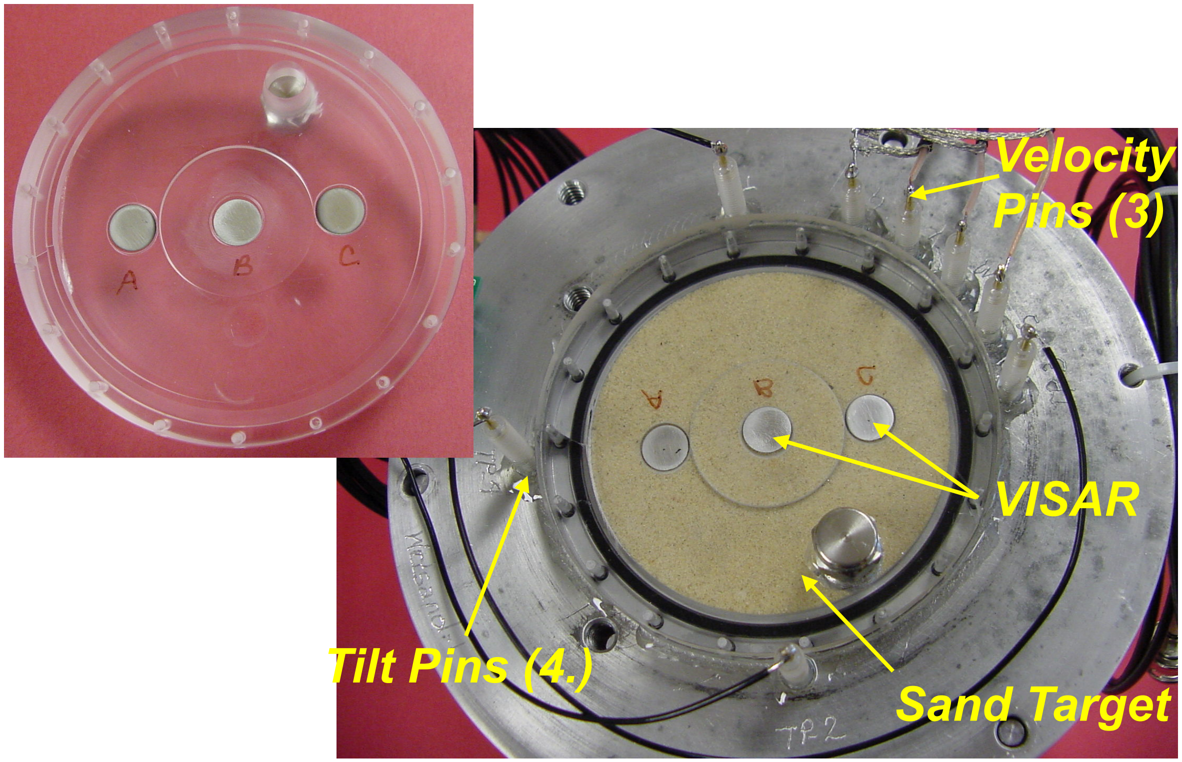

**Intermediate Regime**
all EOS phenomena and particulate behaviors may be active

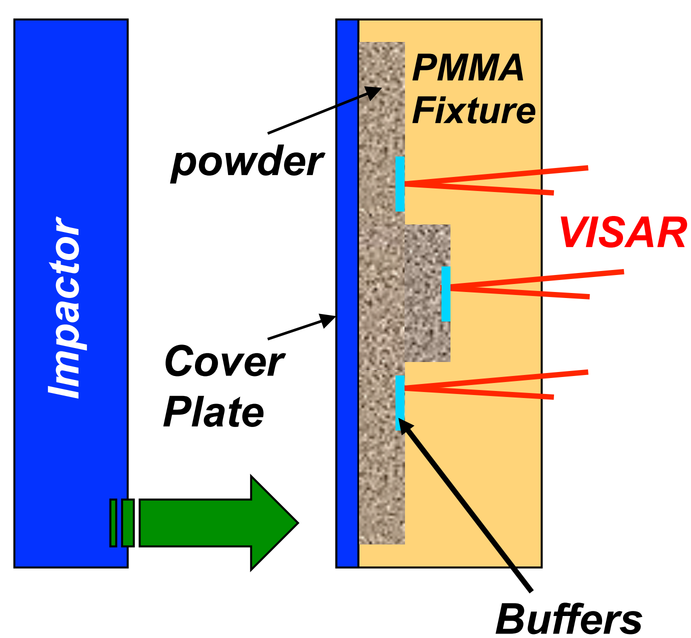
**Compaction Regime**
P, $\sigma$ < Y (10-20 GPa)
particle crushing, fracture, strength of granular compact

- Introduction to Shock and High-Pressure Physics
- Introduction to Granular Materials
- Compaction and Scaling Properties of Waves
- High Pressure EOS – Experiments and DFT Modeling
- The Intermediate Regime – Porosity Enhanced Densification
- Closure and Acknowledgements

# Planar Impact Experiments on Granular Materials



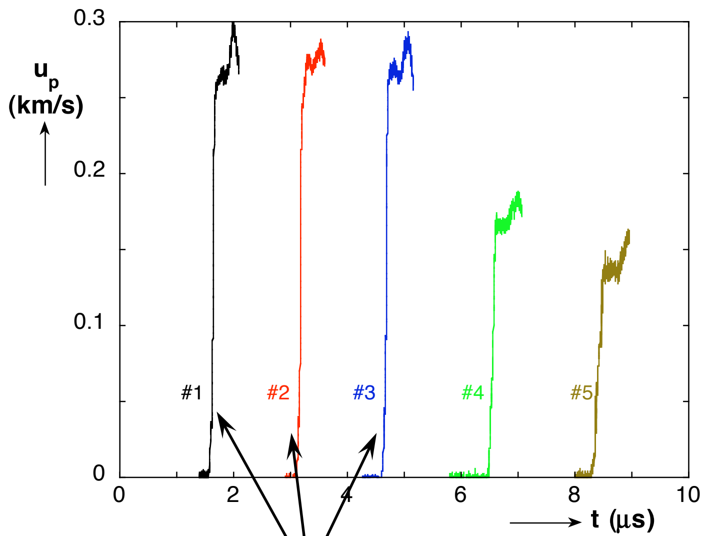



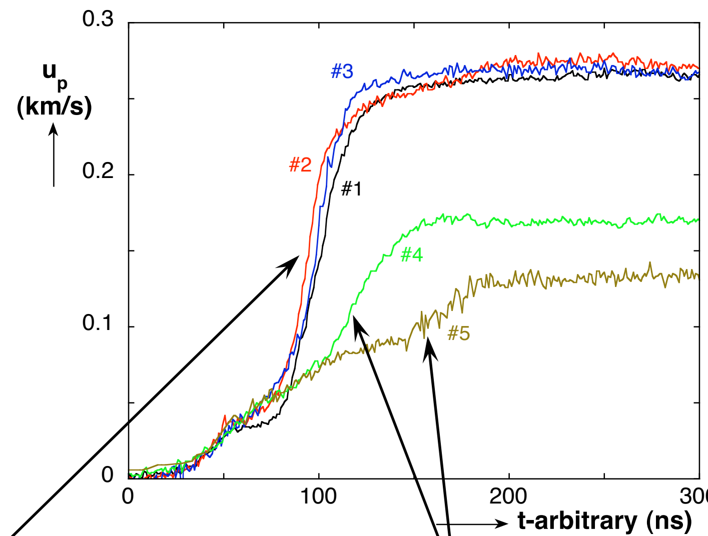

**stepped sample for accurate shock velocity and uniform powder density; sealed capsule allows fluid / powder mixtures**

Vogler, T.J., Lee, M.Y., Grady, D.E., 2007. "Static and dynamic compaction of ceramic powders." *International Journal of Solids and Structures* **44**, 636-658.

Brown, J.L., Thornhill, T.F., Reinhart, W.D., Chhabildas, L.C., Vogler, T.J., 2007. "Shock response of dry sand." in Shock Compression of Condensed Matter – 2007, American Institute of Physics, 1363-1366.

# Measured Steady Waves in WC



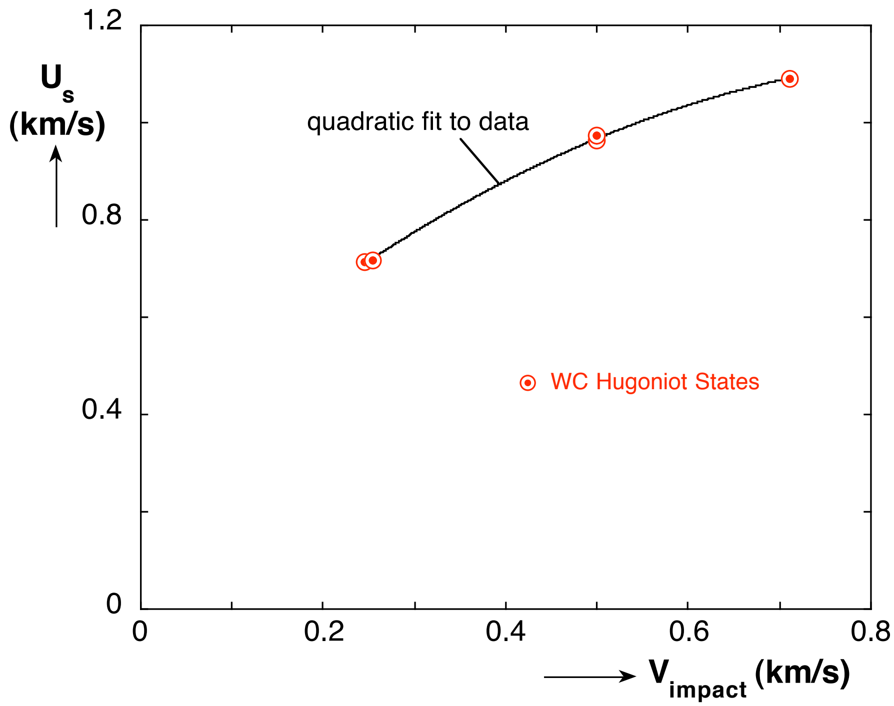

**shock velocity calculated based on powder thicknesses and arrival times**

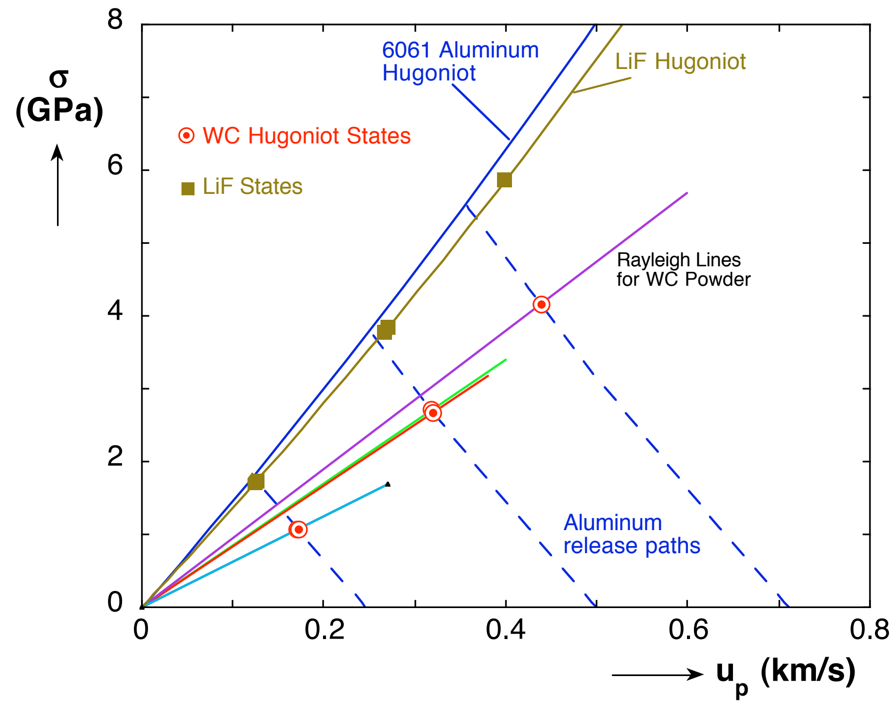
**steady, structured waves**

**attenuated waves**

- seem to be first time-resolved measurements of steady waves in granular materials
- since waves are steady, Rankine-Hugoniot jump conditions can be used even though waves have finite rise times

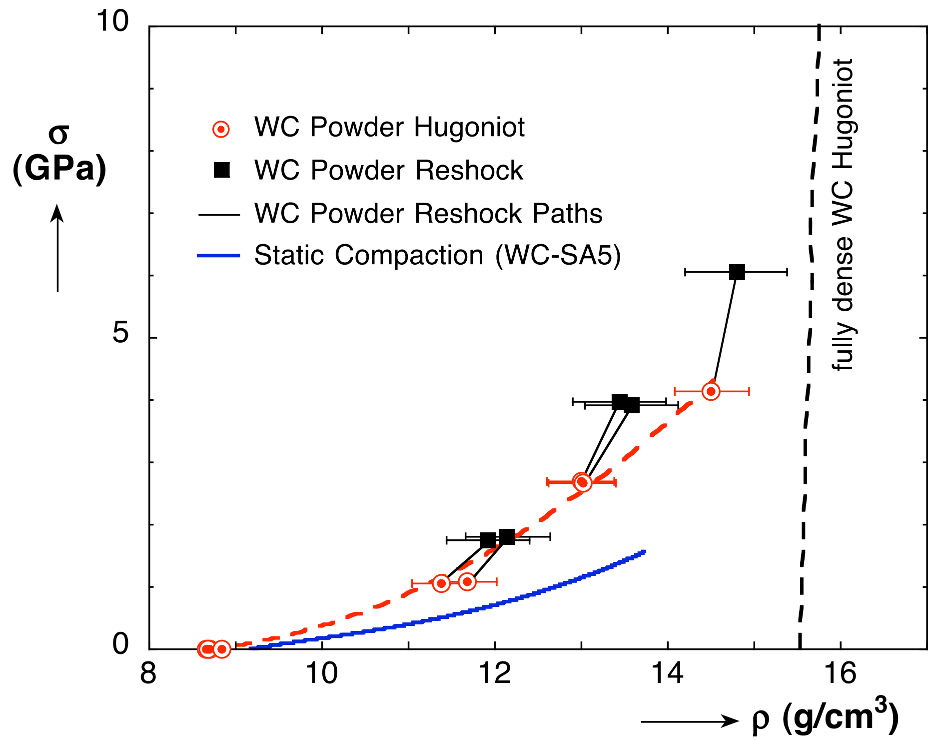
# Shock Velocities and Hugoniot States

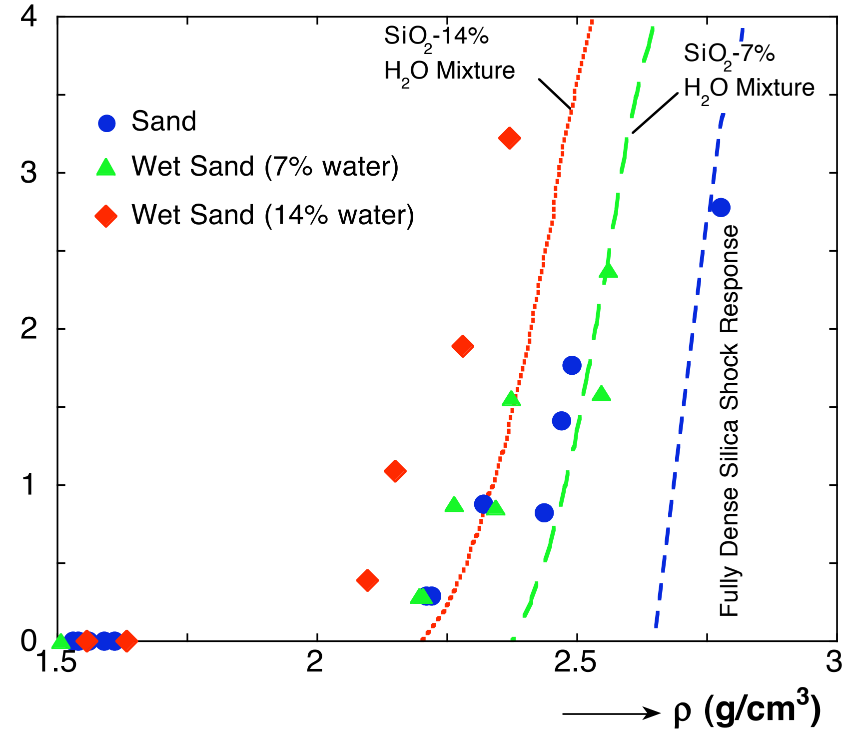



- impedance matching to aluminum impactor used to determine Hugoniot stress and particle velocity ($\sigma = \rho_{oo} U_s u_p$)
- density then calculated from $\rho = \rho_{oo} U_s / (U_s - u_p)$

