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Dynamic Behavior of Granular Ceramics

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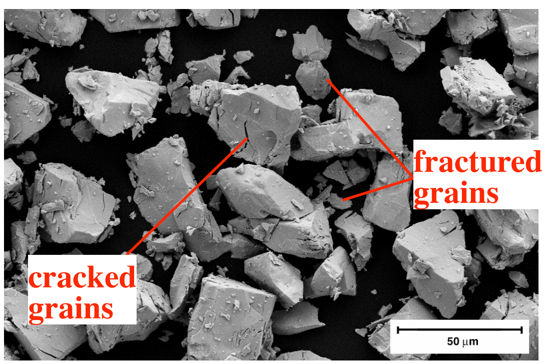

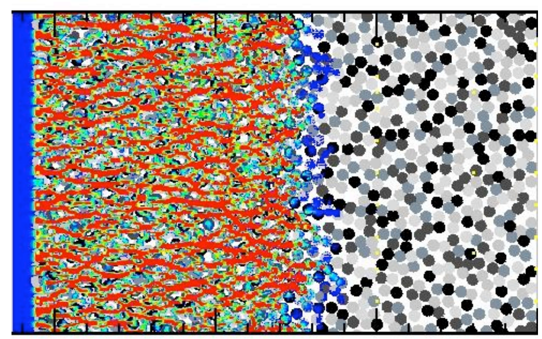

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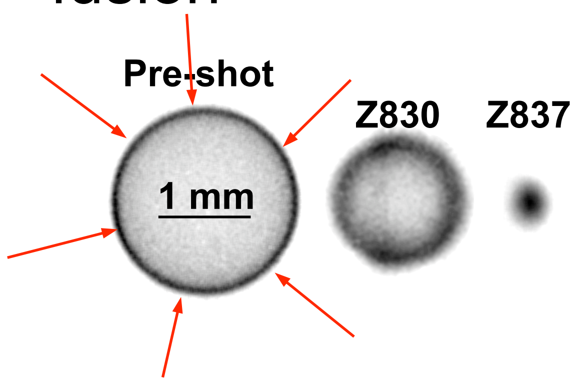
- Introduction to Shock and High-Pressure Physics
- Introduction to Granular Materials
- Planar Impact Experiments
- Mesoscale Modeling
- Scaling Properties of Waves
- Conclusions

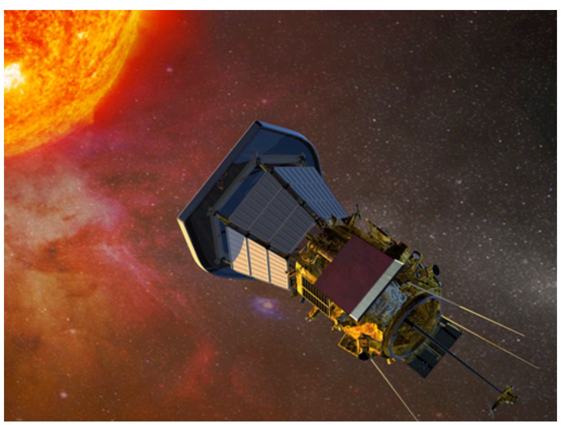
Why Do We Need To Know the Behavior of Materials Under Extreme Conditions?

- weapons applications (warheads, armor, etc.)

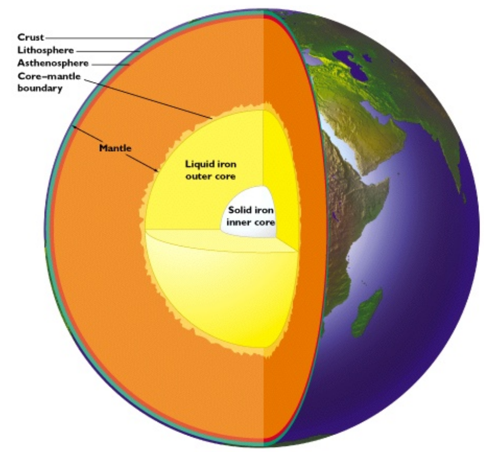
- explosives behavior and applications

- inertial confinement fusion





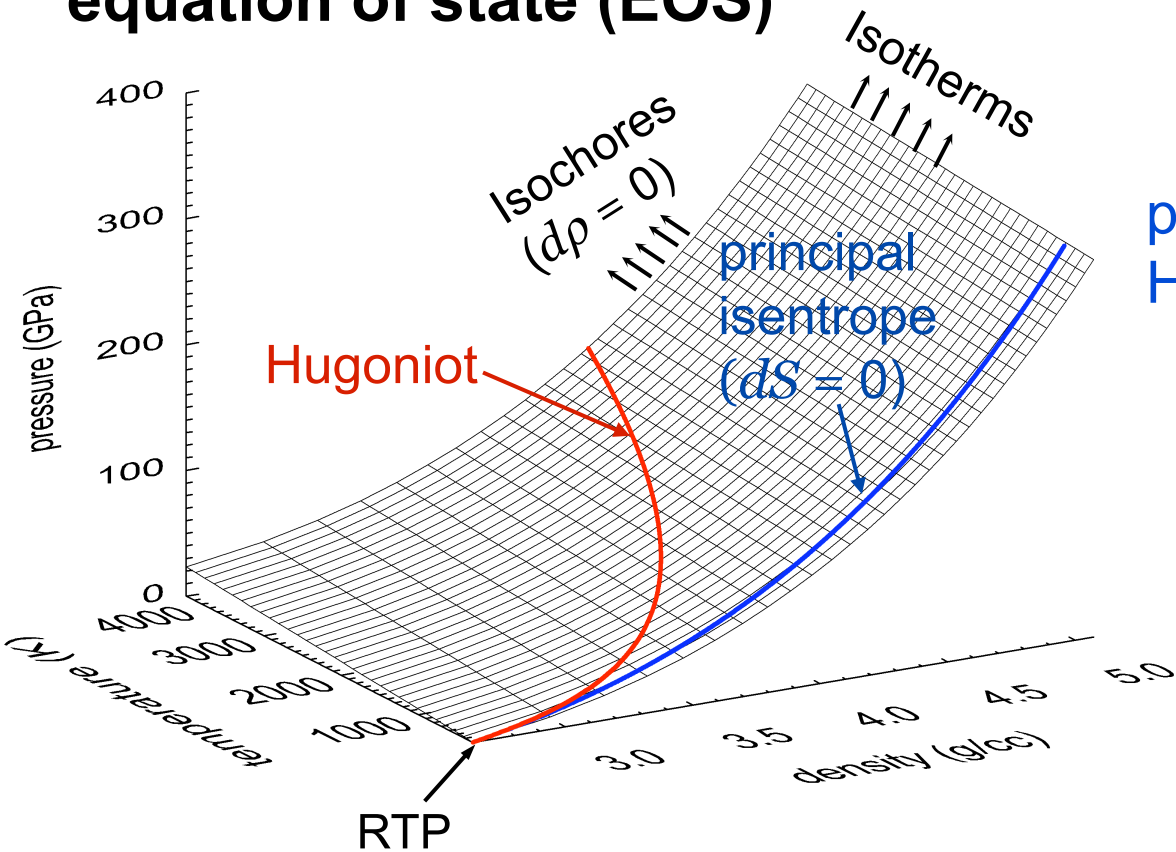
- solar probe
  - 100 μm particles
  - up to 300 km/s velocities
  - P_{max} ~ 100 TPa, T_{max} ~10^6 K



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

Material Behavior: EOS & Constitutive Aspects

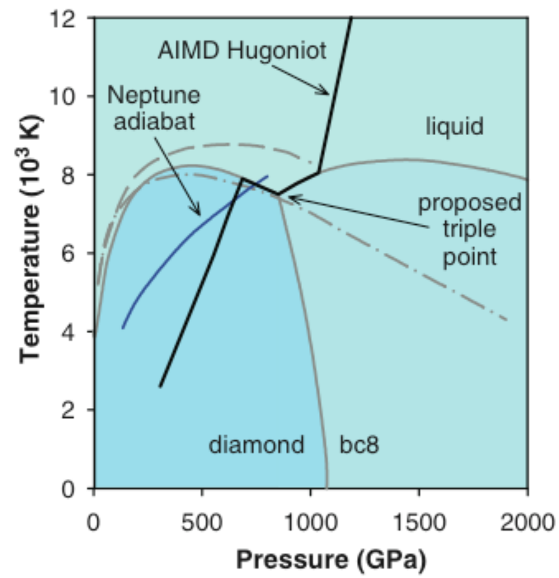
equation of state (EOS)



one thermodynamic state variable as a function of two others:

pressure $P = P(r,T)$

Helmholtz energy $f = f(v,T)$

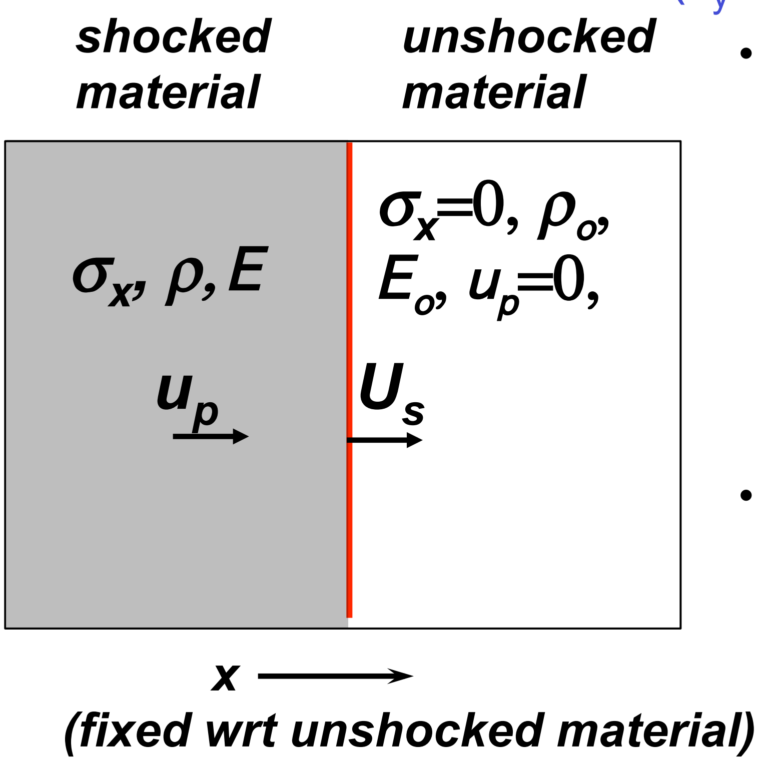


Knudson, M. D., M. P. Desjarlais and D. H. Dolan (2008). "Shock-wave exploration of the high-pressure phases of carbon." *Science* **322**: 1822-1825.

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 *assumed* 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

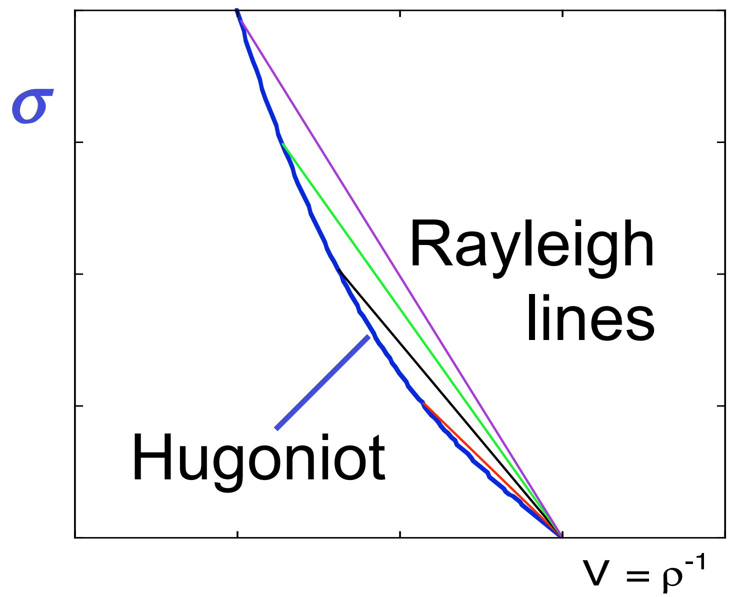
- Five variables: σ_x, u_p, U_s, ρ, and E
- Three conservation relationships (Rankine-Hugoniot jump conditions)
  - By measuring two variables (typically σ_x, u_p, or U_s), the other three can be determined

<u>conservation of</u>

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 <u>collection of end states</u>, not a material response curve

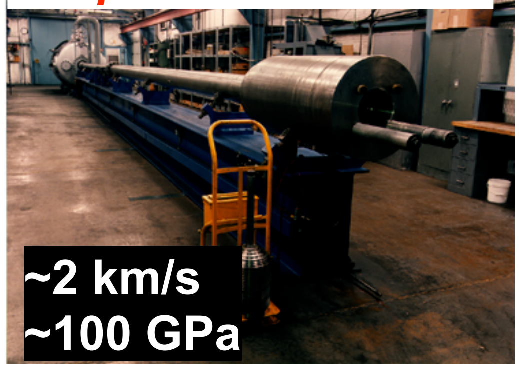
the Hugoniot is not a complete equation of state (EOS)!

Gas Guns to Generate Shock Waves

Shock Thermodynamics Applied Research

Single Stage Gun 100mm

Propellant Gun 89mm

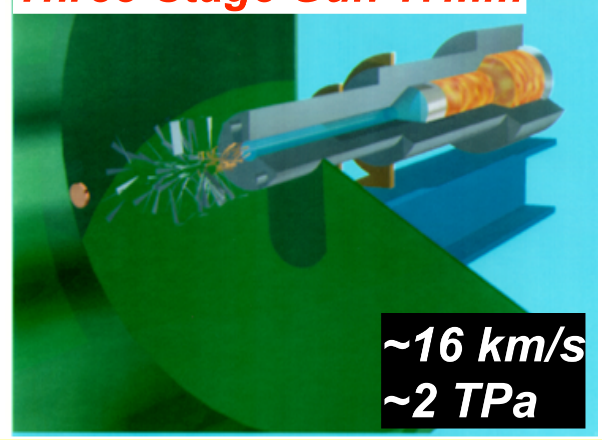


Two-Stage Gun 29mm

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

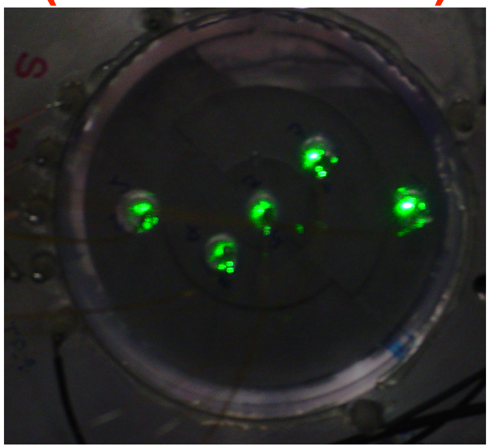


Chhabildas, L. C., Dunn, J. E., Reinhart, W. D., and Miller, J. M. (1993). "An impact technique to accelerate flier plates to velocities over 12 km/s," *Int. J. Impact Eng*. **14**, 121-132.

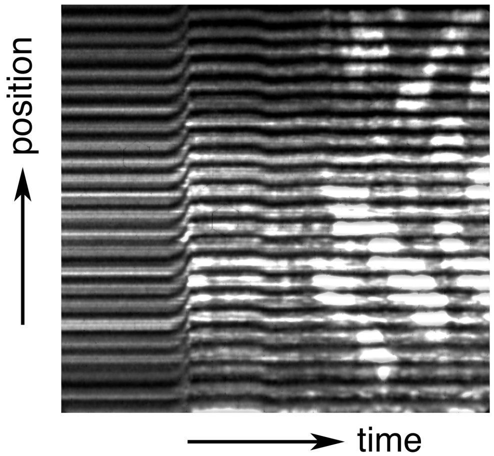
also: explosives, lasers, magnetic loading (Z)

Diagnostics for Dynamic Experiments

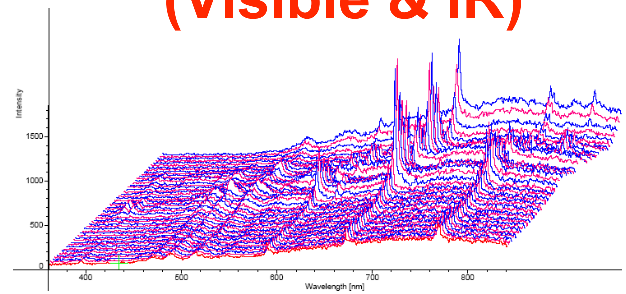
Velocity Interferometry (VISAR & PDV)



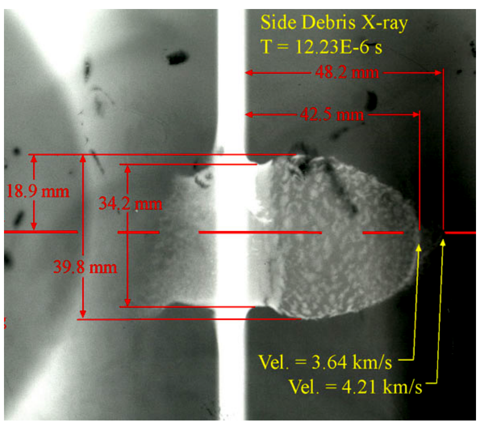
Line-VISAR



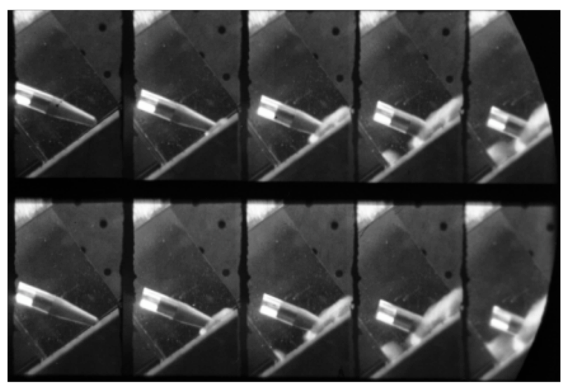
Time-Resolved Spectroscopy (Visible & IR)



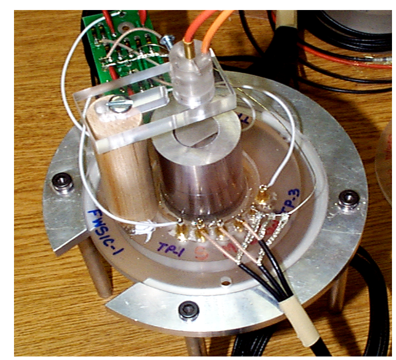
Flash X-rays



High-Speed Photography



Pressure Gauges



Advanced Diagnostics: pRad, synchrotron, etc.

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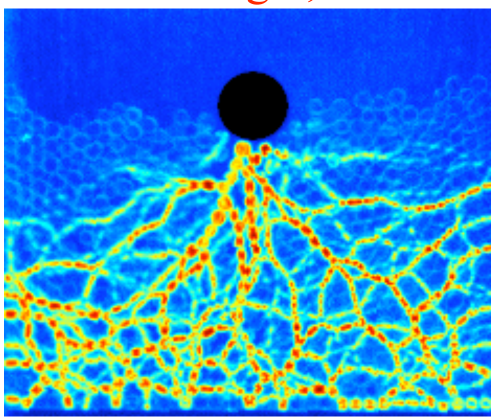
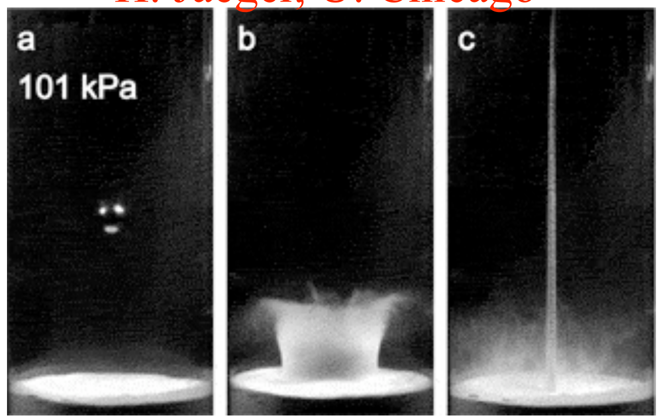
Background on Dynamic Behavior of Granular Materials

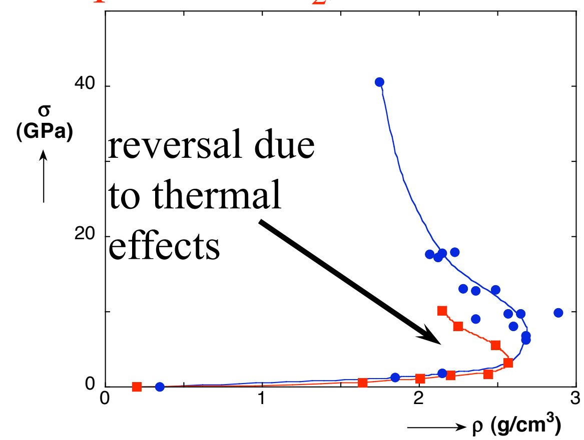
B. Behringer, Duke



H. Jaeger, U. Chicago



porous SiO_2, Trunin et al.

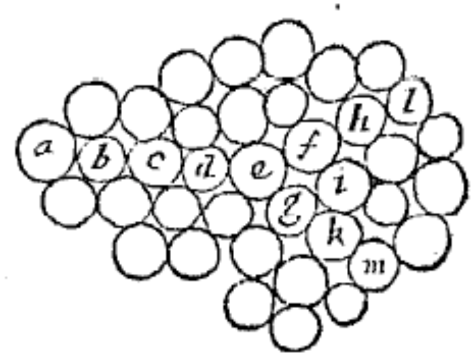


- granular materials display a rich variety of behaviors
- significant experimental and modeling challenges
- extensive quasi-static and low-velocity impact work
- determine thermal behavior through P-V work (Trunin, 2004)
- consolidation studied extensively to optimize loading, etc.
- partial compaction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

Very Early Thoughts on Particulate Materials

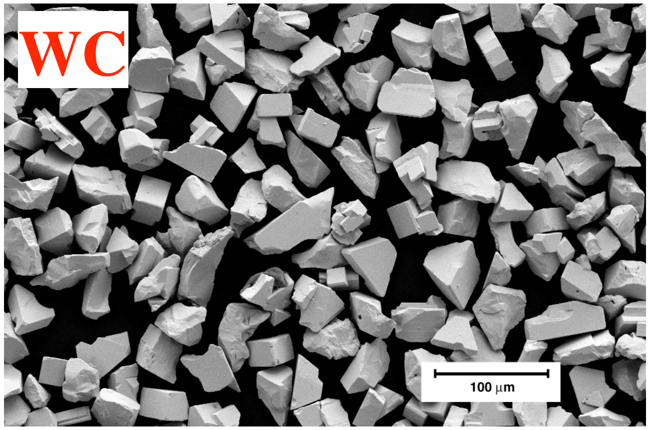
<u>Newton's *Principia*, Book II, 1687:</u>

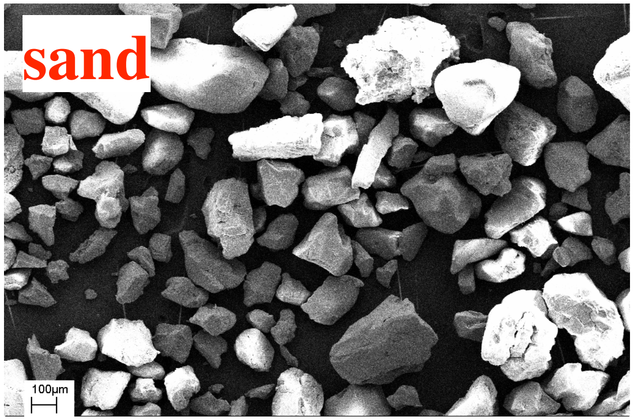
Si jaceant particulæ *a*, *b*, *c*, *d*, *e* in linea recta, poteſt quidem preſſio directe propagari ab *a* ad *e*; at particula *e* urgebit particulas oblique poſitas *f* & *g* oblique, & particulæ illæ *f* & *g* non ſuſtinebunt preſſionem illatam, niſi fulciantur a particulis ulterioribus *h* & *k*; quatenus autem fulciuntur, premunt particulas fulcientes; & hæ non ſuſtinebunt preſſionem niſi fulciantur ab ulterioribus *l* & *m* eaſque premant, & ſic deinceps in infinitum. Preſſio igitur, quam primum propagatur ad particulas quæ non in directum jacent, divaricare incipiet & oblique propagabitur in infinitum; & poſtquam incipit oblique propagari, ſi inciderit in particulas ulteriores, quæ non in directum jacent, iterum divaricabit; idque toties, quoties in particulas non accurate in directum jacentes inciderit. *Q.E.D.*



Investigation of Dynamic Behavior of Granular Ceramics

- investigate dynamic compaction behavior of ceramic powders (WC, sand, Al_2O_3, etc.)
- develop insight into physics of dynamic behavior of these materials and the parameters that influence it
- explore a variety of techniques (quasi-static experiments, mesoscale simulations, etc.) to predict dynamic results
- determine suitability of current models within Sandia codes for simulating dynamic behavior of powders