# Compaction Response for WC and Wet/Dry Sand

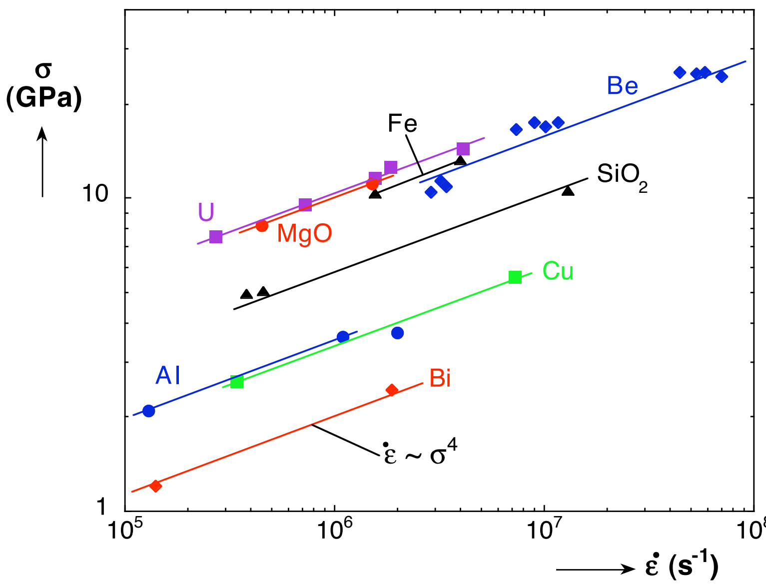


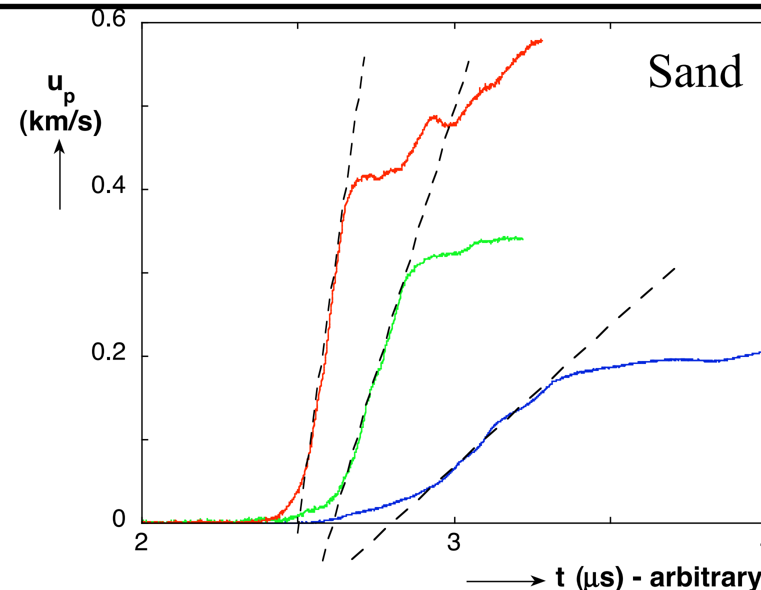



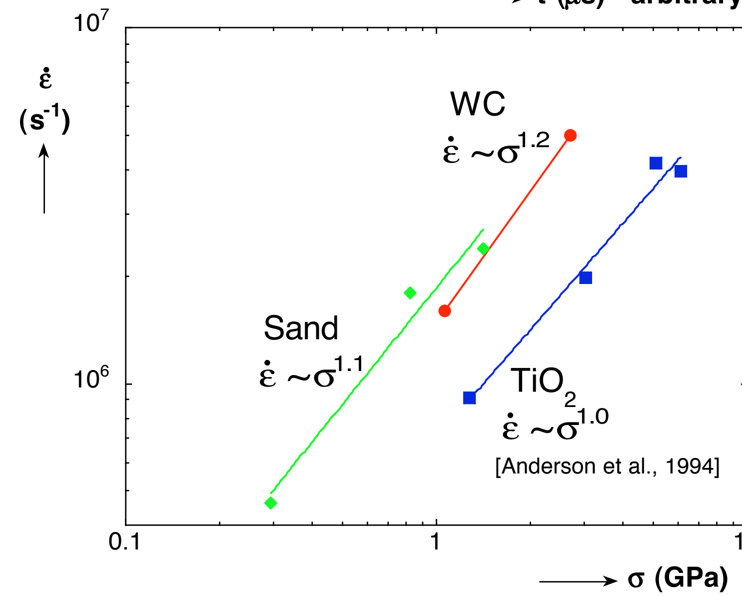

- first reshock state lies above Hugoniot suggesting elastic response of compacted material
- dynamic response is stiffer than static response for WC, about the same for sand

# Scaling Between Rise Time of Wave and Stress

for many fully dense materials (Al, Be, Bi, Cu, Fe, MgO, $SiO_2$, U), rise times of steady waves scale as $\dot{\varepsilon} \sim \sigma^4$ (Swegle & Grady, 1985)



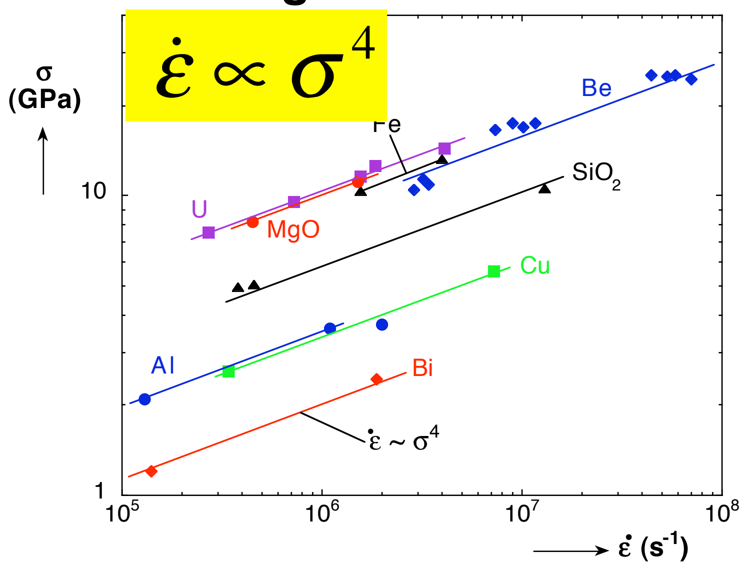



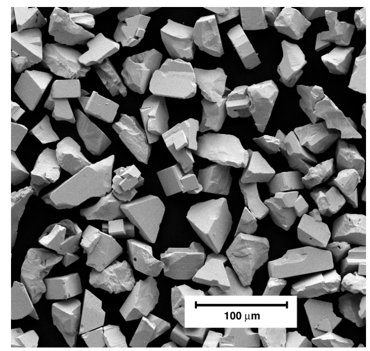




data on three granular ceramics and sugar suggest a linear scaling between stress and strain rate

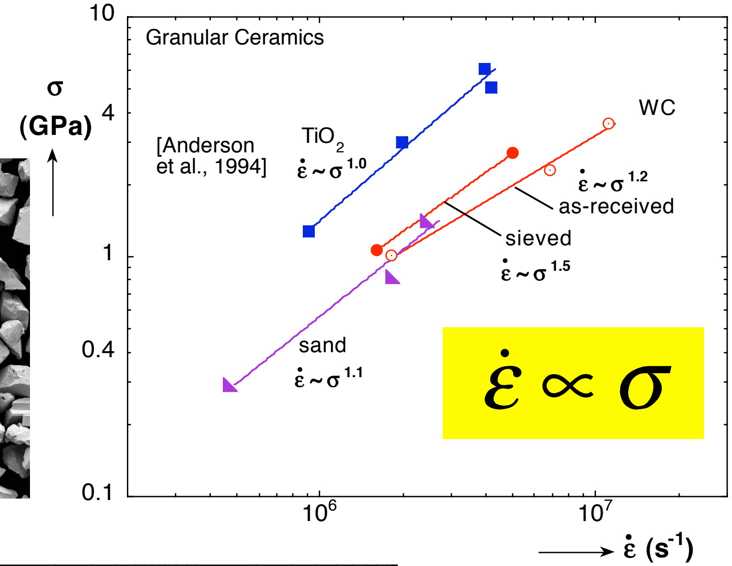
# Scaling of Waves in Materials

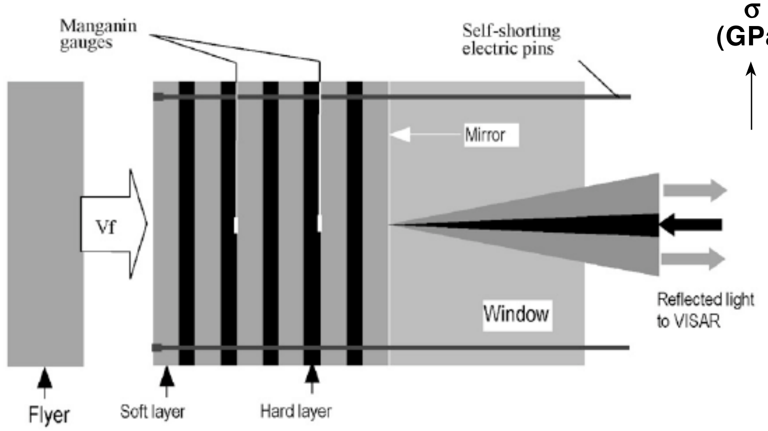
## "Homogeneous" Materials



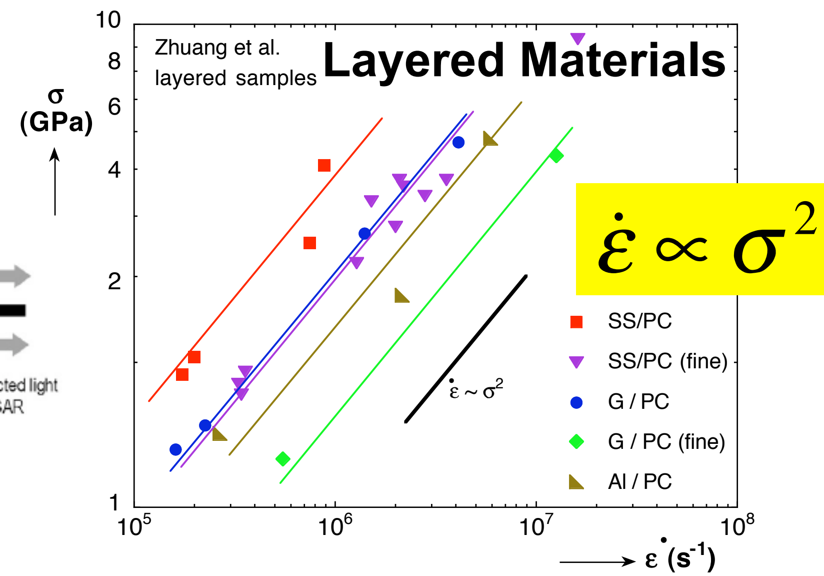




## Granular Materials



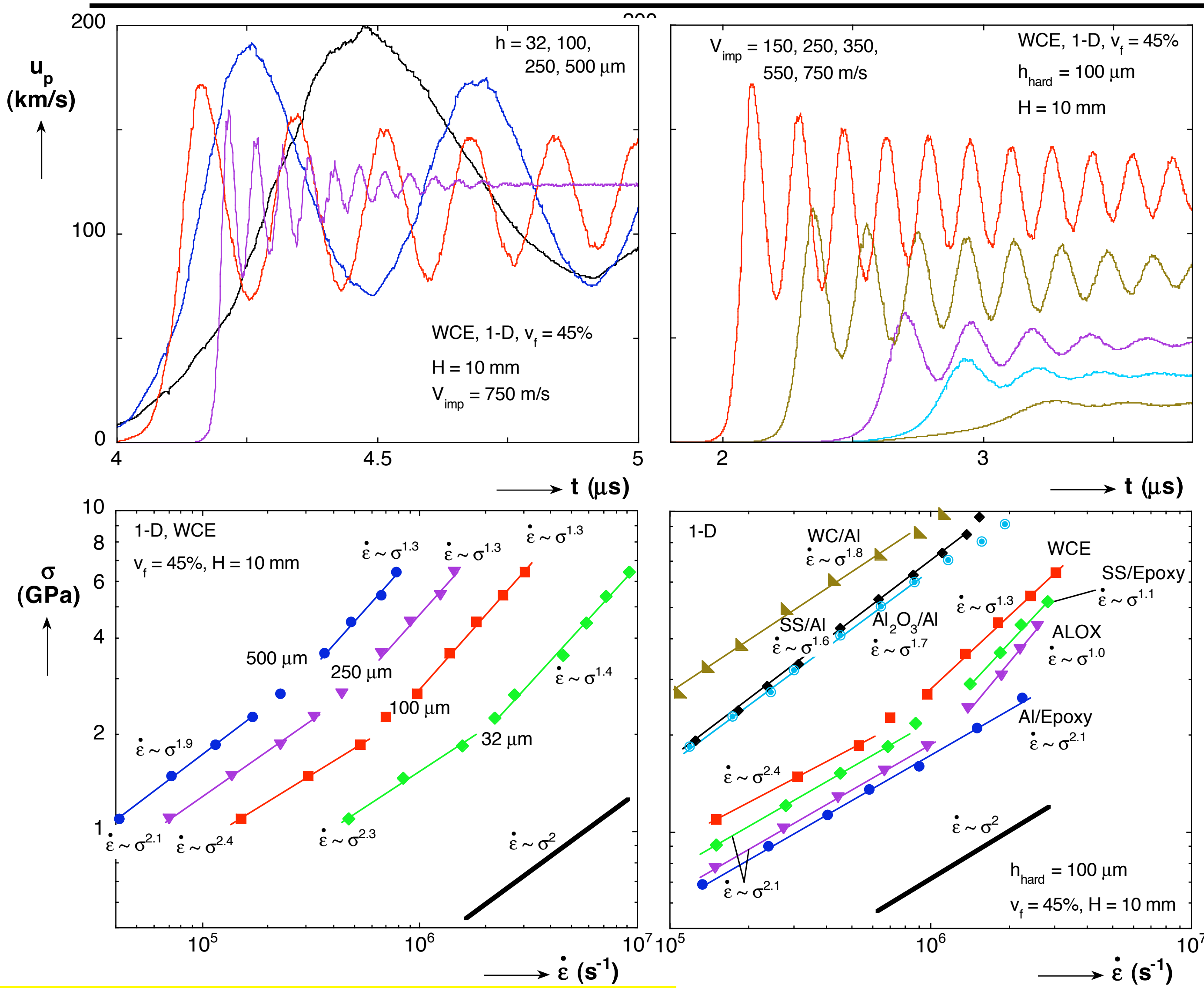




## Layered Materials




particulate composites (e.g. WC/epoxy, ALOX, PBX) show 4th power scaling

# Simulations for Layered Materials
# 1-D CTH Calculations




h ↑ $\dot{\varepsilon}$ ↓

V,σ ↑ $\dot{\varepsilon}$ ↑

also a function of material parameters of layers

Vogler et al. (2012) J. of Applied Physics

# Dimensional Analysis for Layered Materials

variables of problem:

$\sigma$, $\dot{\varepsilon}$, h, $v_f$, C, $(\rho_s,\rho_h)$ or $(z_s,z_h)$

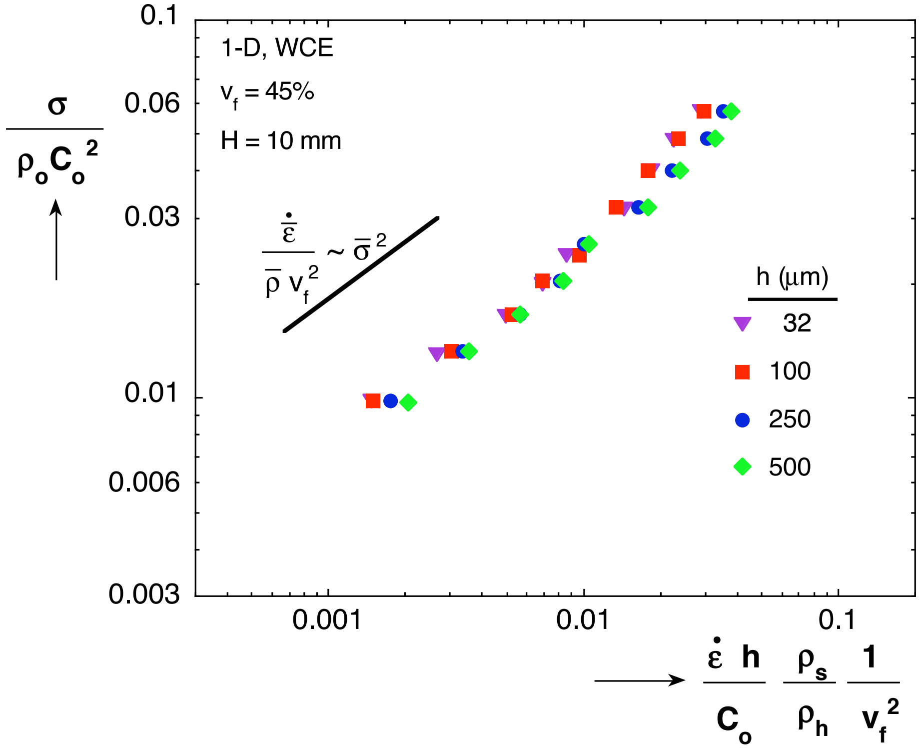
construct non-dimensional groups:

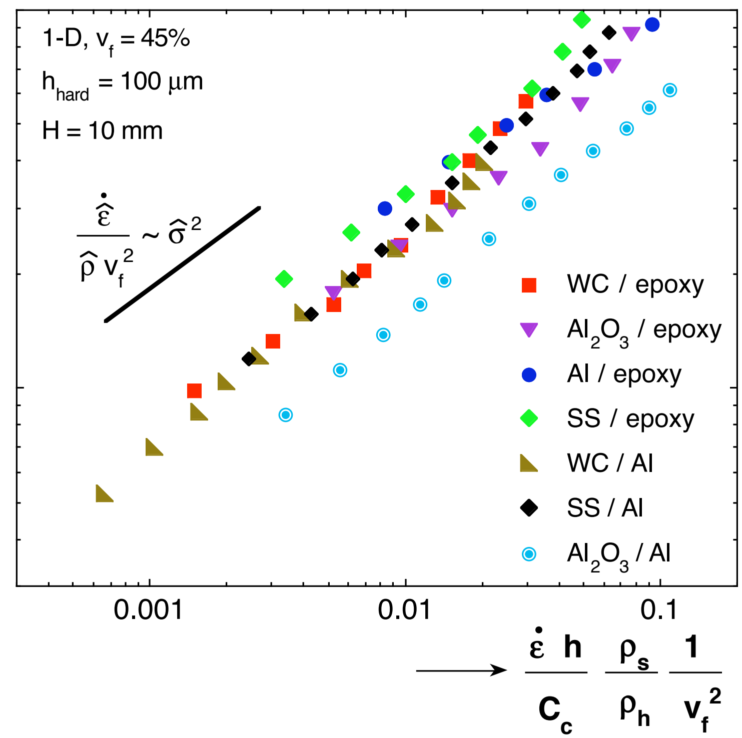
$$\bar{\dot{\varepsilon}} = \left(\frac{\dot{\varepsilon}\, h}{C_o}\right) \qquad \bar{\sigma} = \left(\frac{\sigma}{\rho_o\, C_o^2}\right) \qquad \left(v_f\right) \qquad \bar{\rho} = \left(\frac{\rho_s}{\rho_h}\right)$$

$$C_o = \left(\frac{v_f}{C_h} + \frac{1-v_f}{C_s}\right)^{-1} \qquad C_h, C_s = \begin{cases} C_B \;\; \textit{for polymers and metals} \\ C_L \;\; \textit{for ceramics} \end{cases}$$

$$\rho_o = v_f \rho_h + (1-v_f)\rho_s$$

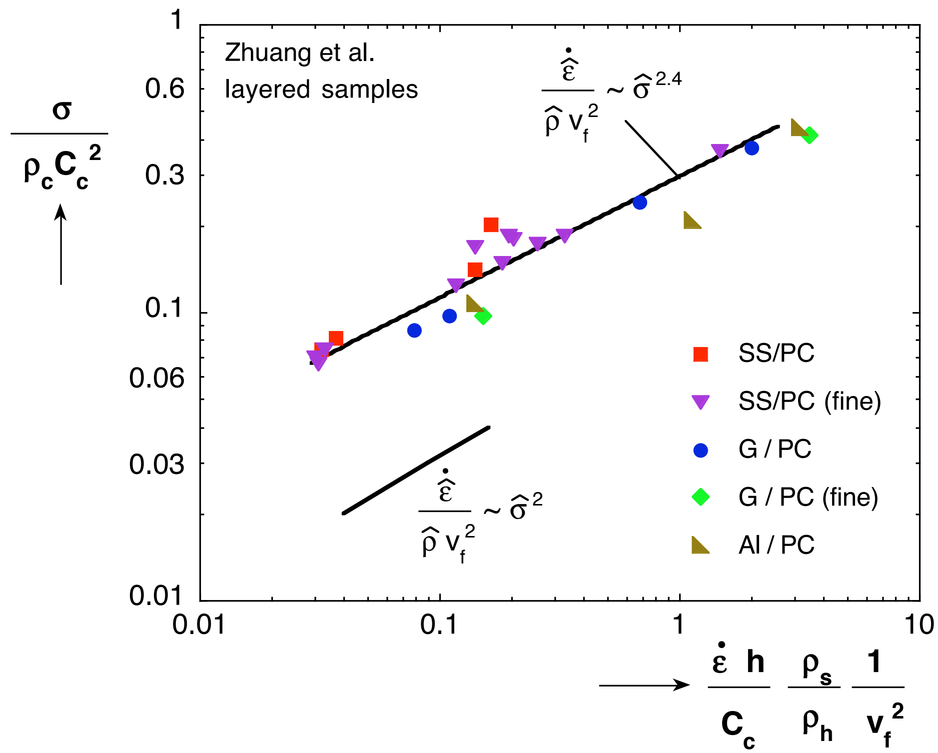
# Non-Dimensional Simulation Results



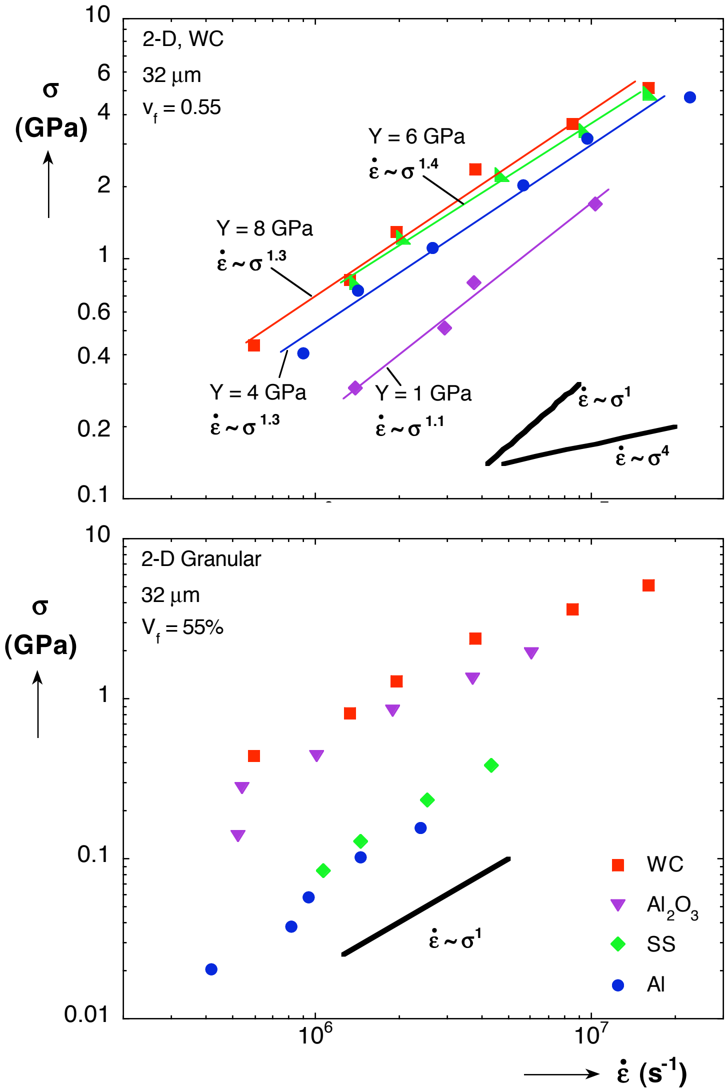

- non-dimensionalization collapses data for different layer thicknesses
- data for different material combinations collapse well using density ratio (with one exception)

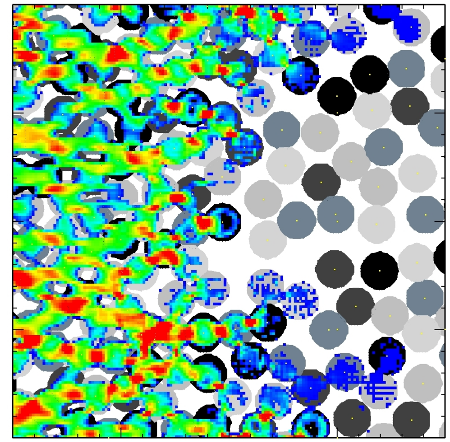
# Non-Dimensionalized Experimental Results




- non-dimensional experimental results also collapse to a single curve (approximately to second power)

# 2-D CTH Simulations of Granular Materials

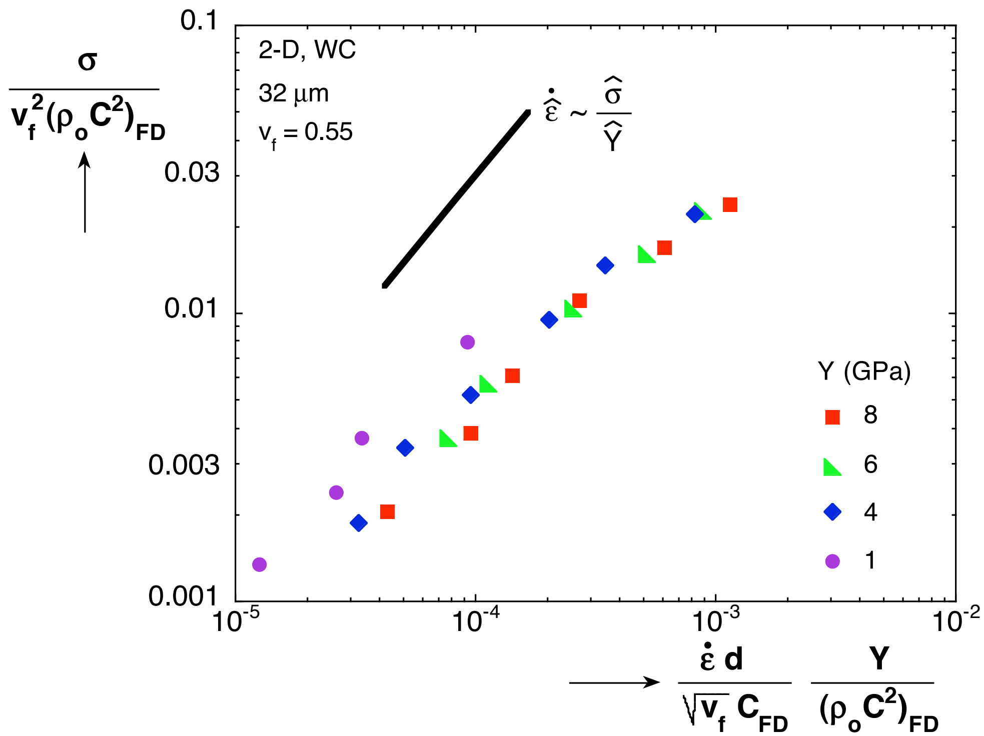


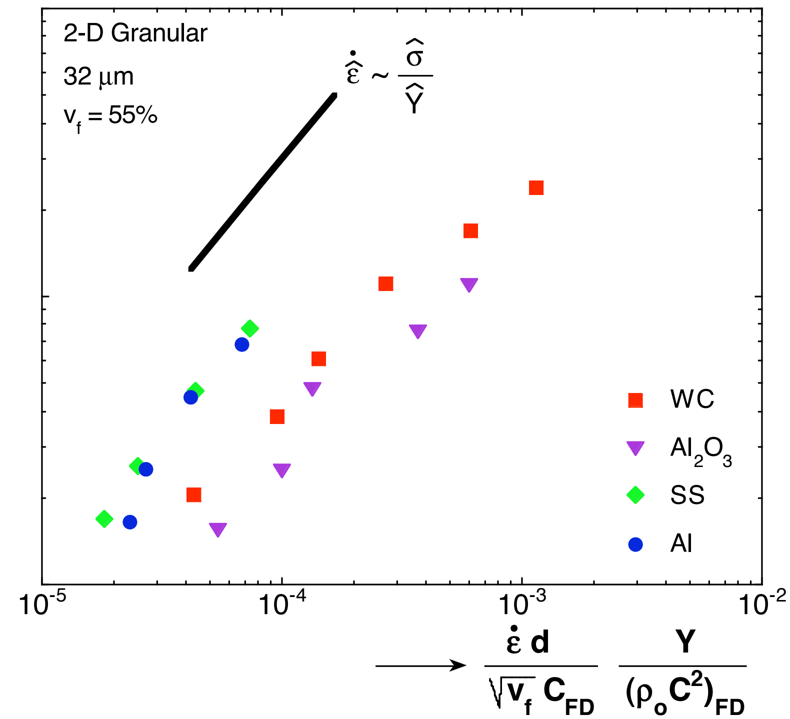



- non-planar shock structure
- CTH simulations reproduce first power scaling
- some dependence on Y, strong material dependence
- non-dimensionalization suggested by Grady (2010):

$$\frac{\sigma}{\dot{\varepsilon}} \propto \left(\frac{\rho_o}{\rho_s}\right)^m \sqrt{\rho_o\, d^2\, \sigma_c}$$