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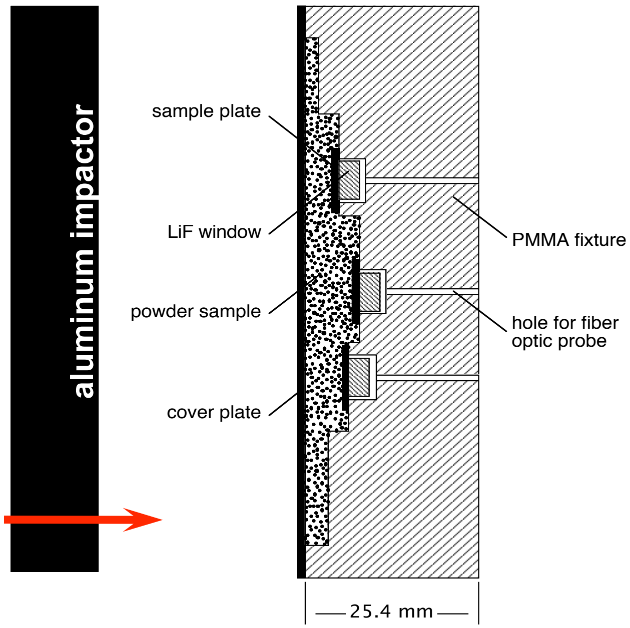
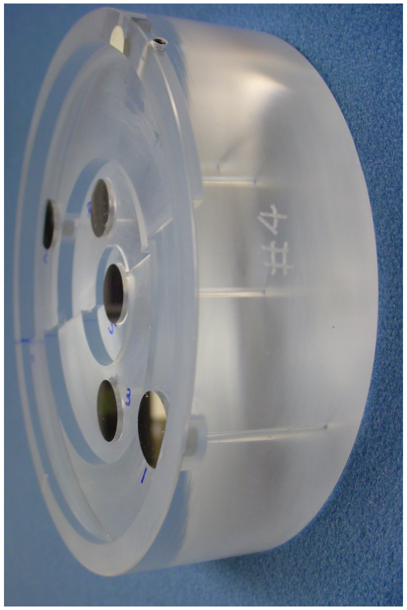
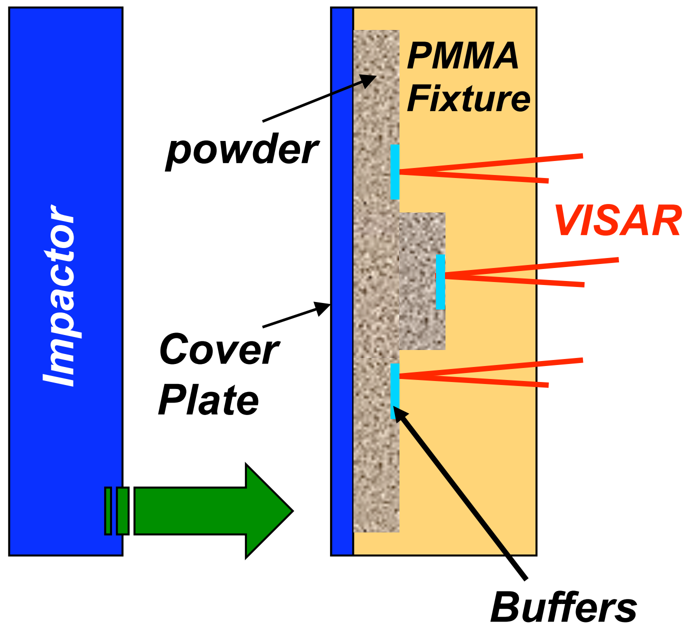
Planar Impact Experiments on Granular Materials







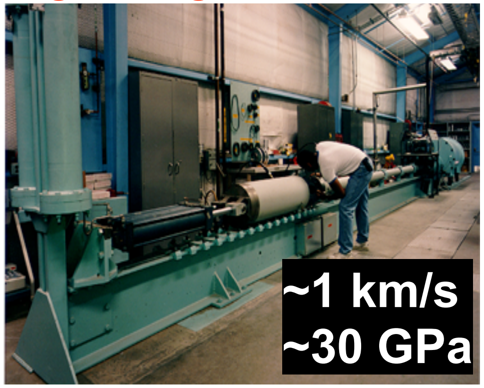
multiple sample thicknesses on the same experiment for accurate shock velocity and uniform powder density; sealed capsule allows fluid / powder mixtures

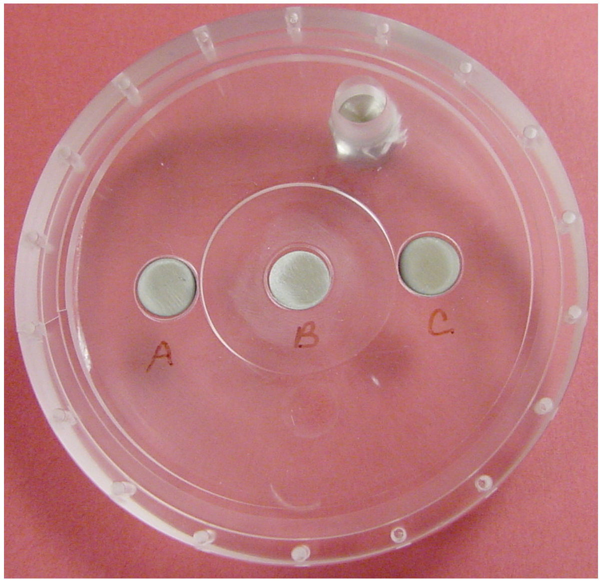
Vogler, T.J., Lee, M.Y., Grady, D.E., 2007. "Static and dynamic compaction of ceramic powders." *International Journal of Solids and Structures* **44**, 636-658.

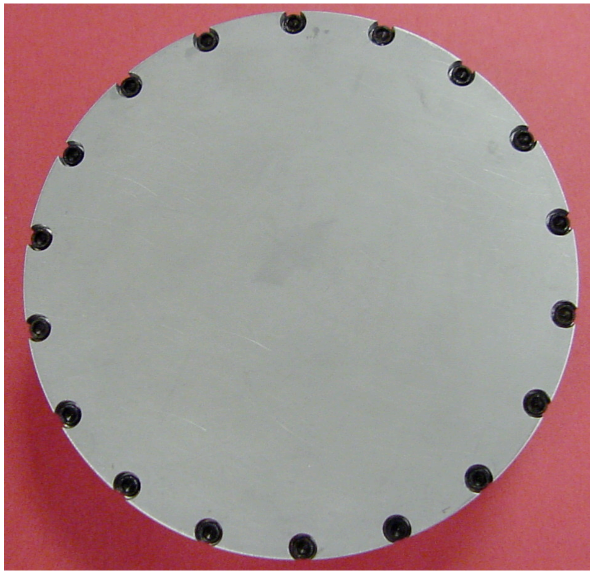
Brown, J.L., Thornhill, T.F., Reinhart, W.D., Chhabildas, L.C., Vogler, T.J., 2007. "Shock response of dry sand." in Shock Compression of Condensed Matter – 2007, American Institute of Physics, 1363-1366.