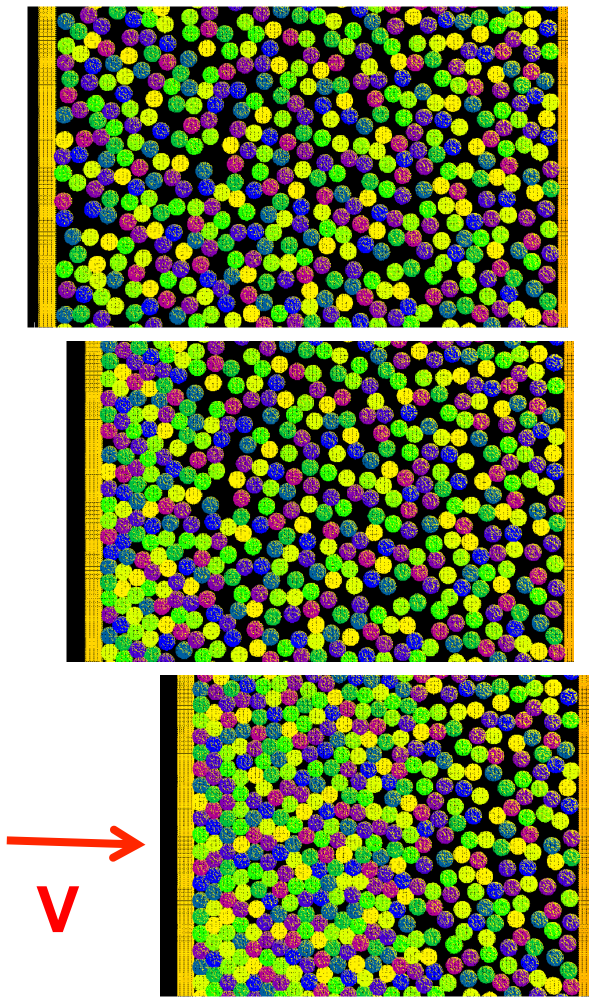
# Non-Dimensionalization of CTH Results



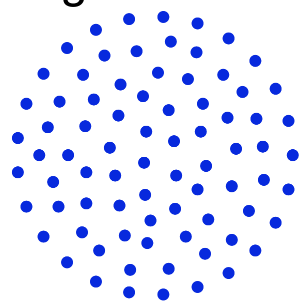



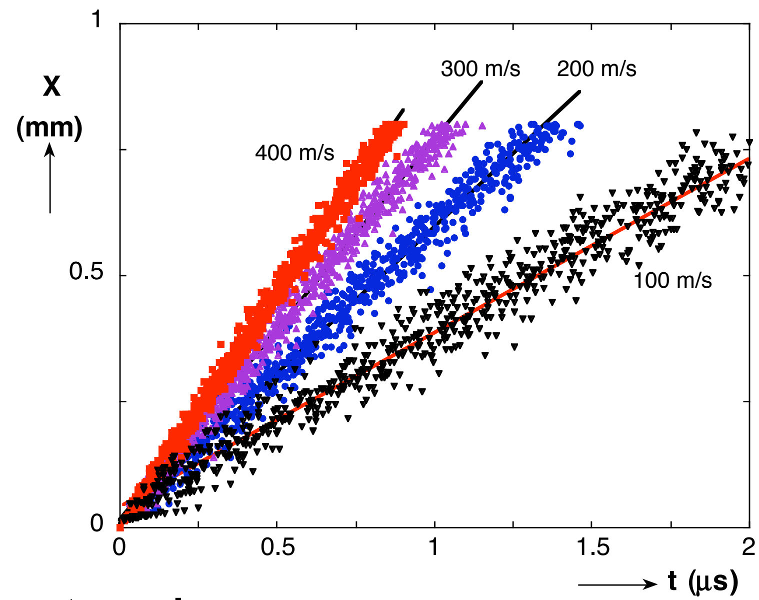

- scale wave speeds by square root of volume fraction (suggested by Steinberg, some validation by Bless)
- Y needed to collapse data, though metals and ceramics separated somewhat

# Results from a Particle-Based Peridynamics Code



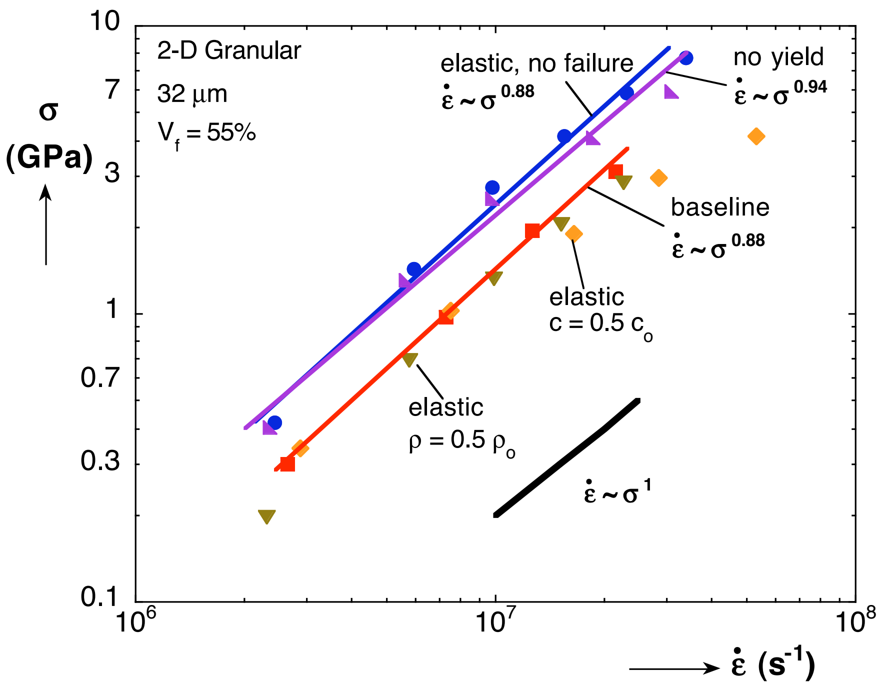

discretization of grains

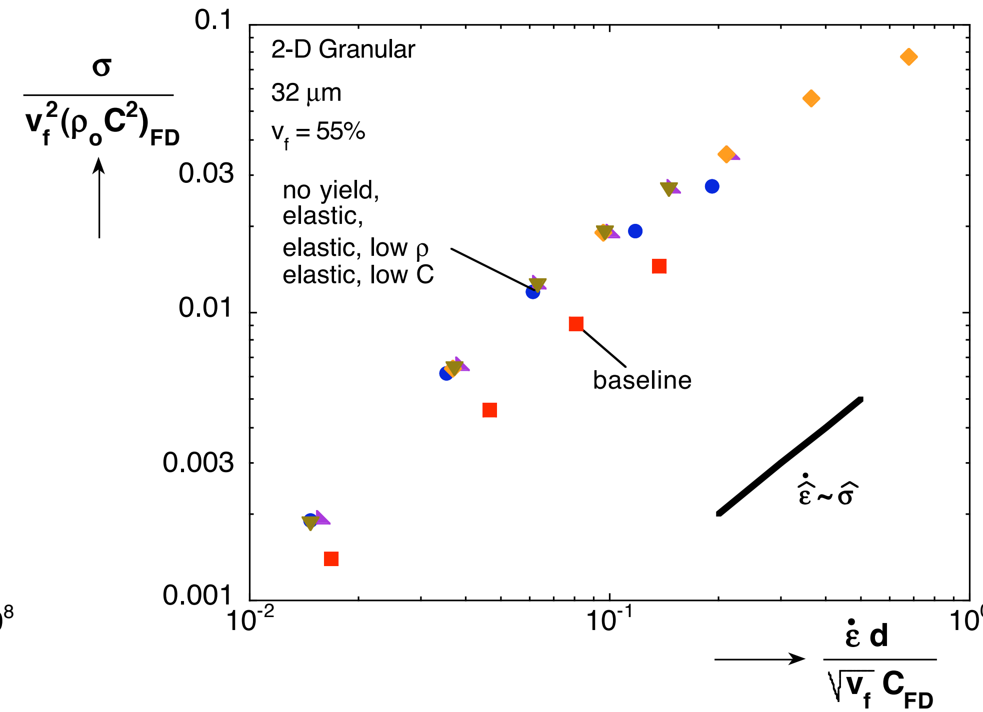





- waves are steady
- wave speed increases with V
- width of band decreases with V
- elastic simulations yield same scaling
  - Grady's scaling doesn't work

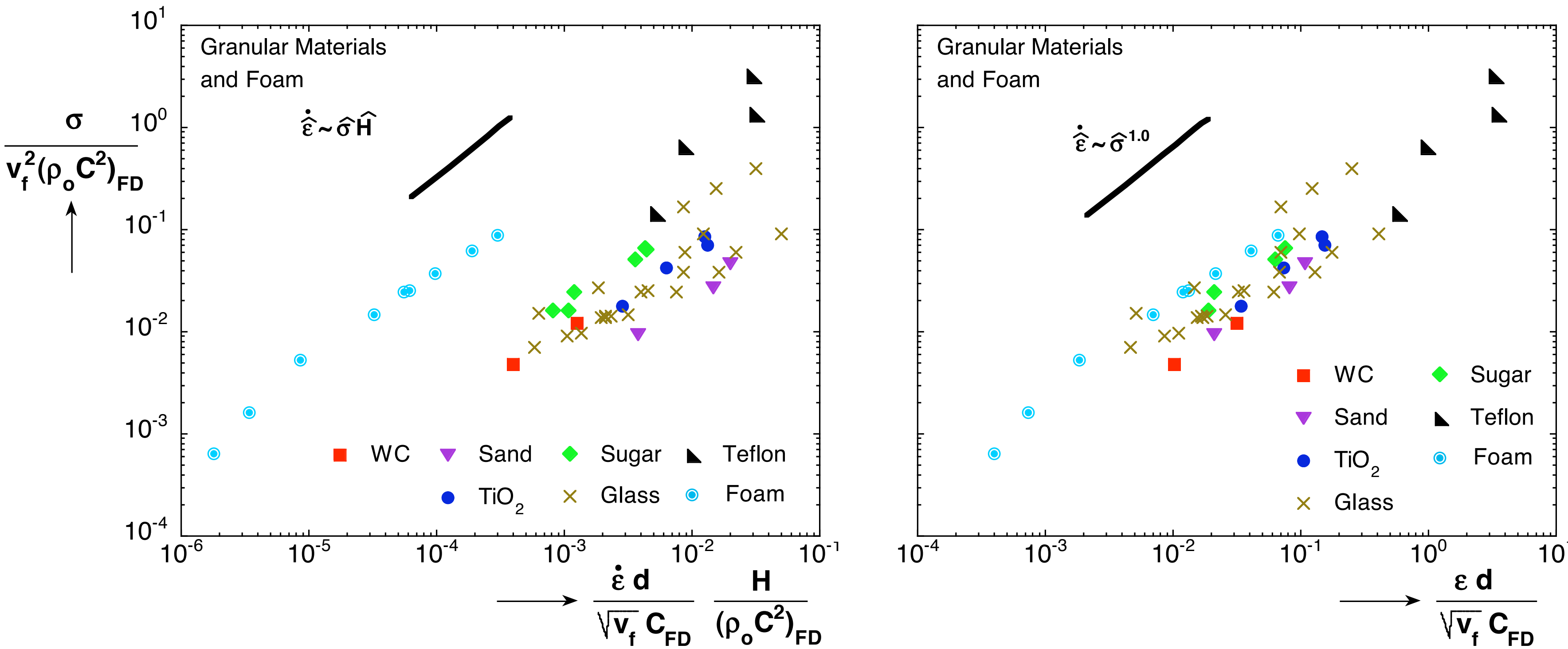
# Non-Dimensionalization of Peridynamics Results




- no strength in problem if material elastic
- fracture does not seem to affect scaling
- elastic-plastic material (baseline) has lower characteristic wave speed → will shift data upward

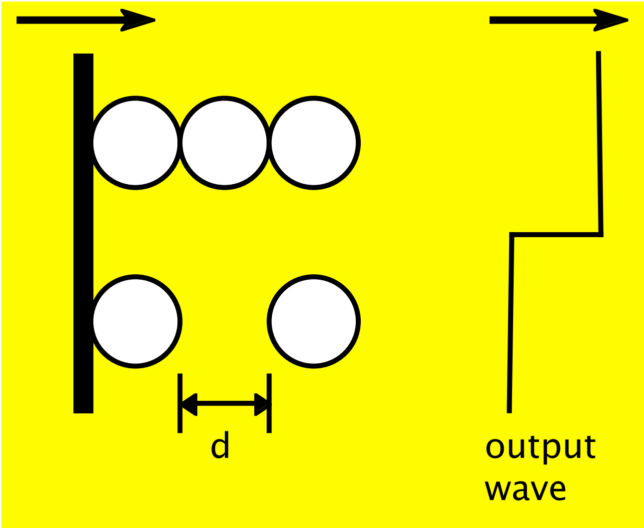
# Non-Dimensionalization of Experimental Results




- use hardness (H) as characteristic strength
- does volume fraction enter in separately?
- collapse is better without H
- polyurethane foam (Zaretsky et al., 2012) consistent

# A Simple Scaling Argument for Granular Materials (1)

$$\varepsilon = \frac{u_p}{U_s}$$ (conservation of mass)



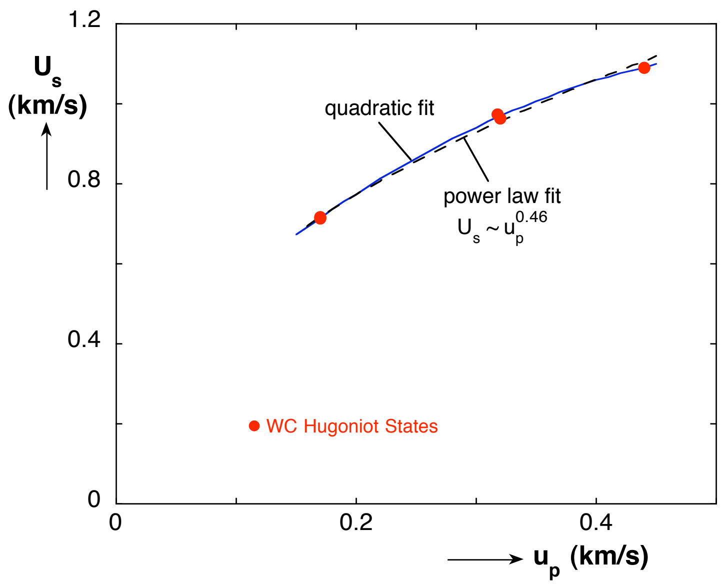

$$\dot{\varepsilon} \propto \frac{\varepsilon}{\Delta t} = \frac{u_p / U_s}{d / u_p}$$

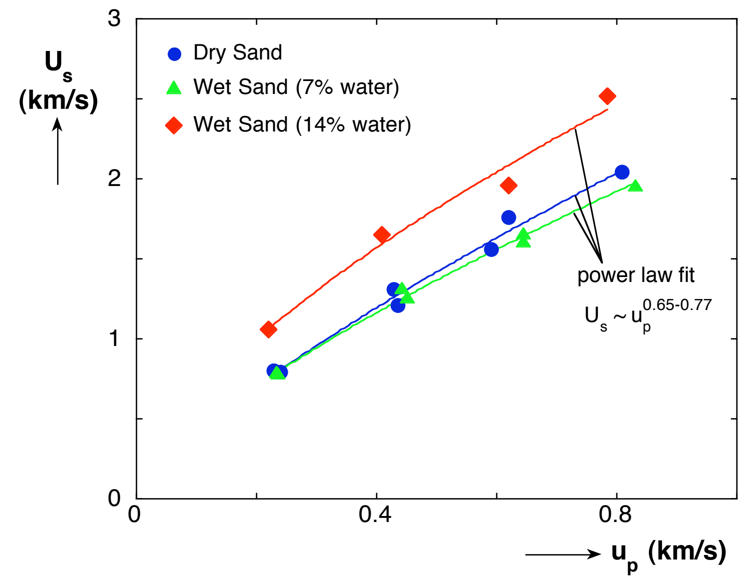
mass traversing pores controls width of shock front

$$\dot{\varepsilon} \propto \frac{u_p^2}{d U_s}$$

# A Simple Scaling Argument for Granular Materials (2)

$$\sigma = \rho_{oo} U_s u_p \qquad \dot{\varepsilon} \propto \frac{u_p^2}{d U_s}$$




$$\underline{if \;\; U_s \propto u_p^{0.5}}$$

$$\sigma \propto u_p^{3/2} \qquad \dot{\varepsilon} \propto u_p^{3/2} \;\Rightarrow\; \boxed{\dot{\varepsilon} \propto \sigma}$$

$$\underline{if \;\; U_s \propto u_p^{0.75}}$$

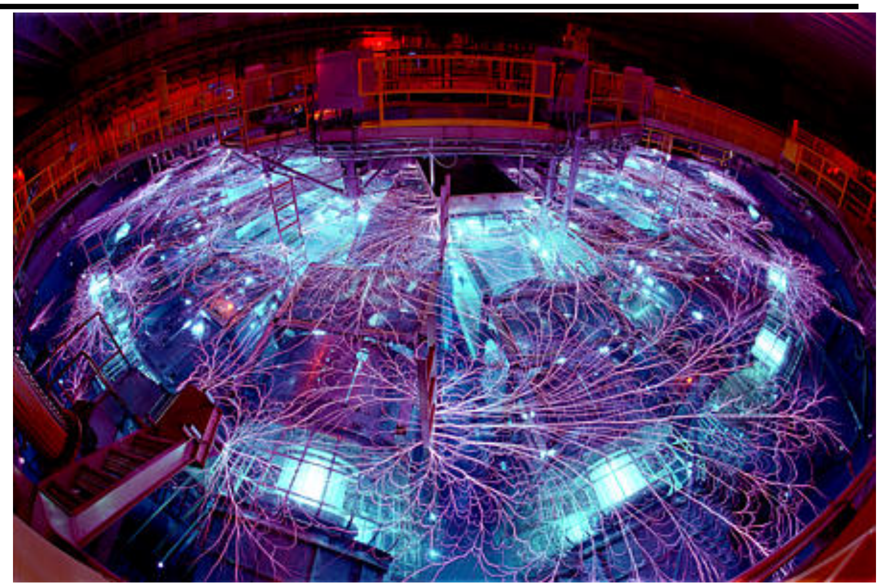
$$\boxed{\dot{\varepsilon} \propto \sigma^{0.7}}$$

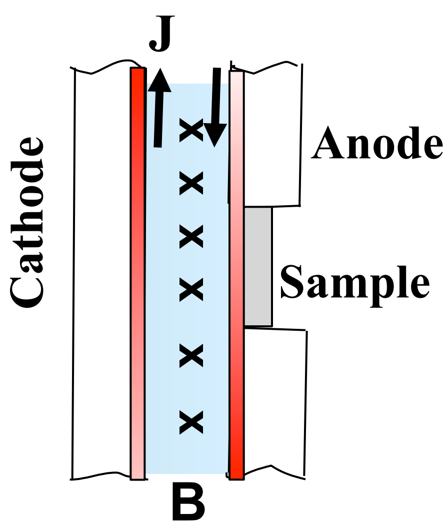
*mass transfer across void is critical aspect, thus granular WC (n=1) and WC/epoxy (n=4) behave very differently*

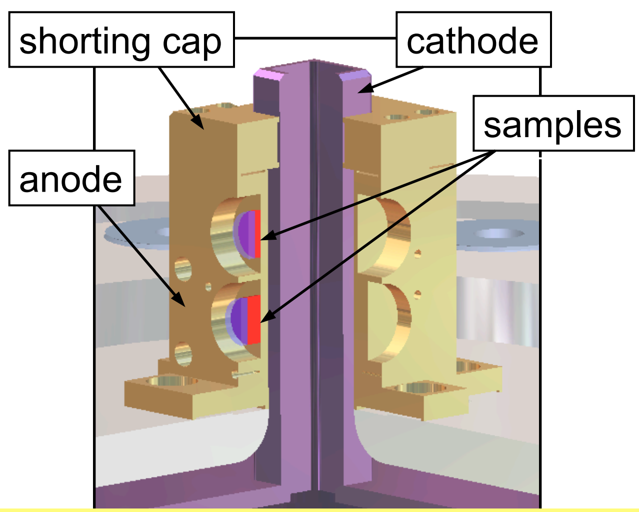
- Introduction to Shock and High-Pressure Physics
- Introduction to Granular Materials
- Compaction and Scaling Properties of Waves
- **High Pressure EOS – Experiments and DFT Modeling**
- The Intermediate Regime – Porosity Enhanced Densification
- Closure and Acknowledgements

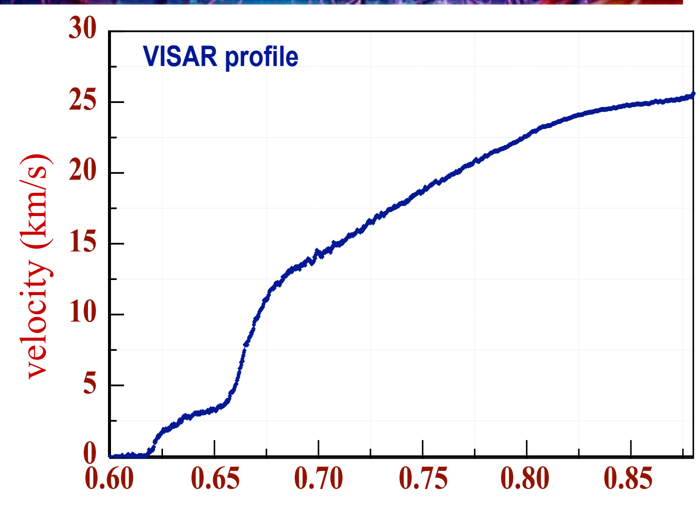
# Z Pulsed Power Machine

- Generates ~26 MA over 100’s of ns
- Utilize current to generate magnetic forces
- Magnetic forces create smooth waves in materials
- Waves used for isentropic loading (to ~400 GPa) and to launch high-velocity flyer plates (to ~40 km/s, pressures > 1 TPa)



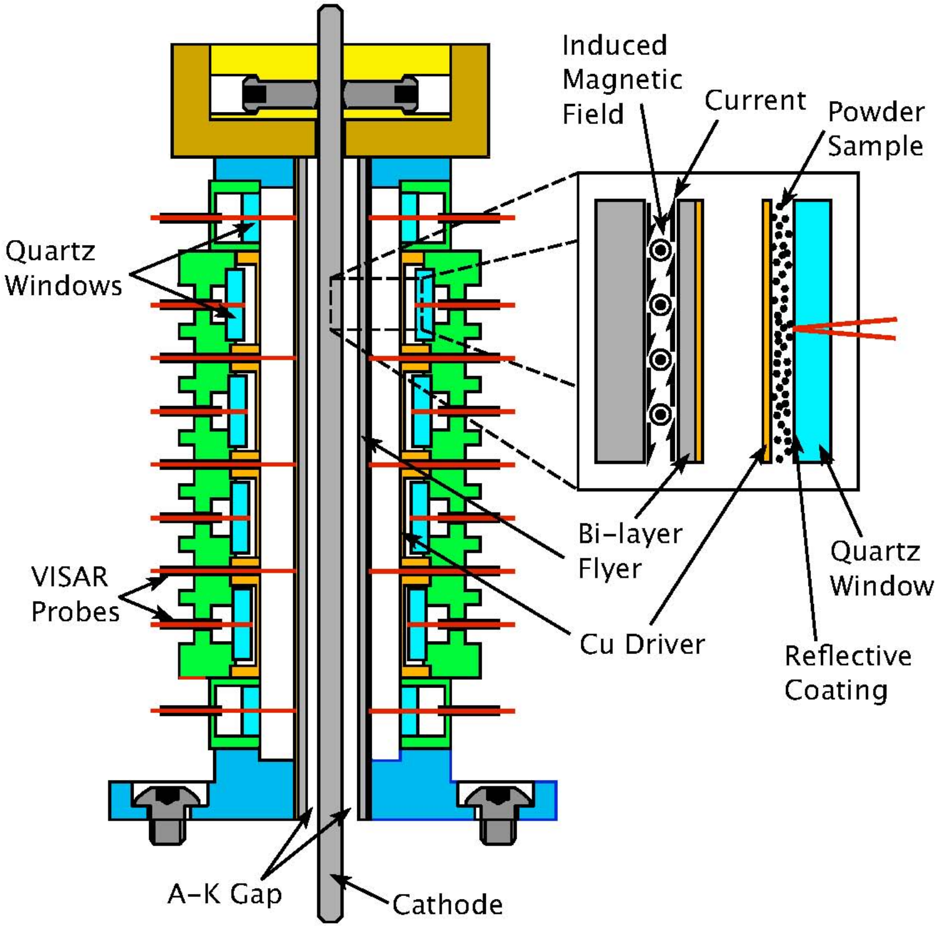


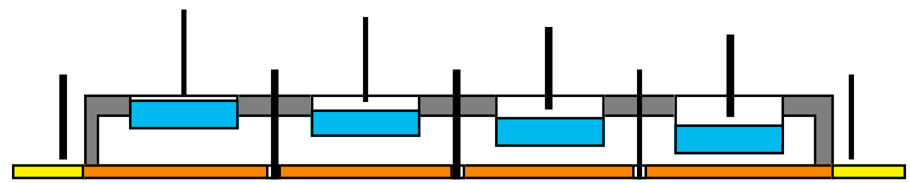




Davis, J.-P., Deeney, C., Knudson, M. D., Lemke, R. L., Pointon, T. D., and Bliss, D. E. (2005). "Magnetically driven isentropic compression to multimegabar pressures using shaped current pulses on the Z accelerator," *Physics of Plasmas* 12, 056310.