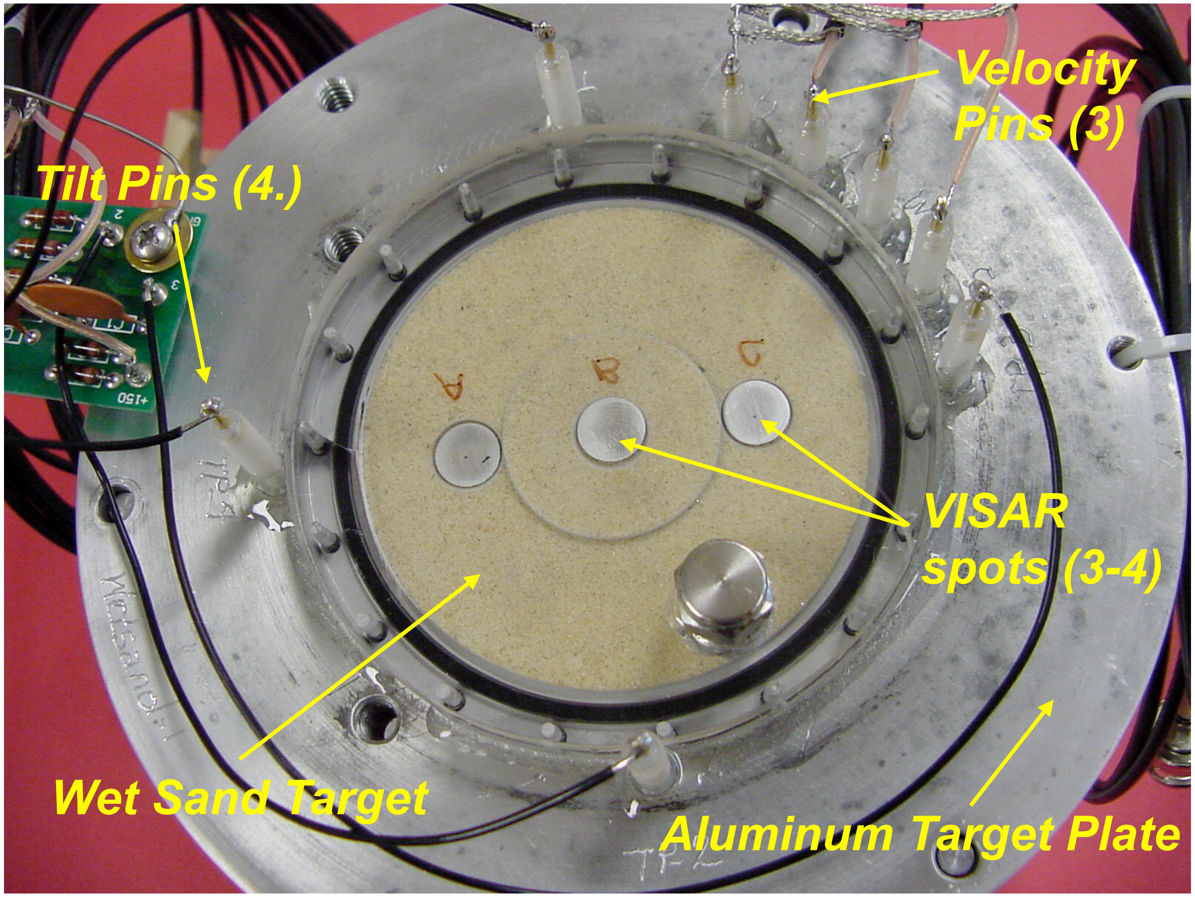
Wet Sand Targets

Single Stage Gun 100mm

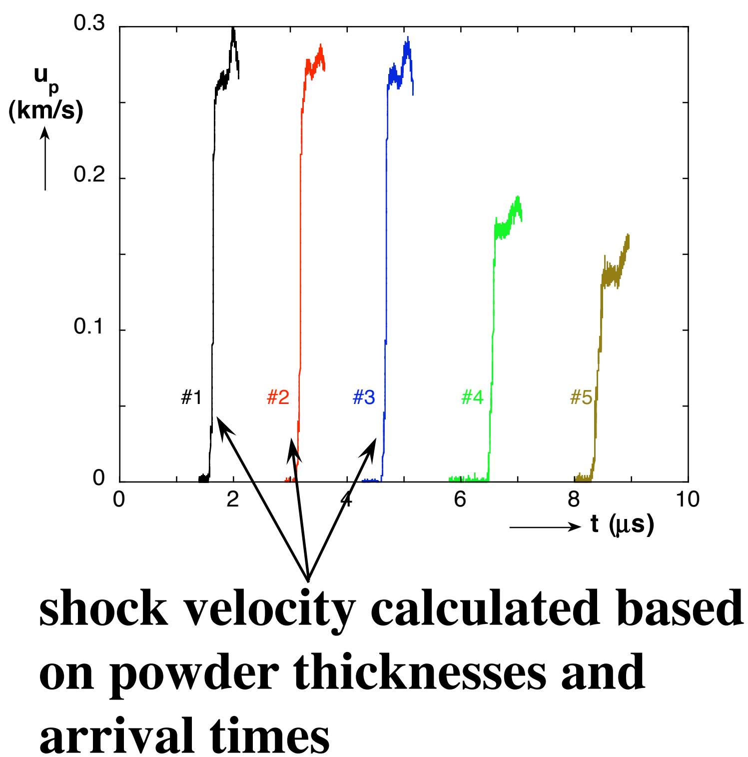


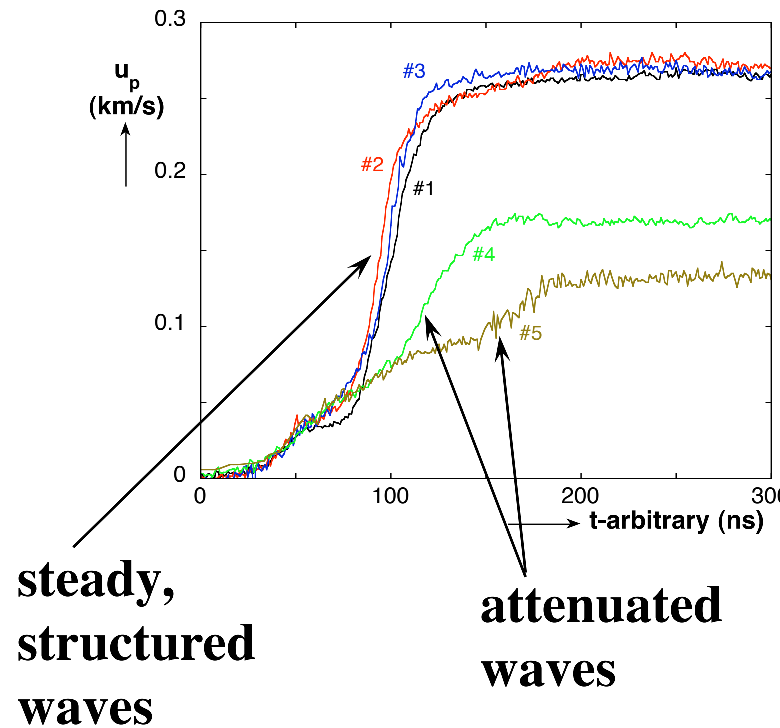






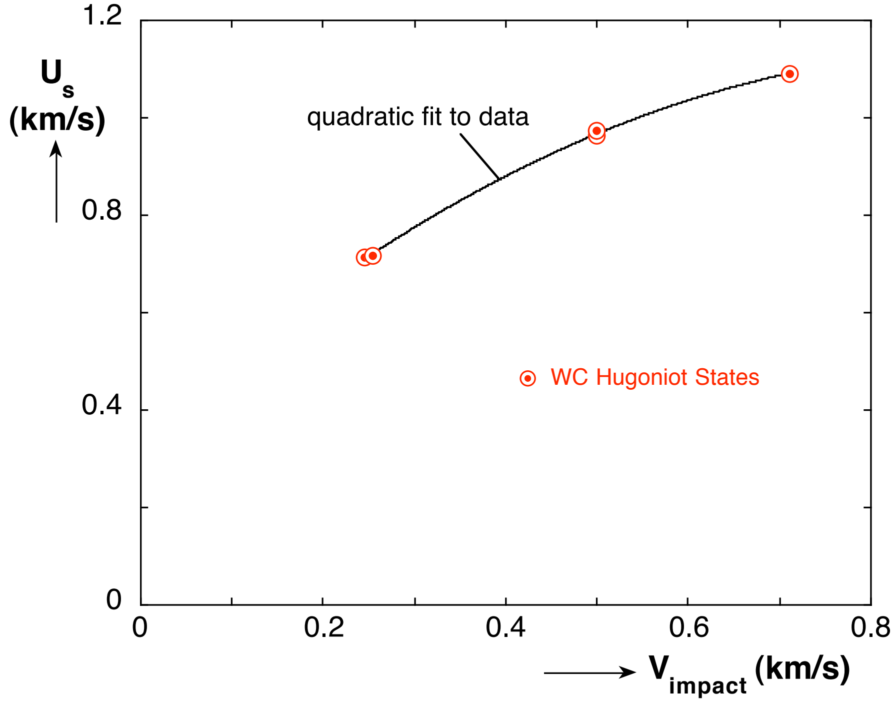
Measured Steady Waves

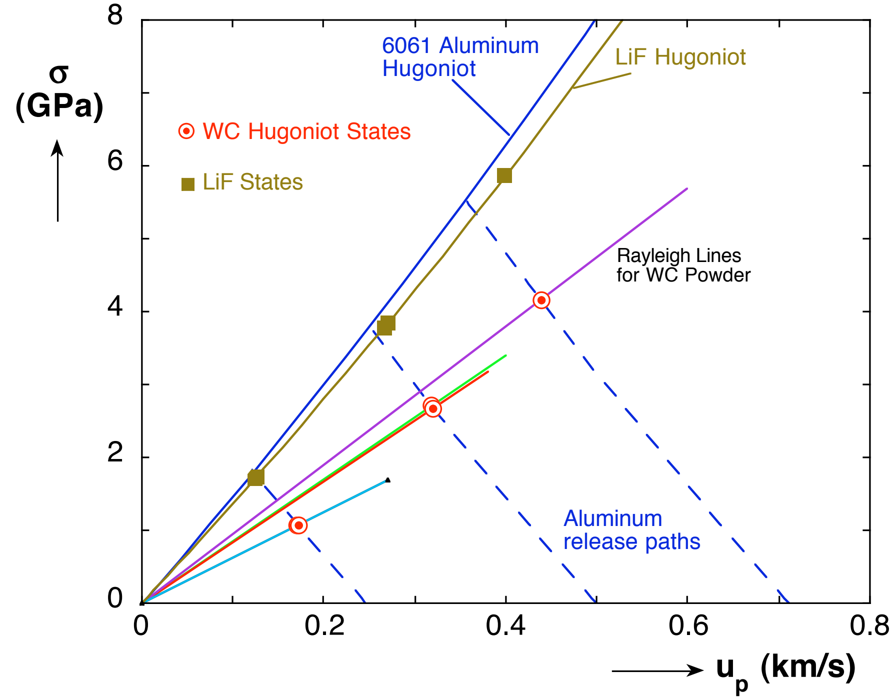




- seem to be first time-resolved measurements of steady waves in granular materials
- since waves are steady, Rankine-Hugoniot jump conditions can be used even though waves have finite rise times

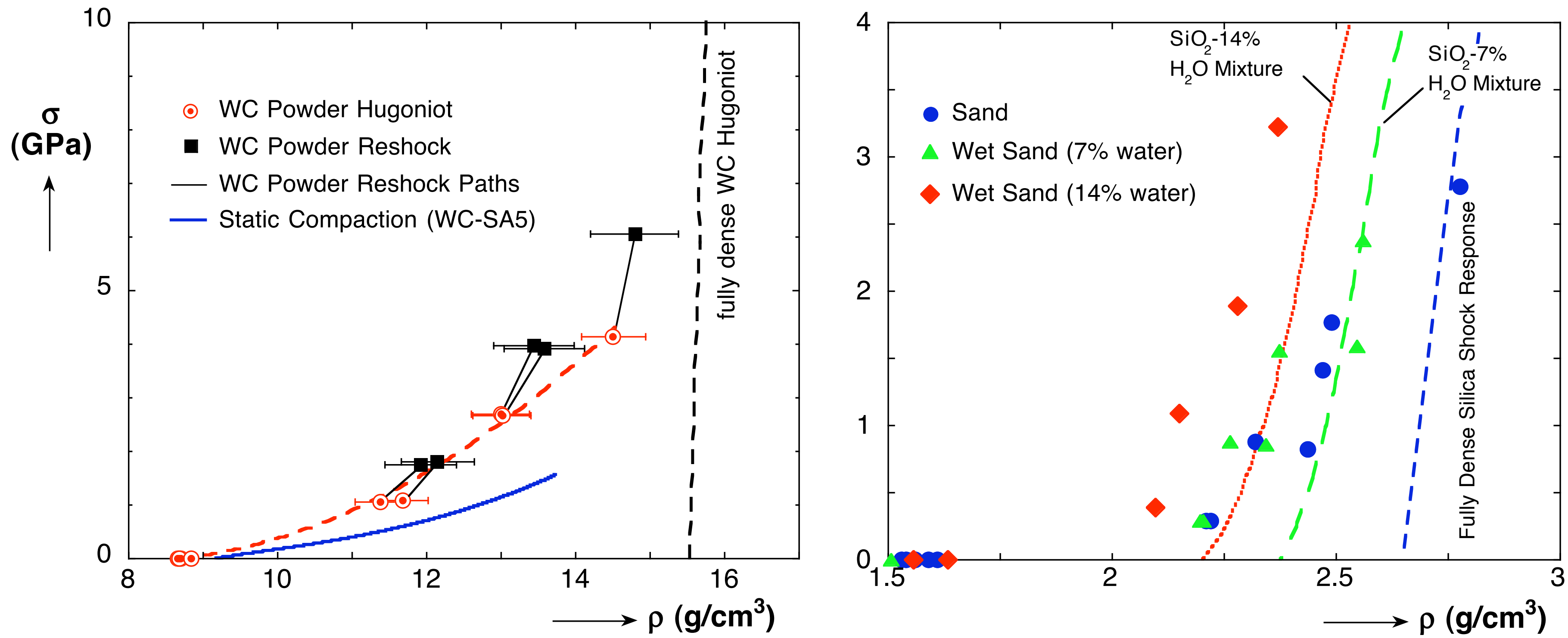
Shock Velocities and Hugoniot States





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

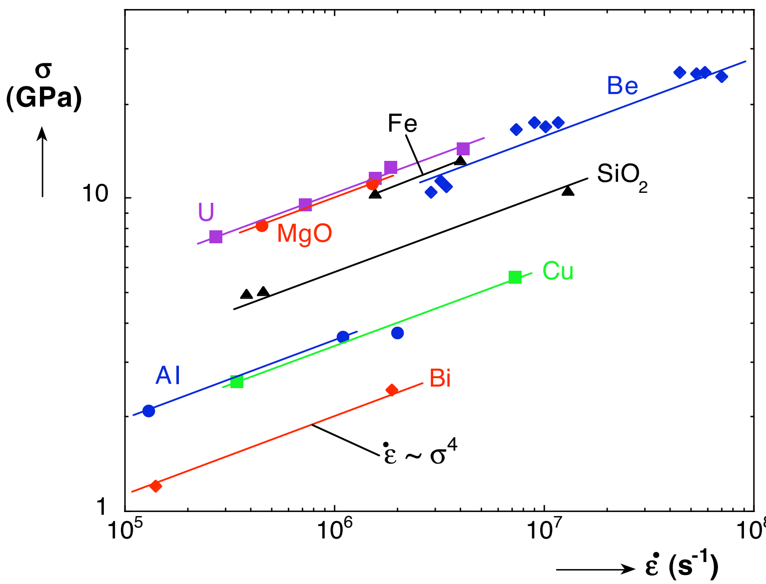
Compaction Response for WC and Wet/Dry Sand

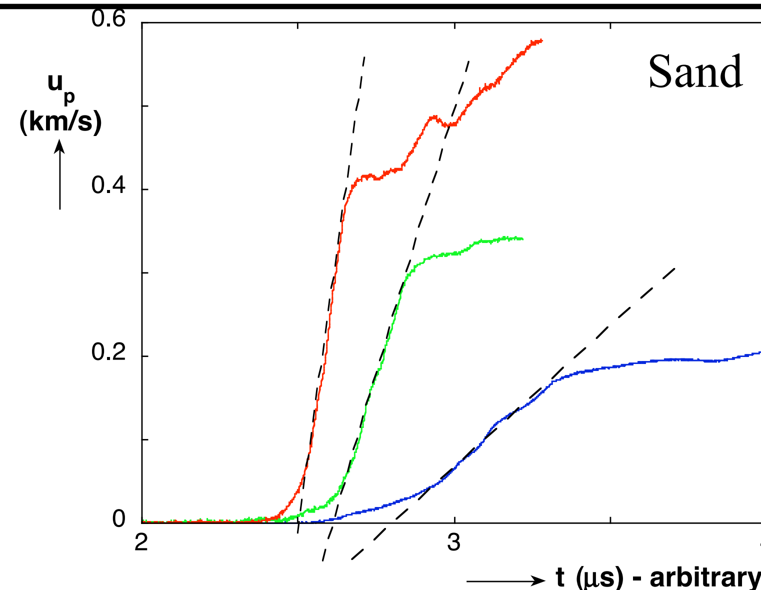


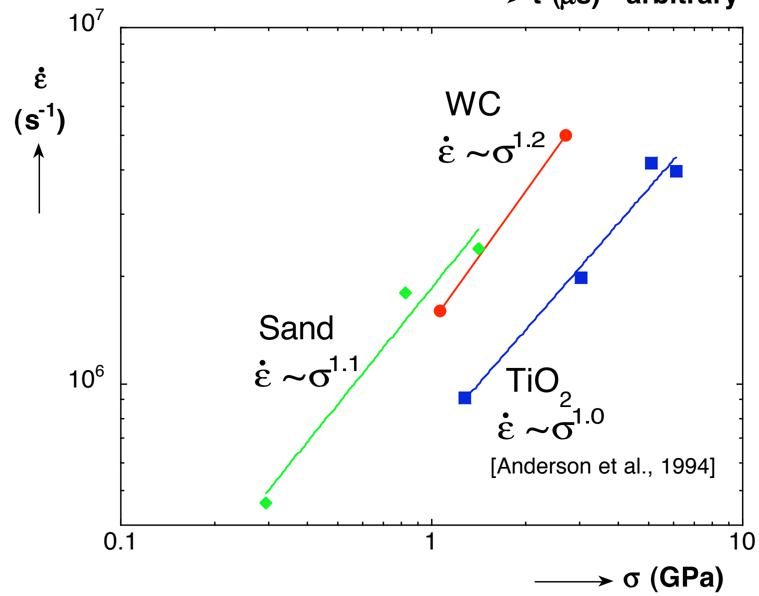
- first reshock state lies above Hugoniot suggesting elastic response of compacted material
- dynamic response is stiffer than static response for WC, about the same for sand

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)