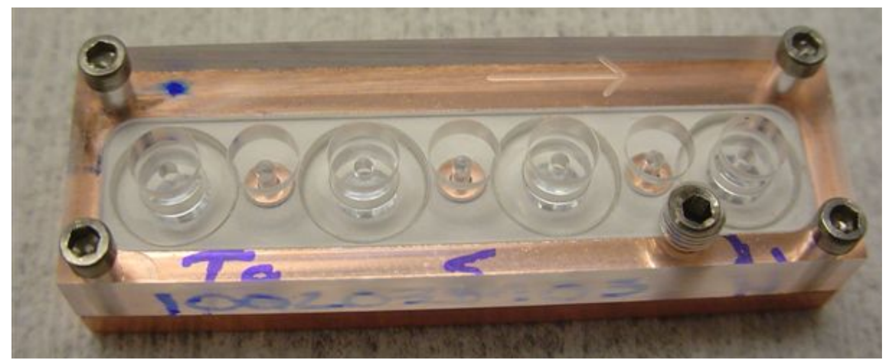
# High Pressure Z Experiments




400, 600, 800, and 1000 micron samples



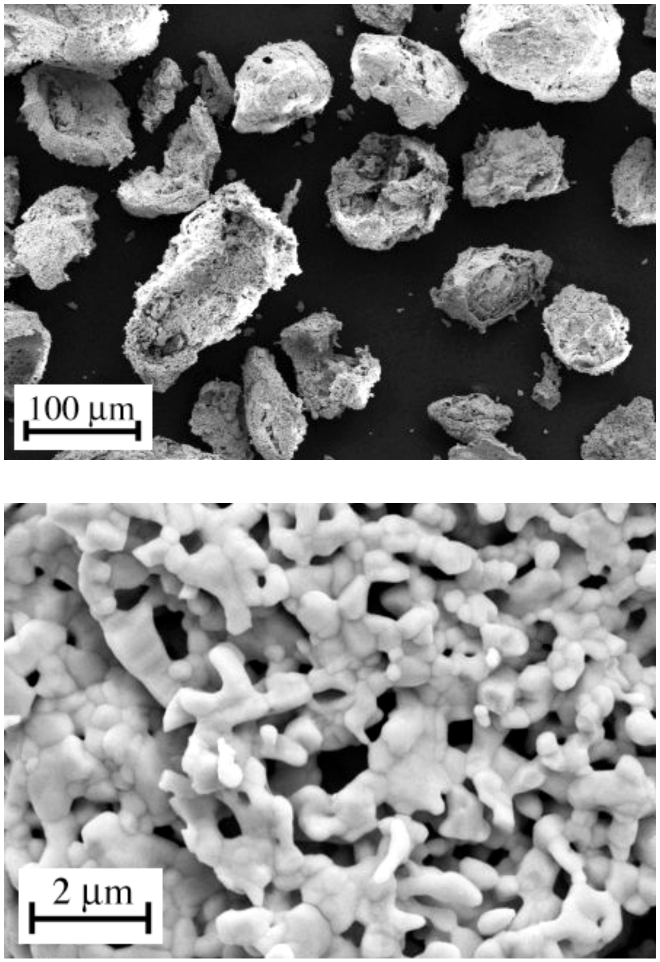
300 micron thick copper driver



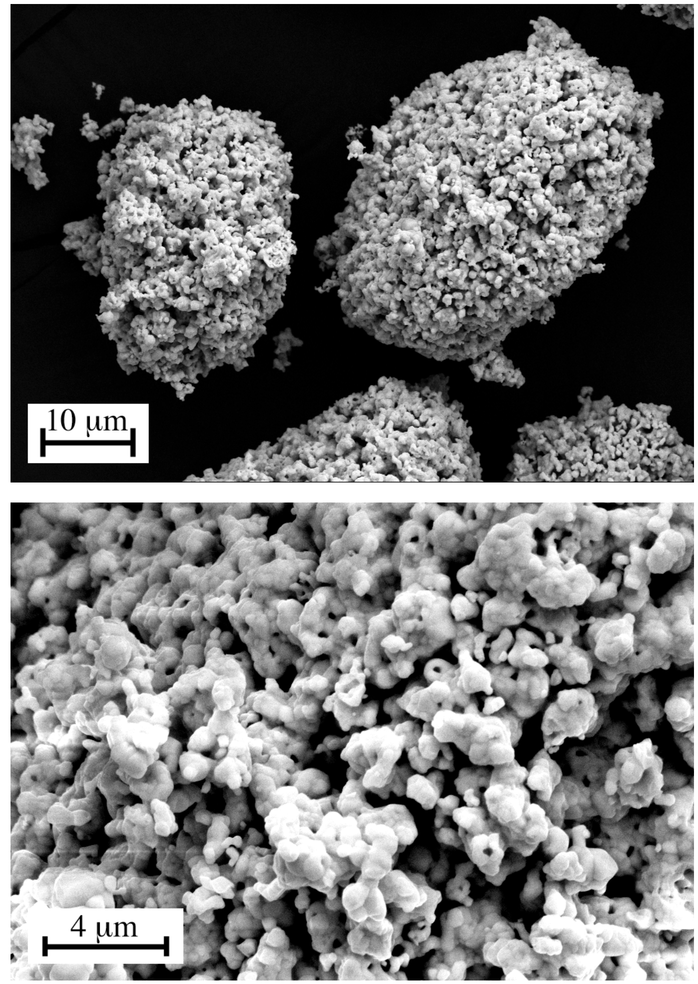
V = 9.9-10.3 and 11.2-11.4 km/s

# Two Different Forms of Granular $Ta_2O_5$

~1.3 g/cc from Cerac




~3 g/cc from American Elements



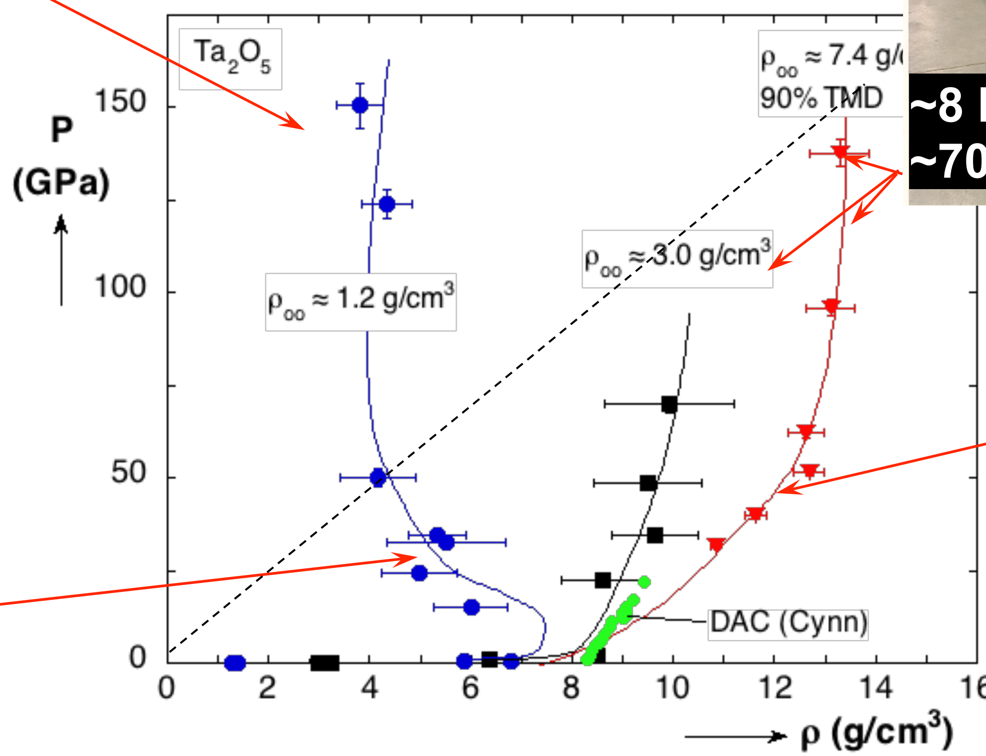

X-ray diffraction shows all material is in orthorhombic phase

*also 90% dense disks from cold pressing or low temperature sintering*

# High-Pressure Shock Results

*Two-Stage Gun 29mm*


Z results




possible phase transformation

lower initial density means material is hotter for a lower pressure

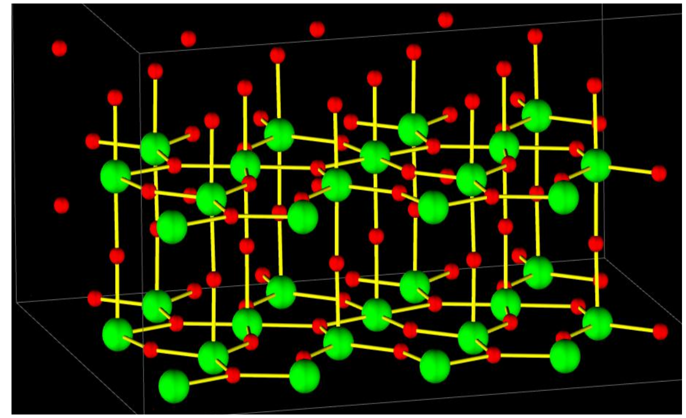
as pressure increases, density decreases

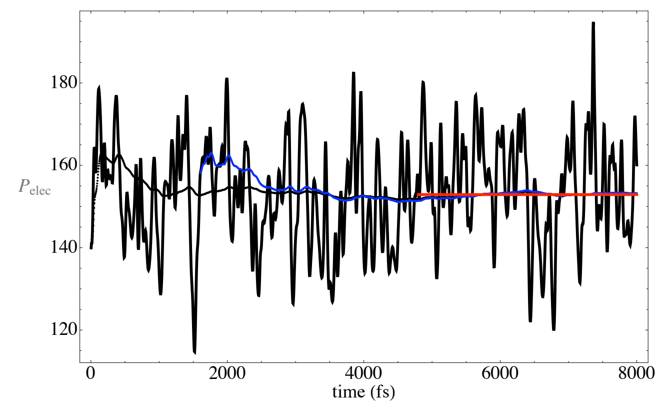
error bars assigned through Monte Carlo technique

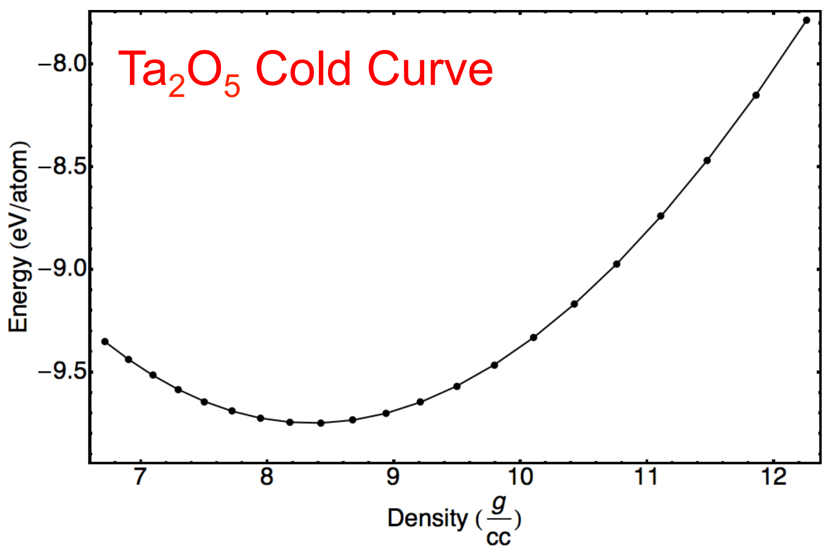
# Density Functional Theory Modeling of Porous Tantala

K. Cochrane
L. Shulenburger
P. Weck

- **solve approximation to Shroedinger's equation**
- **32 Ta atoms and 80 O atoms.**
- **equilibrate for mean P and E**
- **LDA potential with 11 electron Ta pseudo potential and 6 electron O potential**





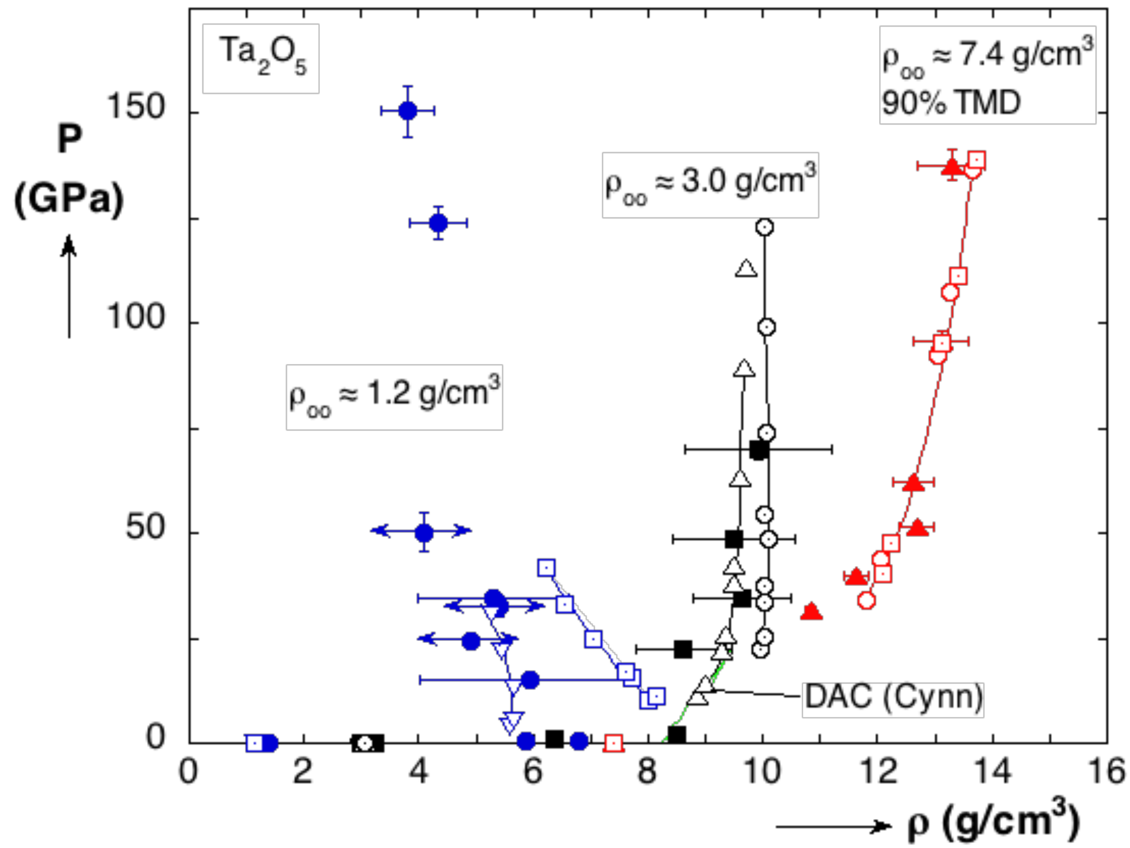




satisfy energy equation to determine Hugoniot state

$$0 = (E - E_o) - \left(\frac{P + P_o}{2}\right)(V_o - V)$$

# Porous Hugoniot Calculated for $Ta_2O_5$ Using DFT

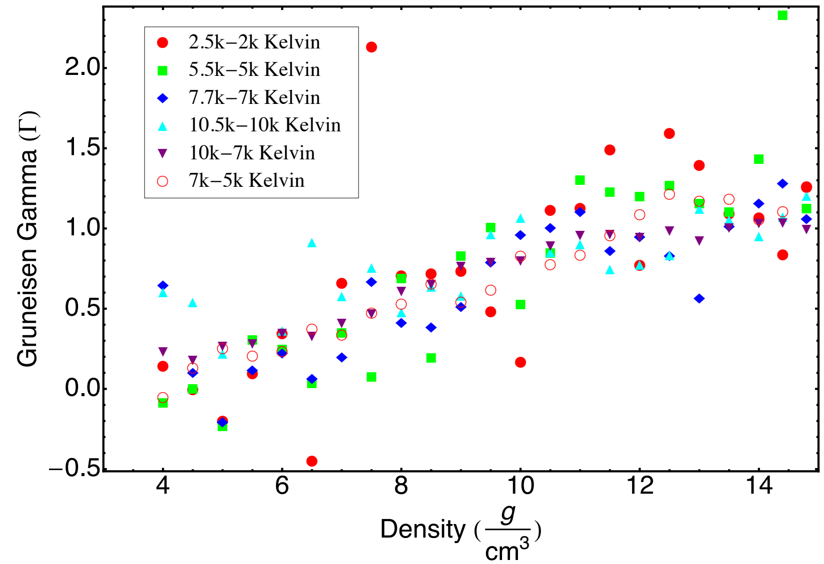
- include the surface energy in energy equation
- $\delta$ = surface energy
- $E_{solid}$ - energy at the reference density
- $P_{solid}$ is the pressure and usually NOT Zero (although experimentally it should be)
- $V_{initial}$ – porous volume
- method of including porosity is empirical but seems to work

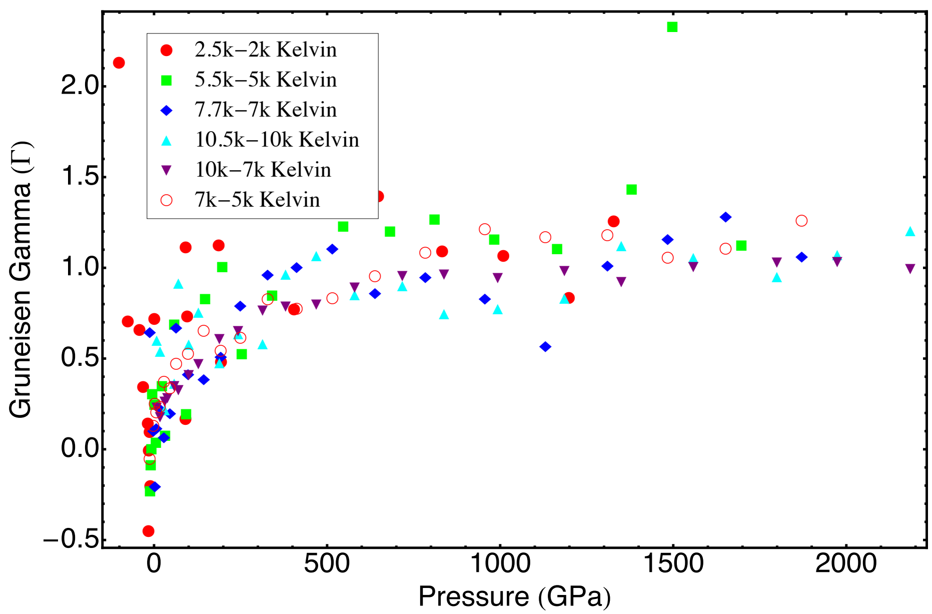


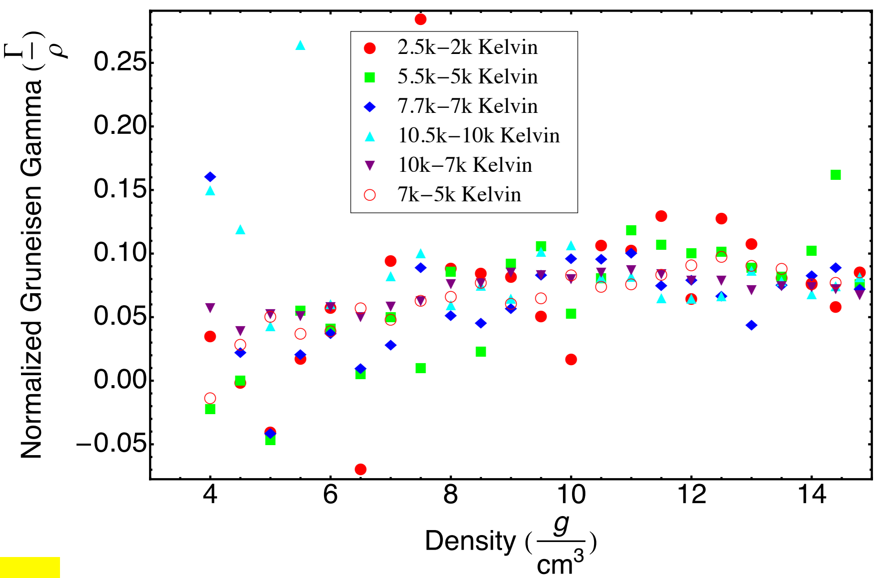

$$0 = \left( E - E_{solid} - \delta \left[ \frac{V_{initial}}{V_{solid}} - 1 \right] \right) - \left( \frac{P + P_{solid}}{2} \right) \left( V_{initial} - V \right)$$