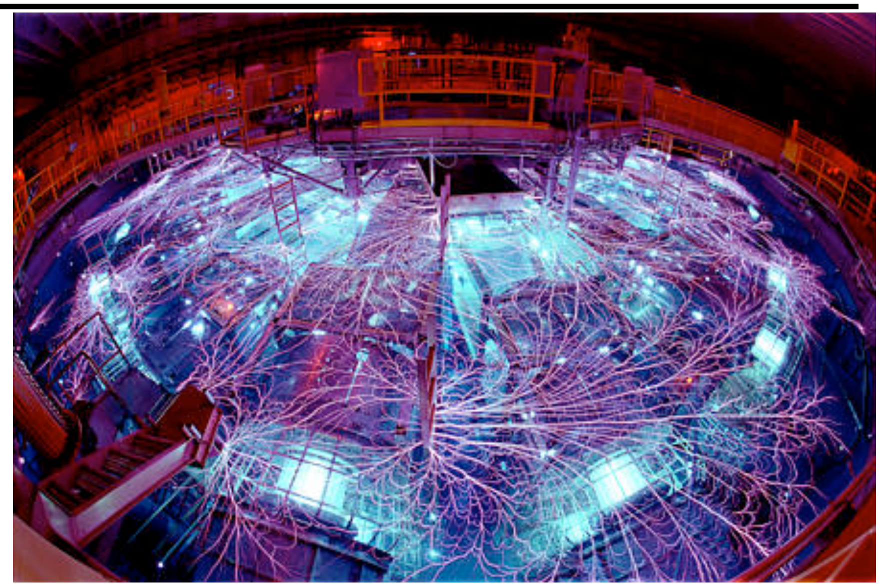


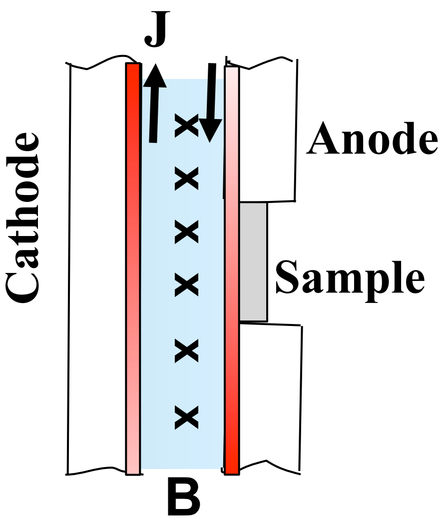


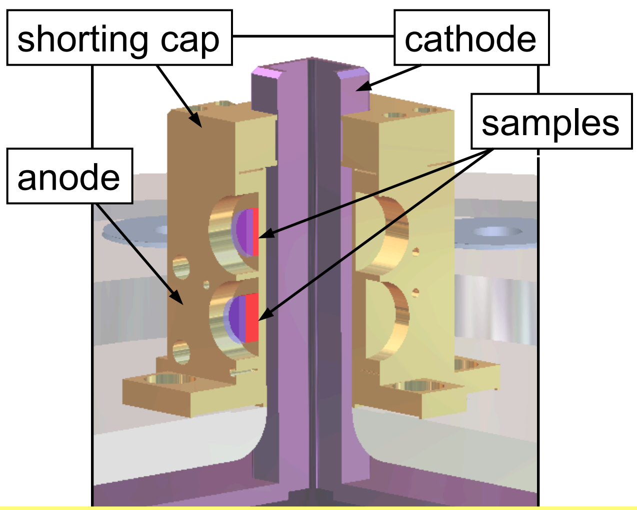
data on three granular ceramics and sugar suggest a linear scaling between stress and strain rate

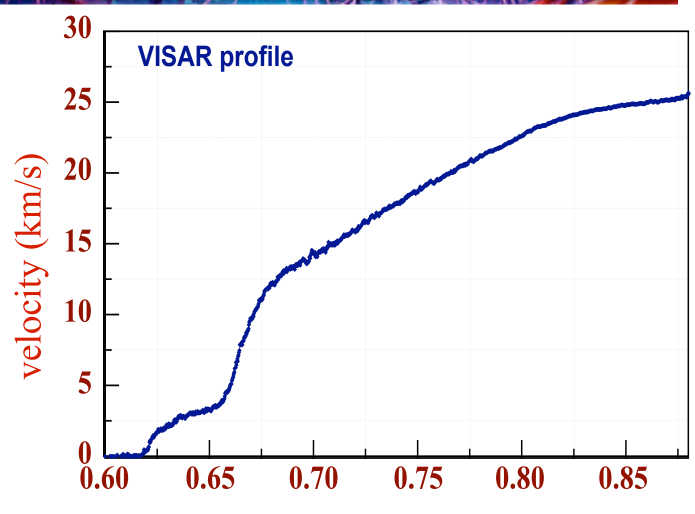
Z Pulsed Power Machine

- **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)**



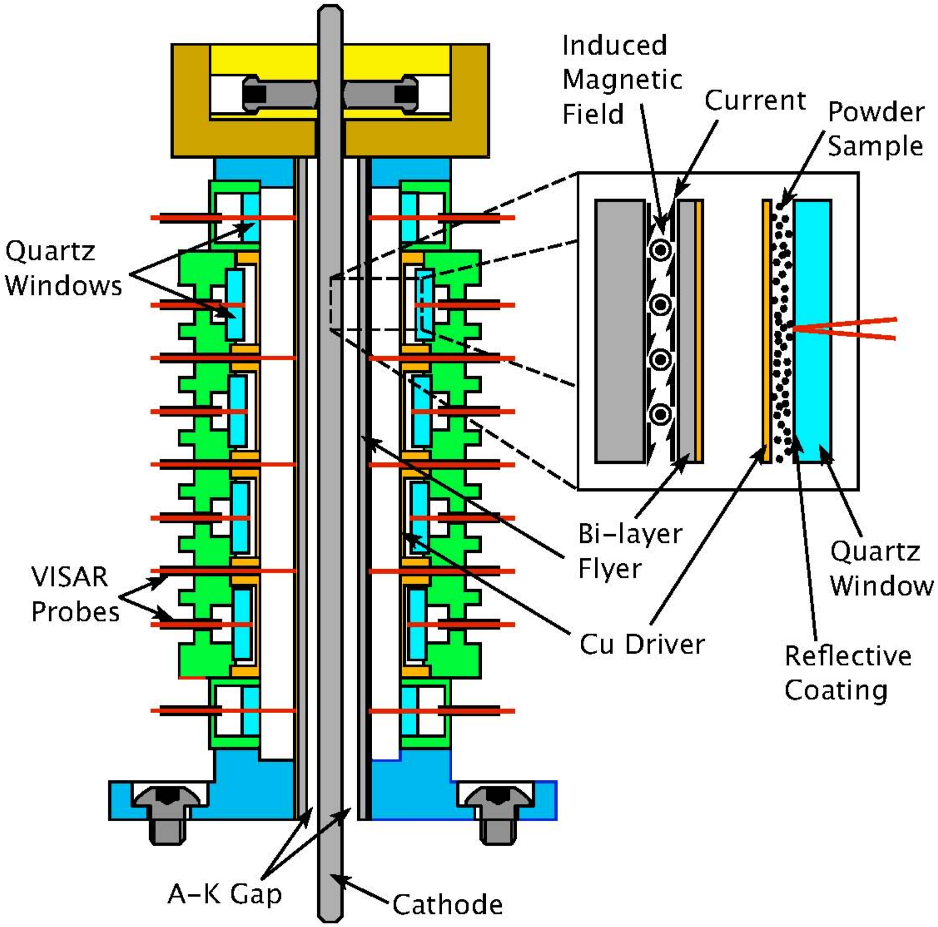




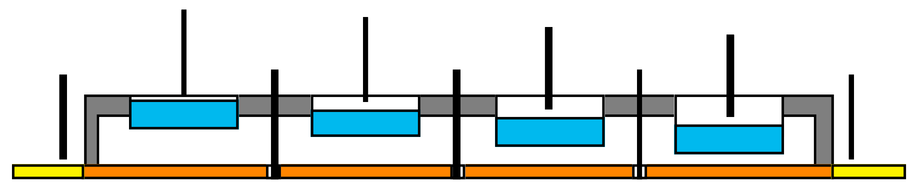


Davis, J.-P., Deeney, C., Knudson, M. D., Lemke, R. L., Pointon, T. D., and Bliss, D. E. (2005). "Magnetically driven isentropic compression to multimegabar pressures using shaped current pulses on the Z accelerator," *Physics of Plasmas* 12, 056310.

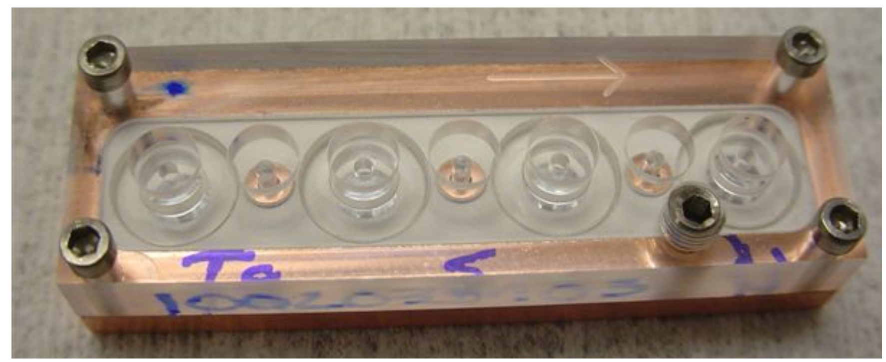
High Pressure Z Experiments



400, 600, 800, and 1000 micron samples



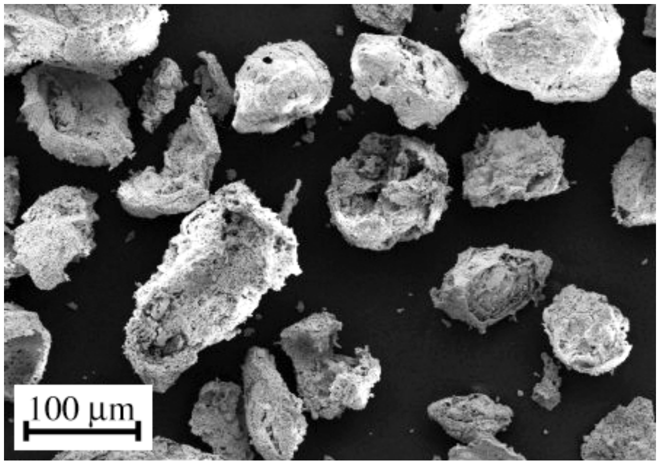
300 micron thick copper driver

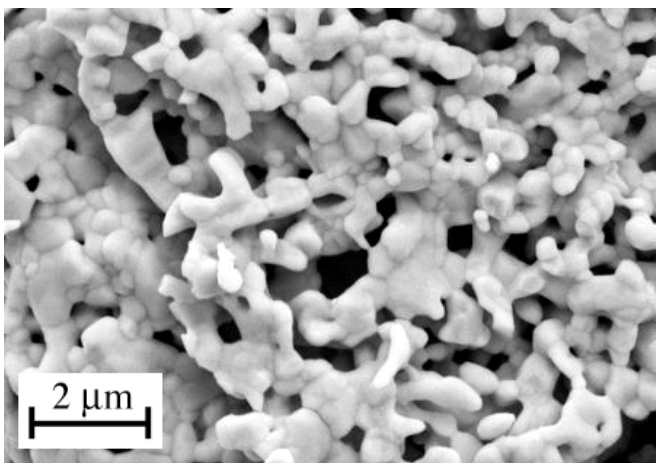


V = 9.9-10.3 and 11.2-11.4 km/s

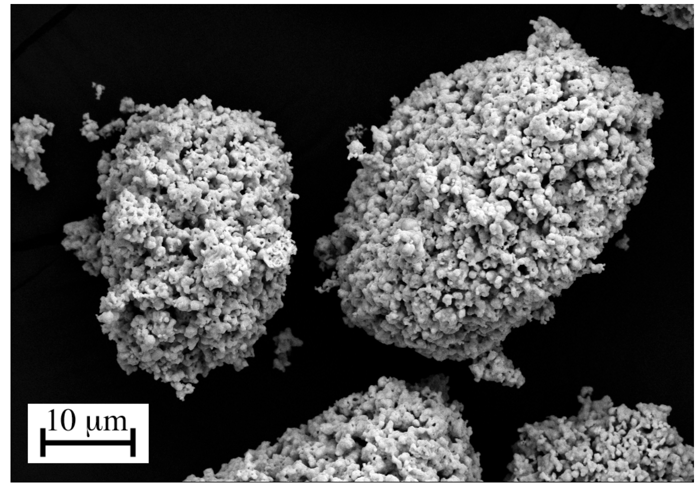
Two Different Forms of Granular Ta_2O_5

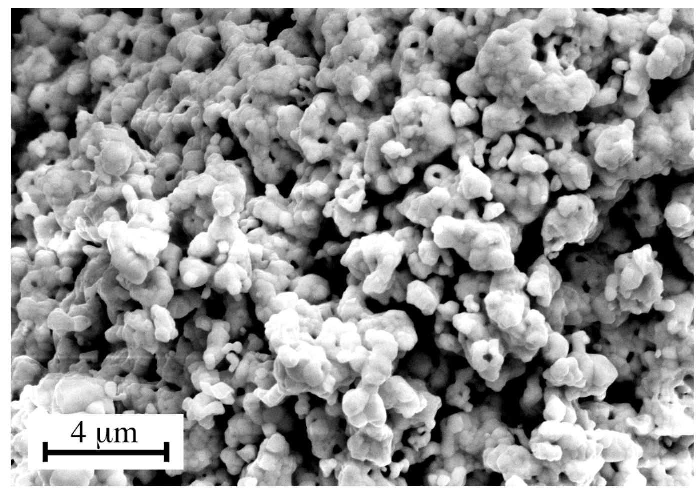
~1.3 g/cc from Cerac





~3 g/cc from American Elements

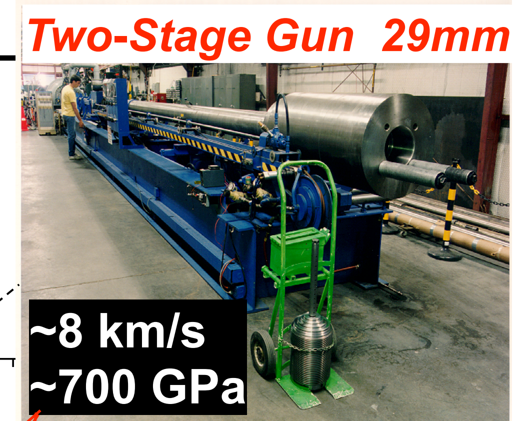




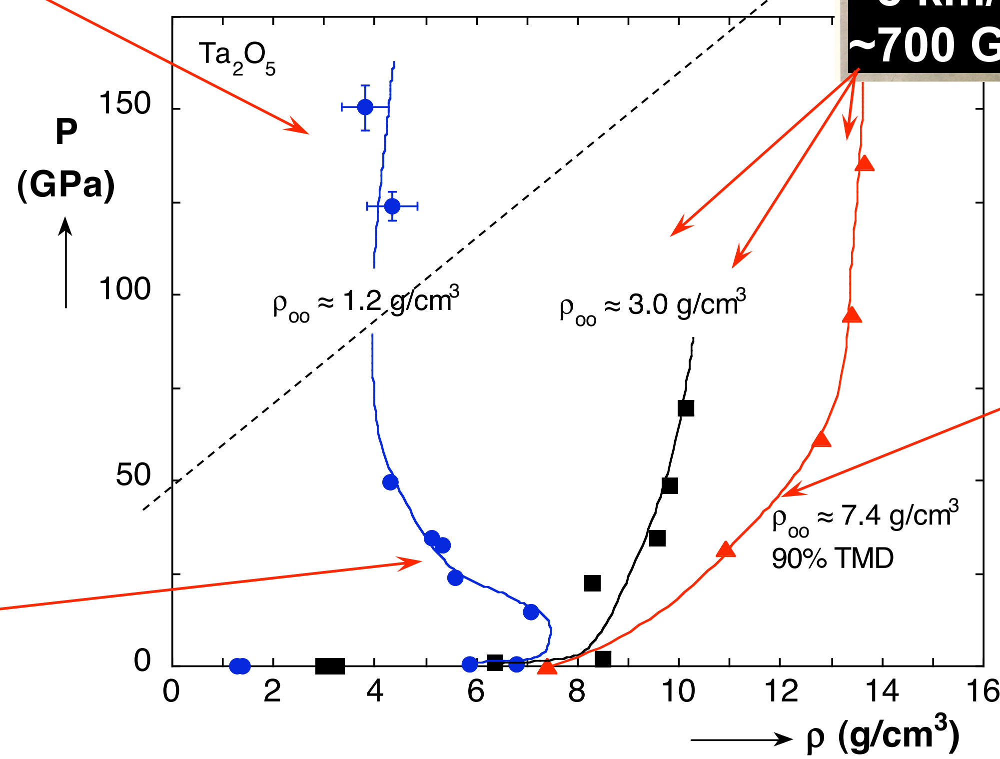
X-ray diffraction shows all material is in orthorhombic phase

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

High-Pressure Shock Results



Z results



possible phase transformation

lower initial density means material is hotter for a lower pressure

as pressure increases, density decreases

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Mesoscale Modeling of Granular Materials: Past Work

- collapsing ring of material under external pressure (Carroll & Holt, 1972; Nesterenko, 2001; Tong & Ravichandran, 1997)

- Williamson (1990) considered a unit cell in a uniform distribution of particles under dynamic loading

- Benson and coworkers (1994-present) studied compaction of granular materials (primarily metals) using a 2-D Eulerian code for a moderate number of grains

- Baer (2002-present) simulated compaction of HMX and sugar (HMX simulant) using a 3-D Eulerian code for a moderate number of particles

- follow approach of Benson et al. for larger number of grains by exploiting parallel computing platforms
- begin with 2-D and determine whether 3-D is necessary

Mesoscale Modeling of Granular Materials

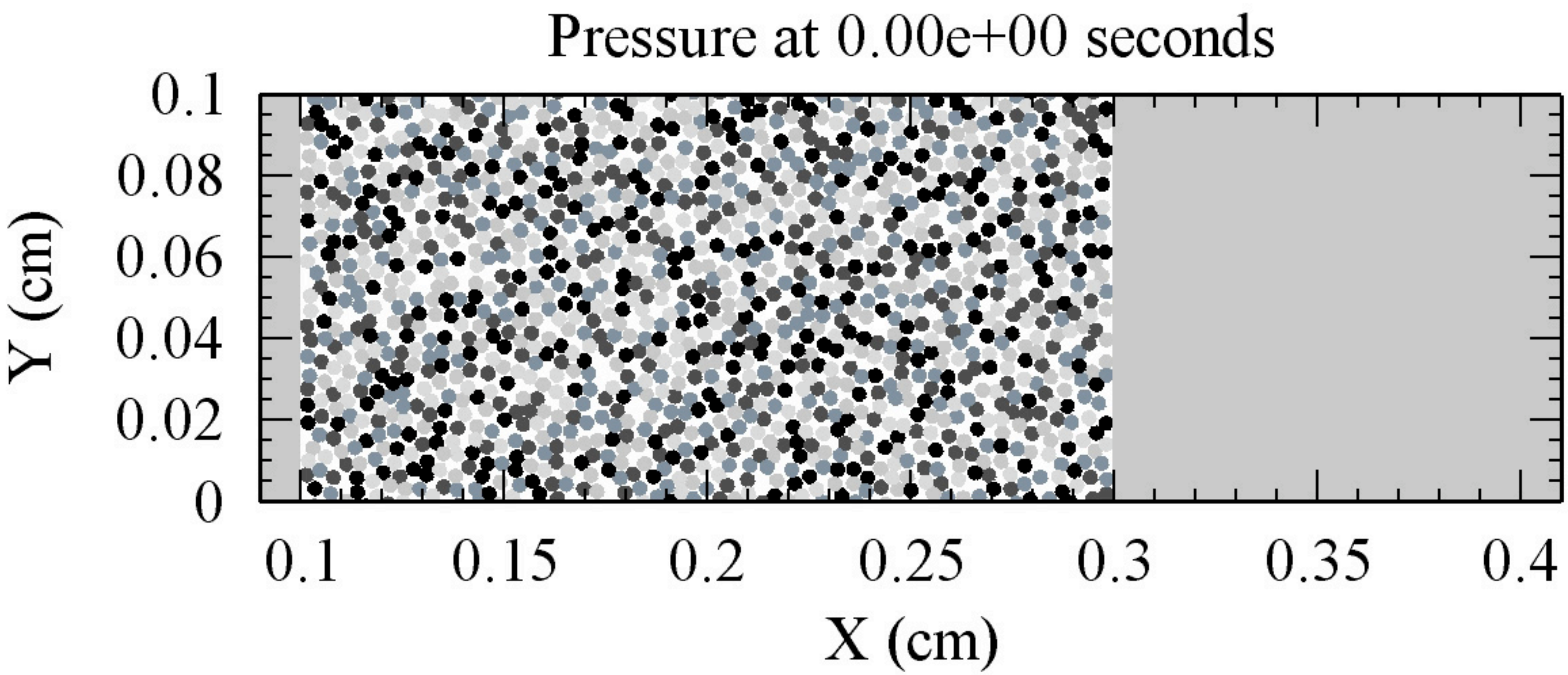
- particles idealized as circles (rods) for initial work
- constant velocity boundary condition applied
- run in CTH (explicit Eulerian finite difference code)
- Mie-Gruneisen EOS, elastic-perfectly plastic strength for WC

Borg, J.P., Vogler, T.J., (2008). "Mesoscale calculations of the dynamic behavior of a granular ceramic." *International Journal of Solids and Structures* **45**, 1676-1696.

Borg, J. P. and T. J. Vogler (2009). "Aspects of simulating the dynamic compaction of a granular ceramic." *Modeling and Simulation in Materials Science and Engineering* ***17: 045003.***

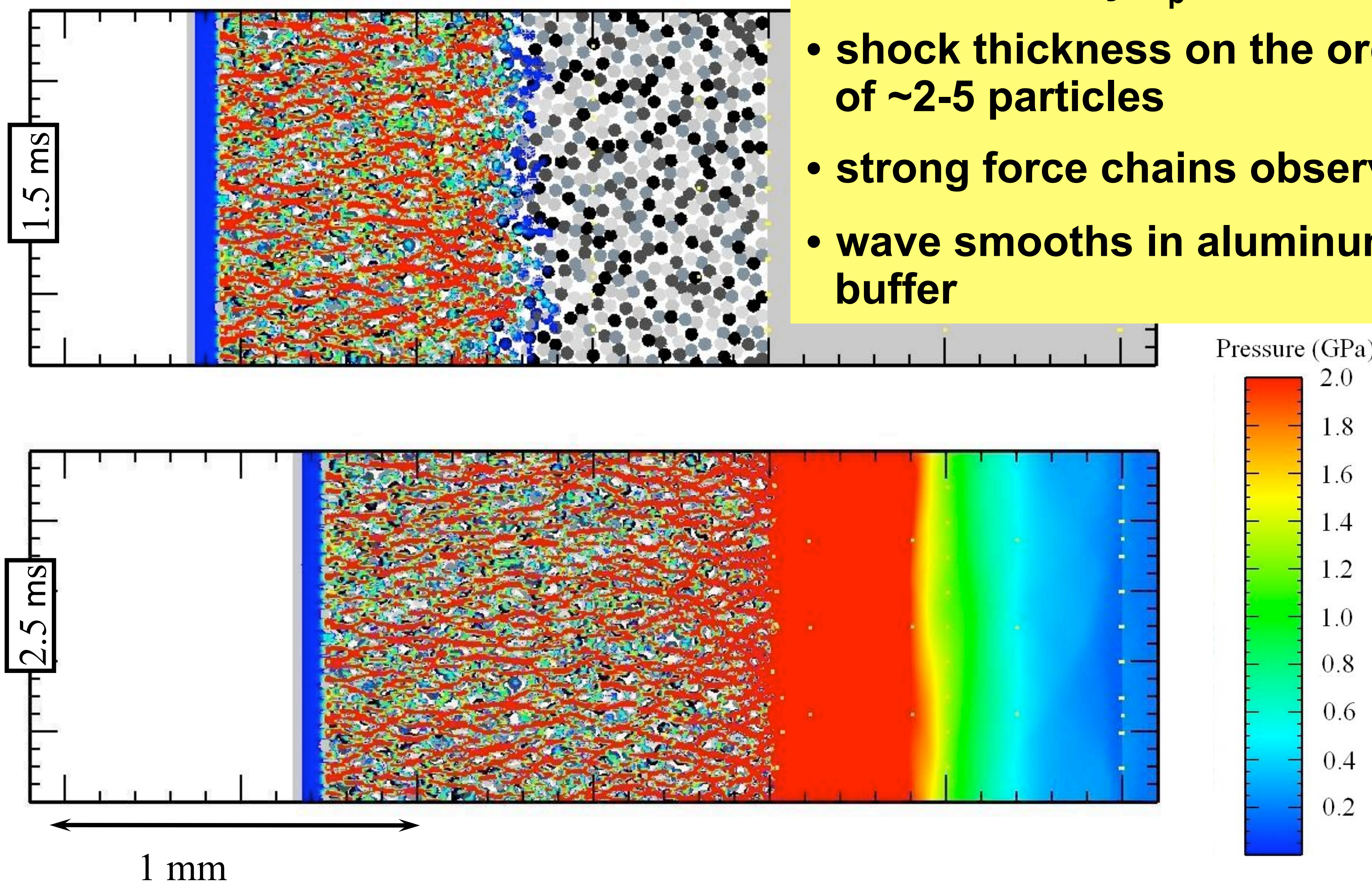
get at underlying physics of granular materials