# Values for the Gruneisen Γ Extracted from DFT

- We can extract trends for Γ
- Γ is not constant as a function of density
- Γ is constant as a function of pressure at higher pressure
- Γ is constant as a function of temperature



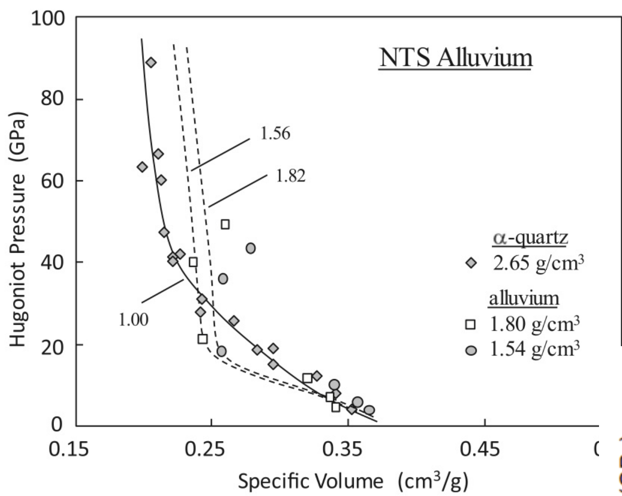

Cochrane et al. (2014), Proceedings APS-SCCM

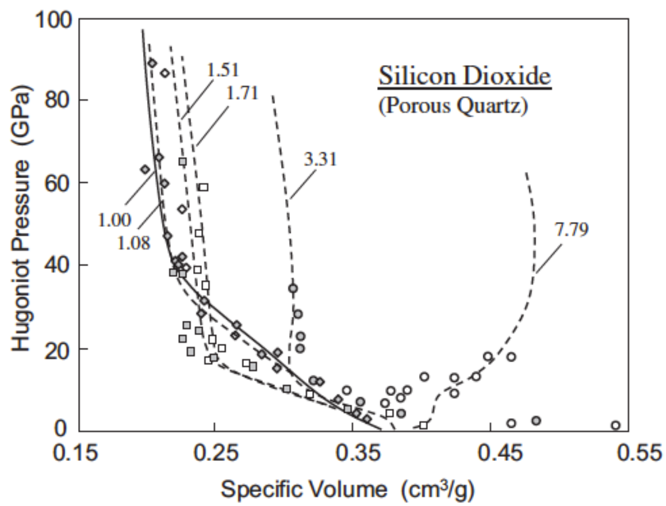
- Introduction to Shock and High-Pressure Physics
- Introduction to Granular Materials
- Compaction and Scaling Properties of Waves
- High Pressure EOS – Experiments and DFT Modeling
- The Intermediate Regime – Porosity Enhanced Densification
- Closure and Acknowledgements

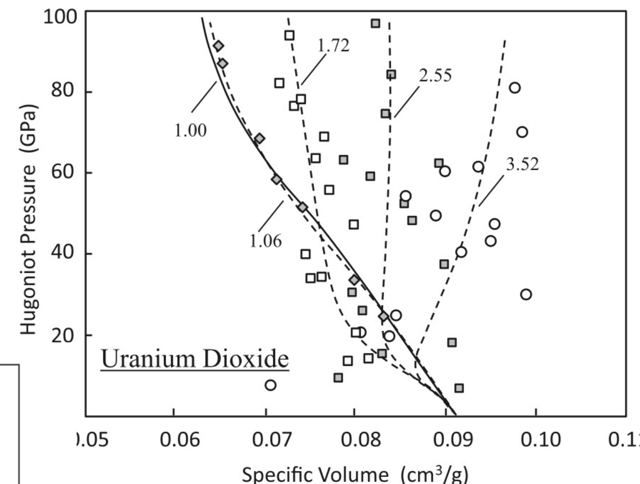
# Porosity Enhanced Densification Observed in Some Porous Ceramics

Some porous material can reach higher densities than the fully-dense form shocked to the same pressure

Grady et al. proposed that void collapse can cause phase transformations to occur at lower pressure due to enhanced shear stresses




Lane et. al, PRB, 2014

# Molecular Dynamics (NEMD) Methodology

**Solve Newton's equations**

$$m_i \frac{d^2\mathbf{r}_i}{dt^2} = \mathbf{F}_i$$

$$\mathbf{F}_i = -\nabla V_i$$

**Mathematical Formulation**

Classical Mechanics

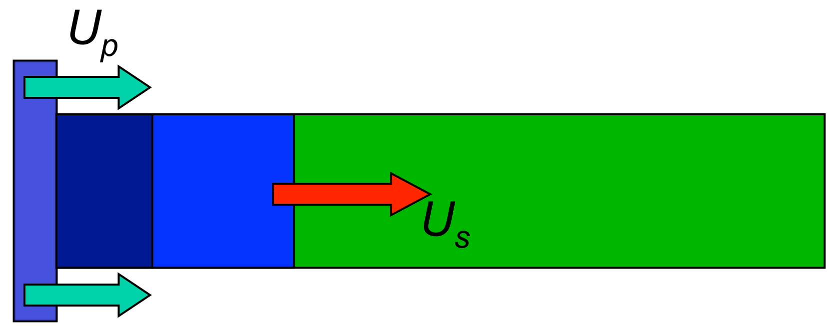
Atoms are Point Masses: $\boldsymbol{r}_1, \boldsymbol{r}_2, ..... \boldsymbol{r}_N$

Positions, Velocities, Forces: $\boldsymbol{r}_i, \boldsymbol{v}_i, \boldsymbol{F}_i$

Potential Energy Function = $V_i(\boldsymbol{r}^N)$

**Sandia's LAMMPS code is spatially parallel**

**L**arge-scale **A**tomic/**M**olecular **M**assively **P**arallel **S**imulator




Warm piston driving into 300 K single-crystal Silicon along <111> and <100>

Systems 13.1 x 13.1 x 320 $nm^3$ and periodic

Timescales 60 to 150 ps

Modified Embedded Atom Method (MEAM) of M. I. Baskes et al.

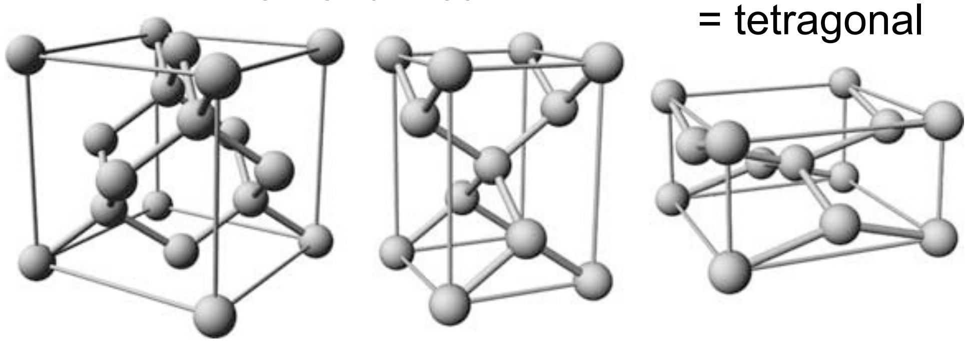
- Uses a two-body and environment dependent term.

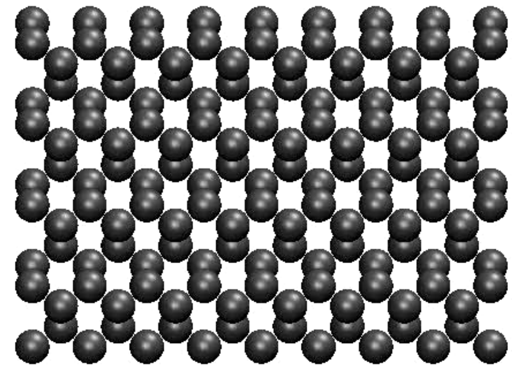
Voids are introduced either by carving out atoms from a single crystal, or by building up polycrystals from nano-grains

# Silicon as a Model System

Diamond = cd

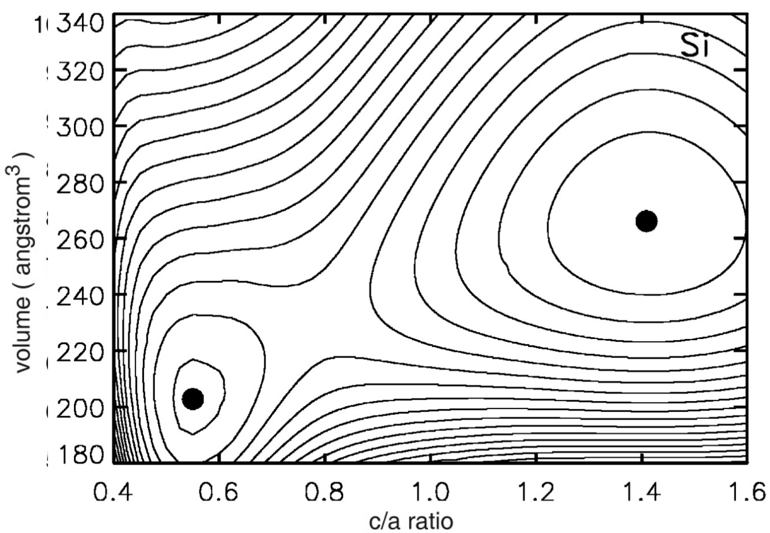
β-tin = bct
= tetragonal

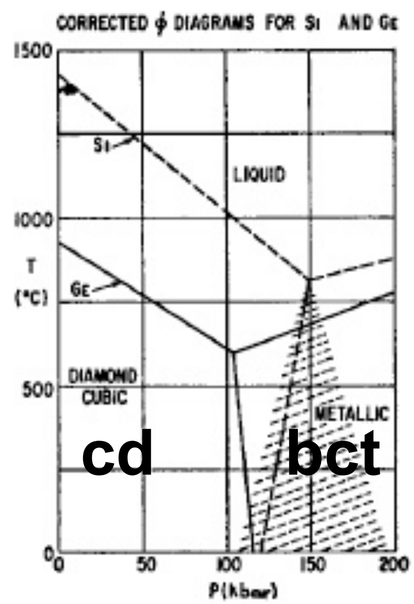




DFT

**Gaal-Nagy, et al., Comp. Mat. Sci., 30, 1**




**Bundy, J. Chem Phys., 41, 3809**

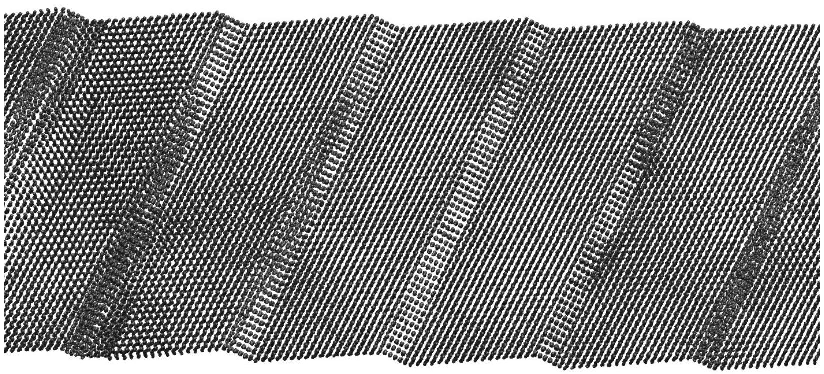
Silicon goes through a low temperature solid-solid phase transition from diamond to tetragonal in molecular dynamics simulation.

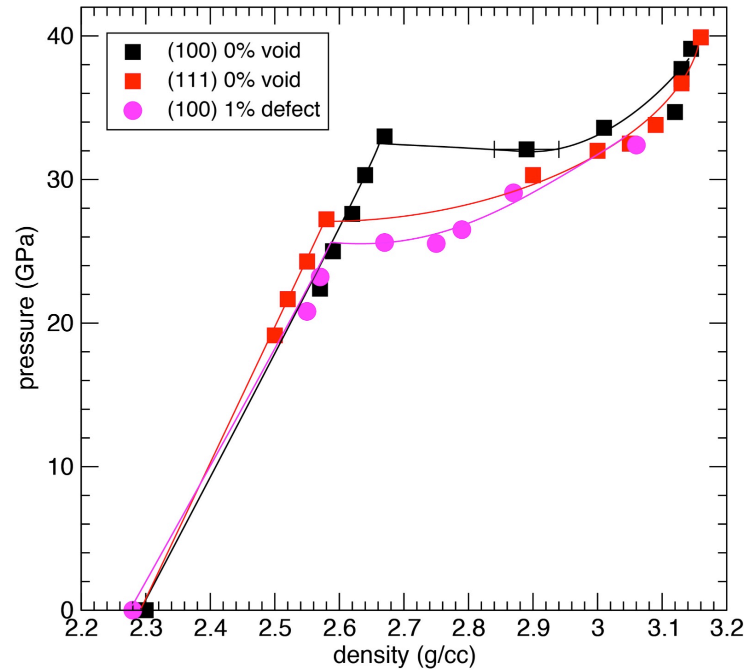
Voids can be introduced through helium implantation and annealing

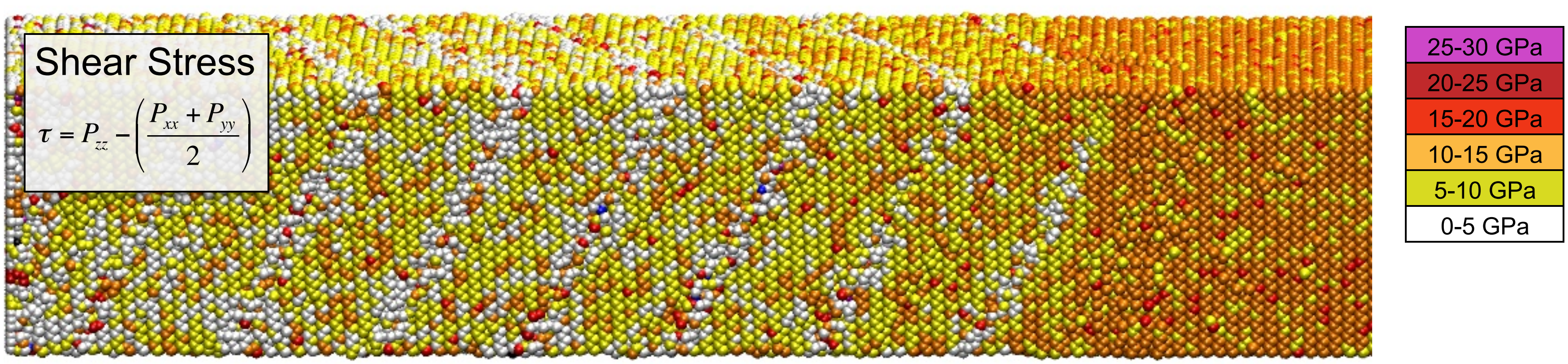
# Fully-Dense Silicon Undergoes a Partial Phase Transition

Silicon is an important covalent solid known to undergo a solid-solid phase transition.