Computational Dynamic Compaction

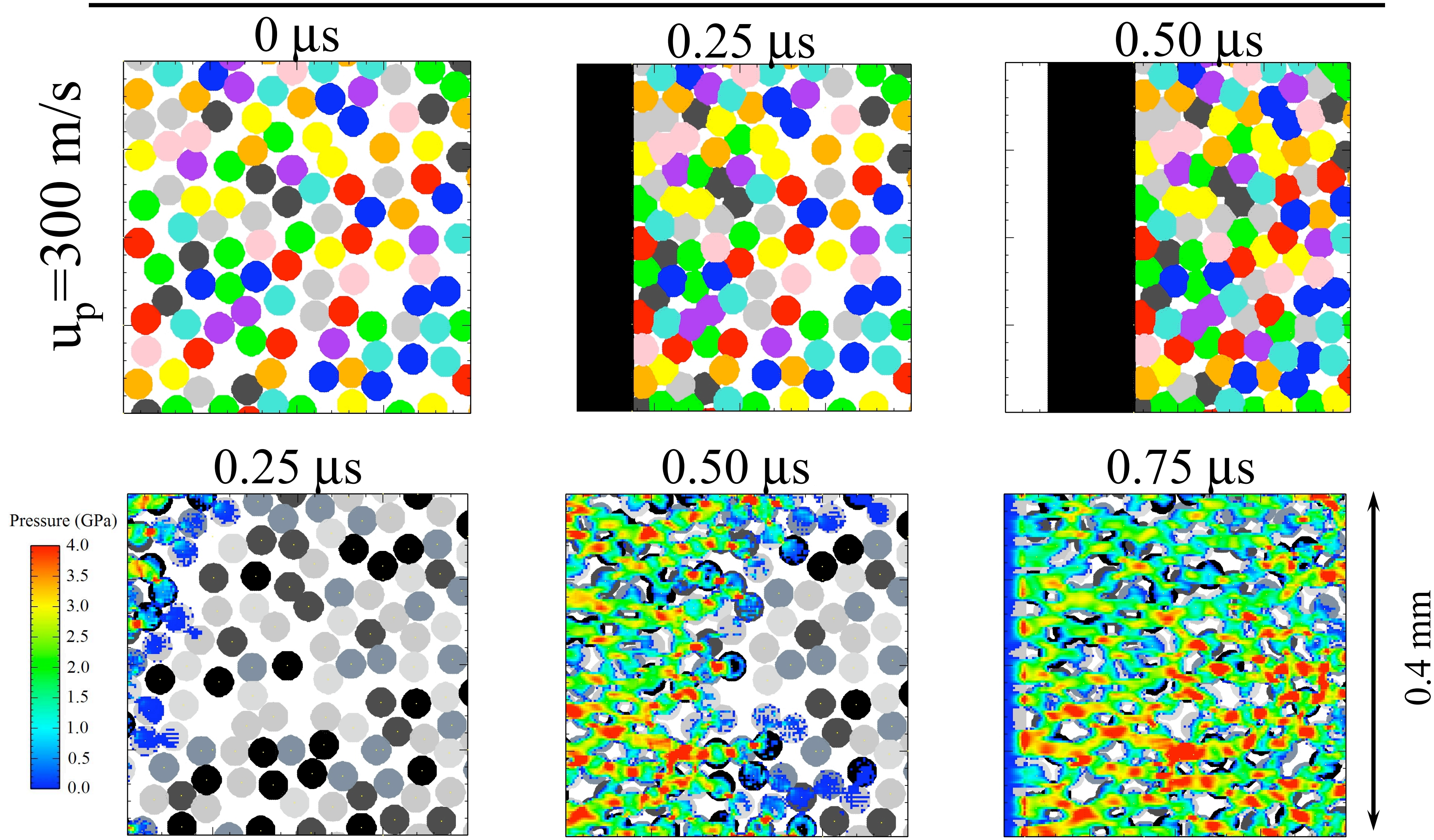


Computational Dynamic Compaction

- driver velocity u_p=300 m/s
- shock thickness on the order of ~2-5 particles
- strong force chains observed
- wave smooths in aluminum buffer

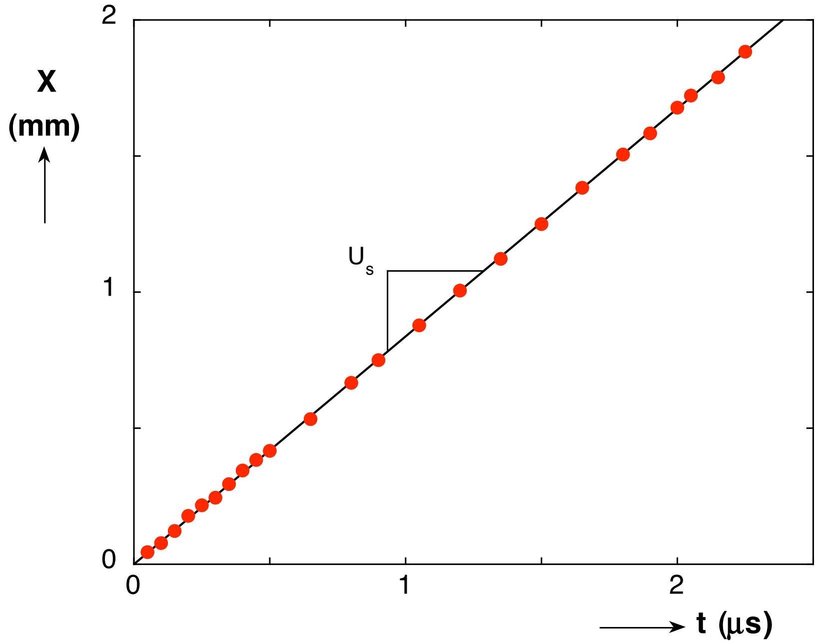


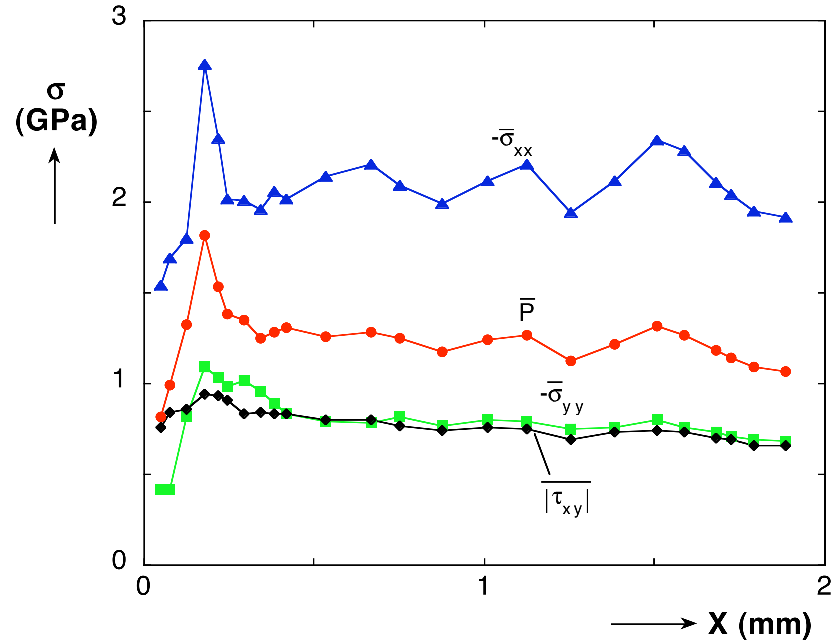
Close-Up of Compaction Process



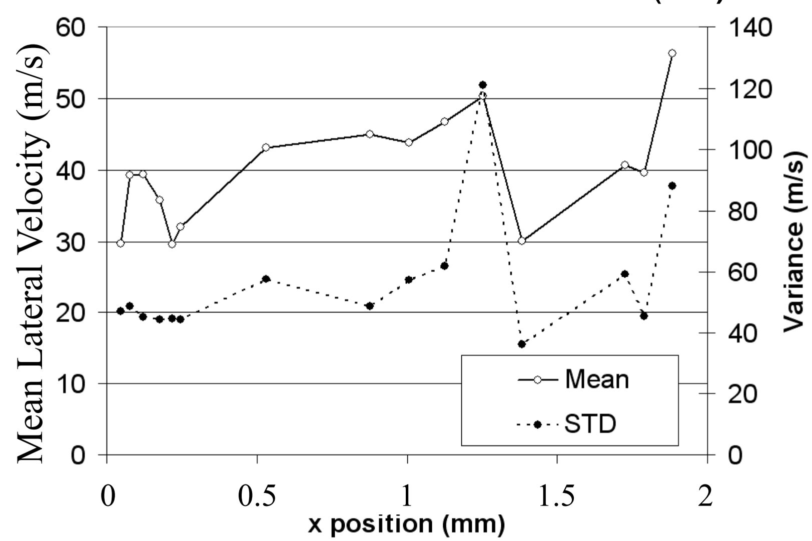
no jetting or vortices so deformation is "*quasi-static*"
(Benson et al., 1997)

Properties of Propagating Wave

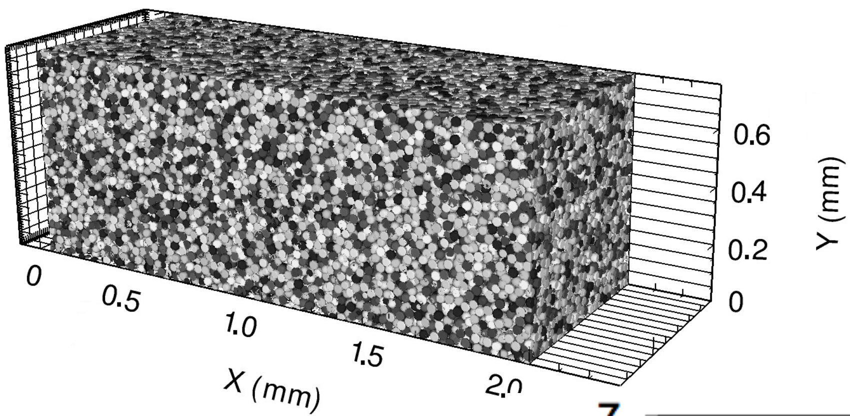




- arrival time of wave suggests steadiness at all times
- stresses in wave front indicate nearly 0.5 mm required to reach steady state
- lateral motion >10% of longitudinal velocity