Recent work in germanium and silicon has shown a shear-induced transition from diamond (cd) to a tetragonal (bct) phase is observed in MD simulation.



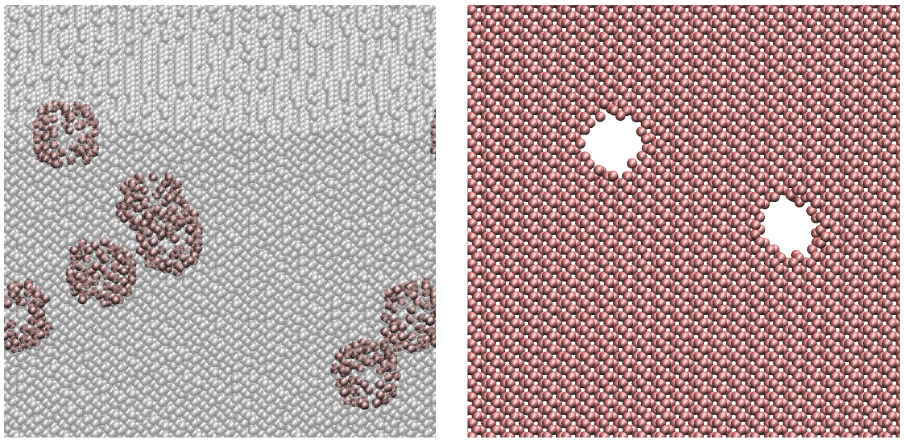


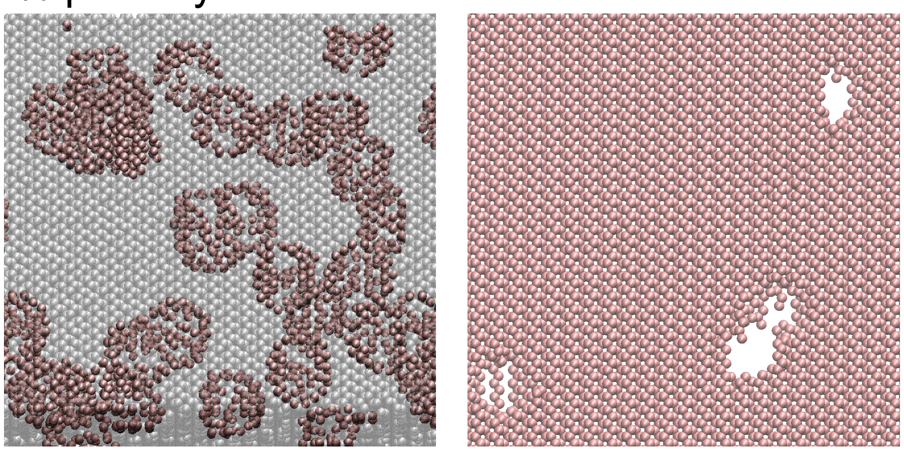
# Low Porosity Silicon Behaves Like Silicon with Defects

Low porosity systems created by cutting randomly spaced 1 nm diameter spherical voids from single-crystal silicon.

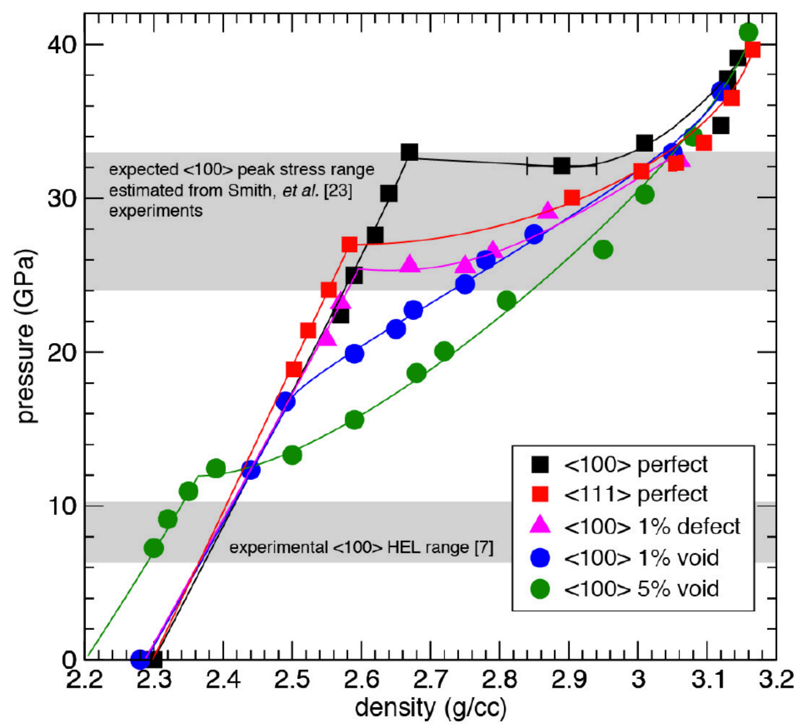
1% porosity: (left) cut voids



5% porosity: cut voids



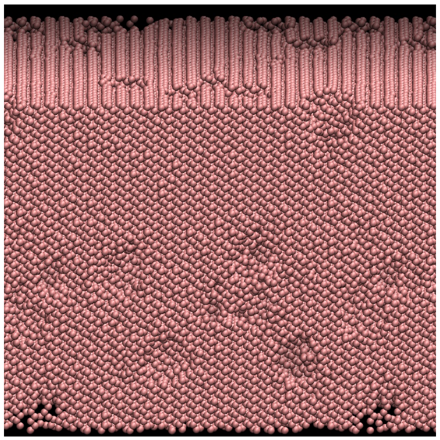
Hugoniot density rises at lower pressure as seen in experiments, then joins the principal Hugoniot at higher pressures.

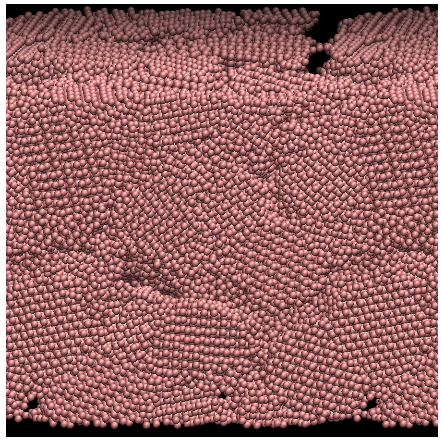


# High Porosity Silicon Displays Porosity Enhanced Densification

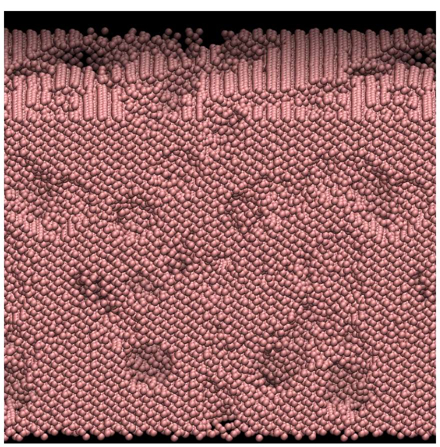
High porosities are made by cutting 1 nm spherical voids from single crystal, or as a polycrystal of 4 nm spherical grains, w/ overlap removal, and annealing.

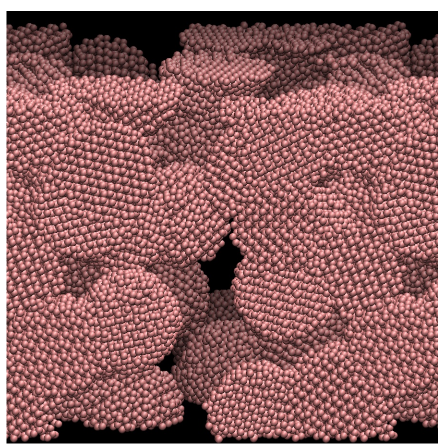
25% porosity: (l) cut voids, (r) polycrystal spheres



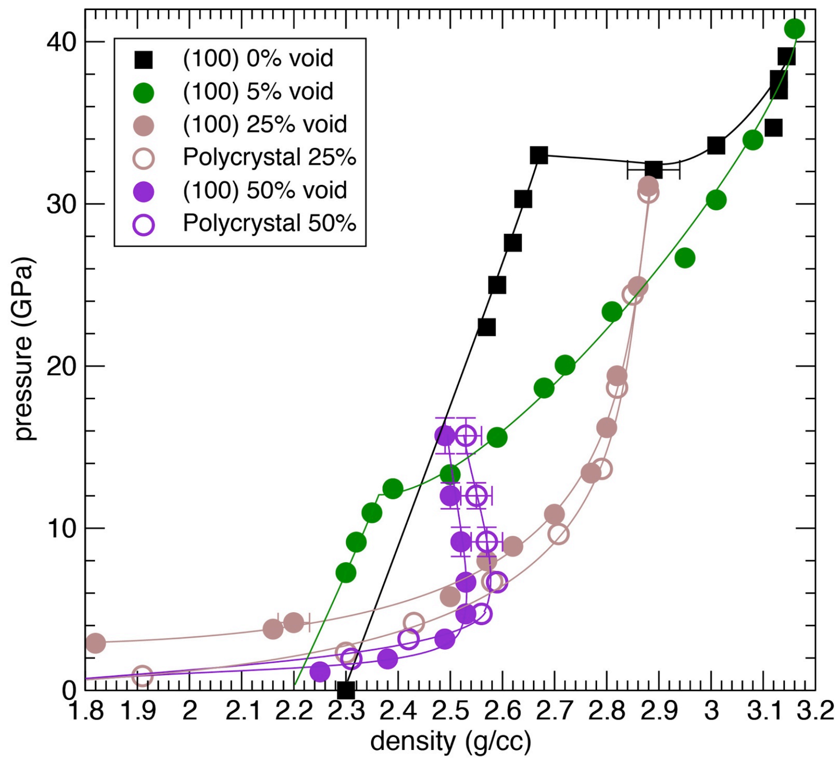


50% porosity: (l) cut voids, (r) polycrystal spheres



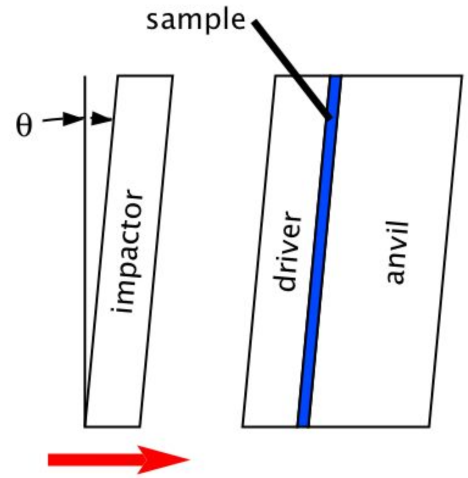


The Hugoniot density quickly collapses in the polycrystal, and slightly more slowly in the void-cut single crystal before rising steeply due to heating from rapid void collapse.

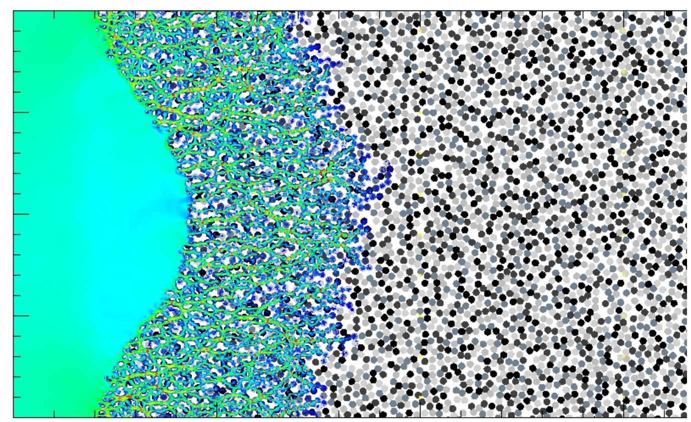


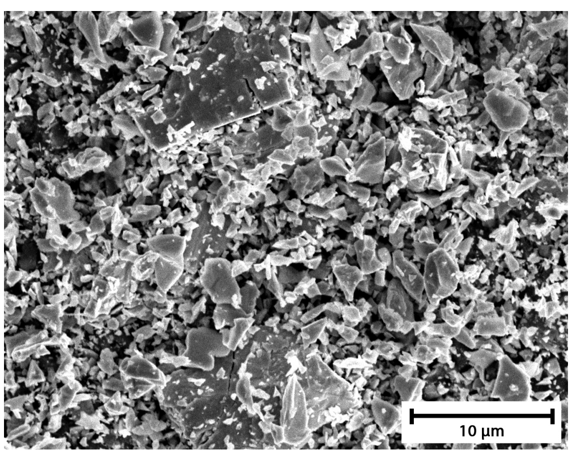
- **Introduction to Shock and High-Pressure Physics**
- **Introduction to Granular Materials**
- **Compaction and Scaling Properties of Waves**
- **High Pressure EOS – Experiments and DFT Modeling**
- **The Intermediate Regime – Porosity Enhanced Densification**
- **Closure and Acknowledgements**

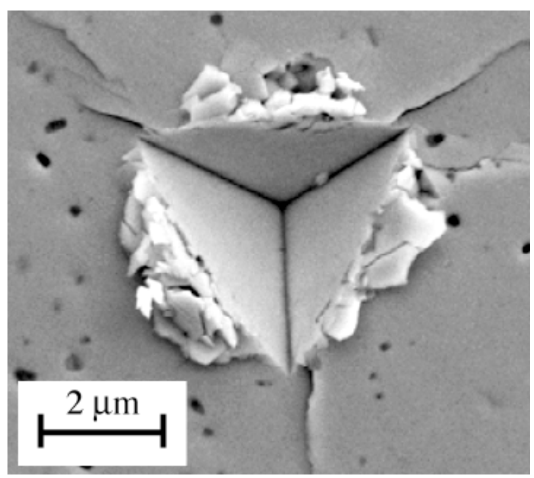
# Topics Not Covered




- **pressure-shear loading and other approaches for measuring strength**
- **role of particle fracture**
- **mesoscale modeling**
- **EOS for granular materials and mixtures in the high-pressure regime**
- **perturbation decay experiments**





# Acknowledgements


J.P. Borg, C. Lammi, J. Foster - mesoscale modeling

M. Lane - molecular dynamics modeling

K. Cochrane, P. Weck, L. Shulenburger - DFT

W.D. Reinhart, T.F. Thornhill, J. Martinez, R. Palomino, H. Anderson - STAR facility gas gun experiments

Z - the large crew for design, assembly and operations; S. Root, R. Lemke, M. Knudson for design & analysis

D. Sandoval, K. Lappo - validation experiments

T. Buchheit - nanoindentation

J.R. Asay, L.C. Chhabildas, D.E. Grady - decades of shock physics experience