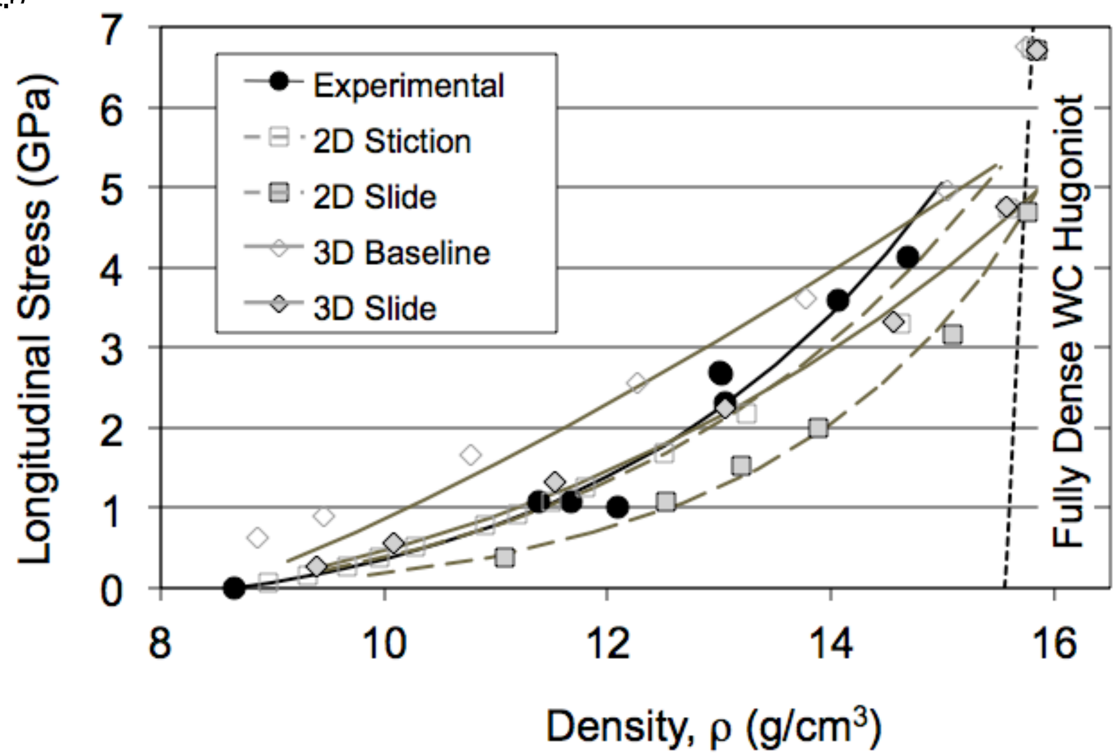
Response of 2-D and 3-D Models



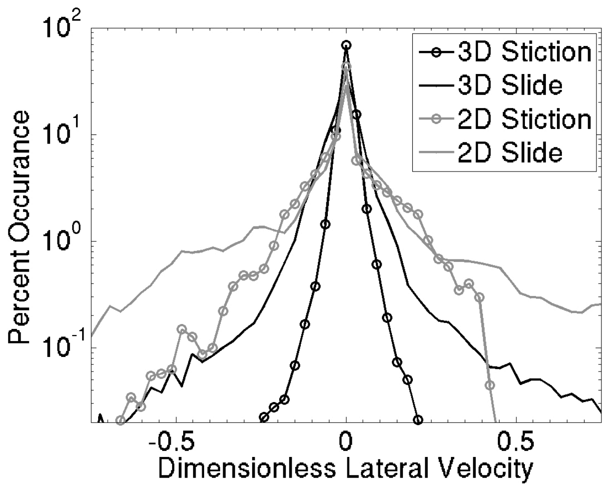
$$\sigma = \rho_o U_s u_p$$

$$\rho = \rho_o \frac{U_s}{U_s - u_p}$$

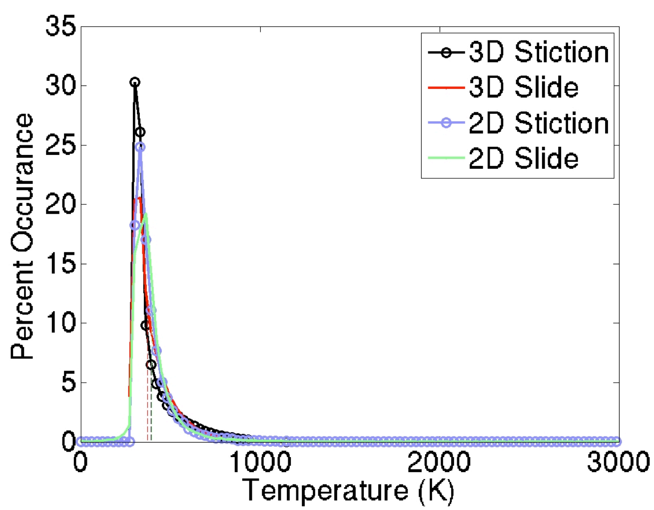
2-D Stiction and 3-D Slide match experimental results best

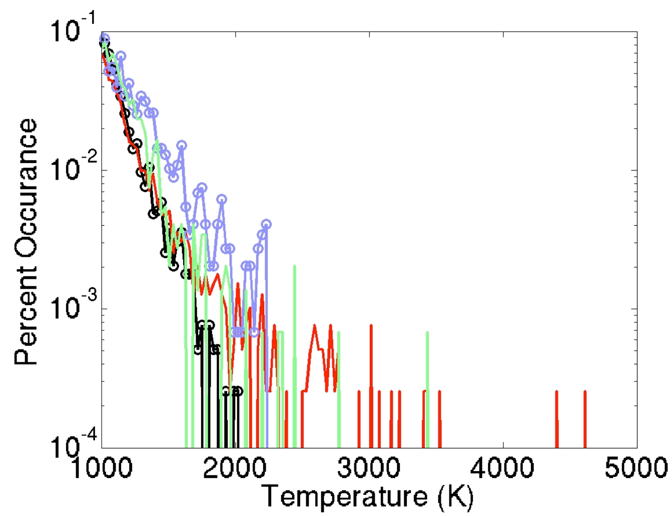


Distributions from 2-D and 3-D Calculations

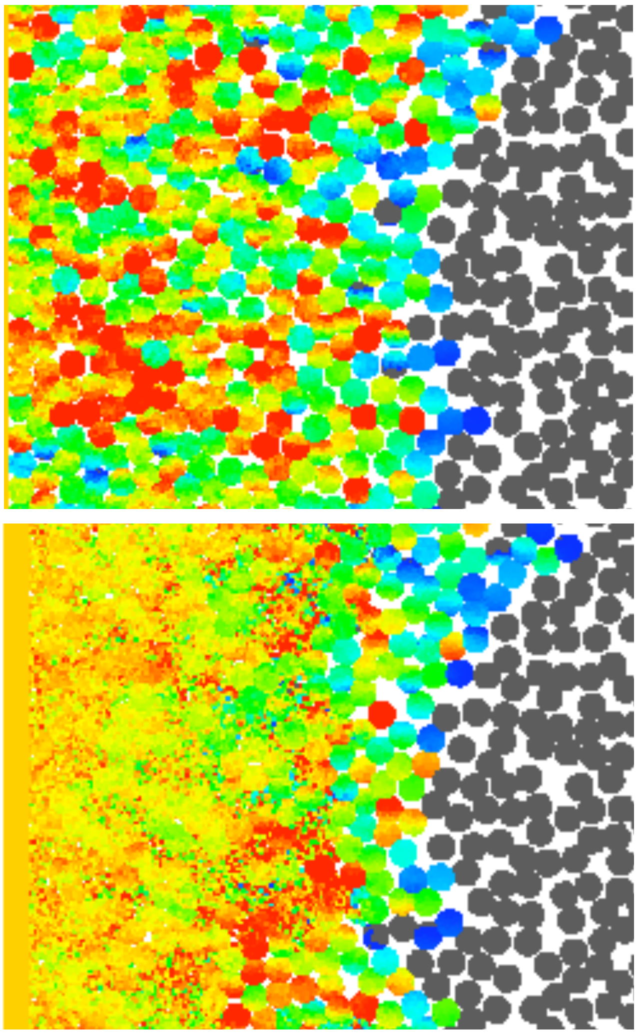


- fields are smoother in 3-D
- larger lateral velocity and temperature in 2-D simulations

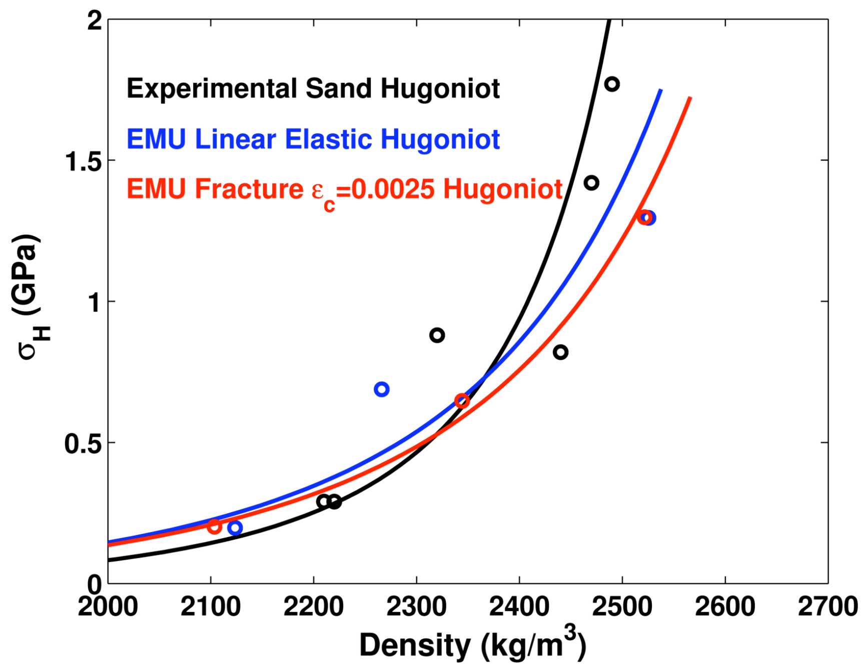




Mesoscale Calculations with Peridynamics



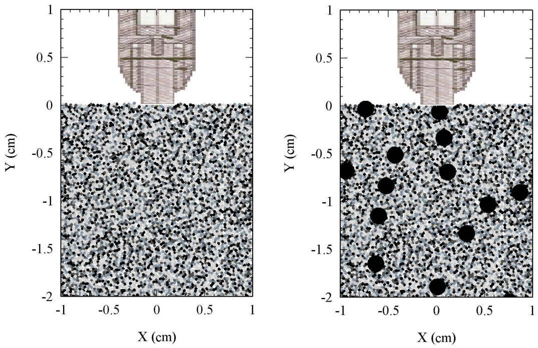
EMU - Parallel, particle-based implementation of peridynamics (Silling, S. A. (2000). *J. Mech. Phys. Solids 48, 175-209*.
includes fracture and contact missing from CTH



Lammi, C.J., and Vogler, T.J. (2011). "Mesoscale Simulations of Granular Materials with Peridynamics," in *Shock Compression of Condensed Matter – 2011*, American Institute of Physics, 1467-1470.

“System Level” Work providing insight into other problems

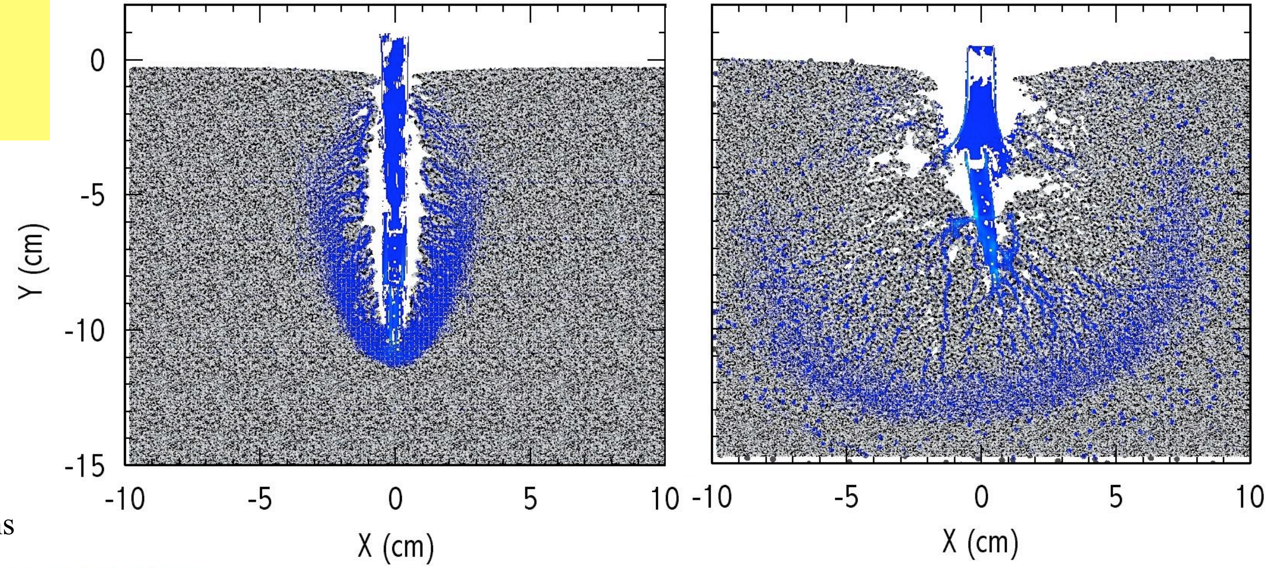
Borg, J. P. and T. J. Vogler (2008). "Mesoscale simulations of a dart penetrating sand." *Int. J. of Impact Engineering* ***35: 1435-1440.***



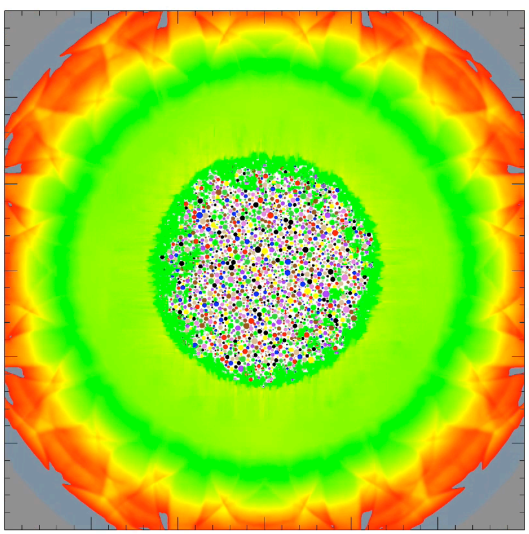
224 mm Sand with 1.6 mm grains

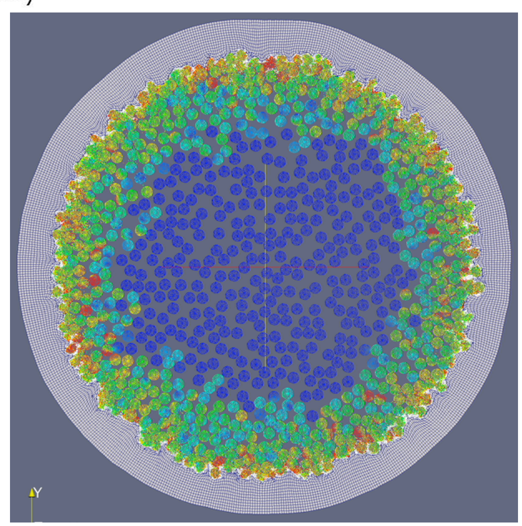
224 mm uniform sand

224 mm sand with 1.6 mm



CTH



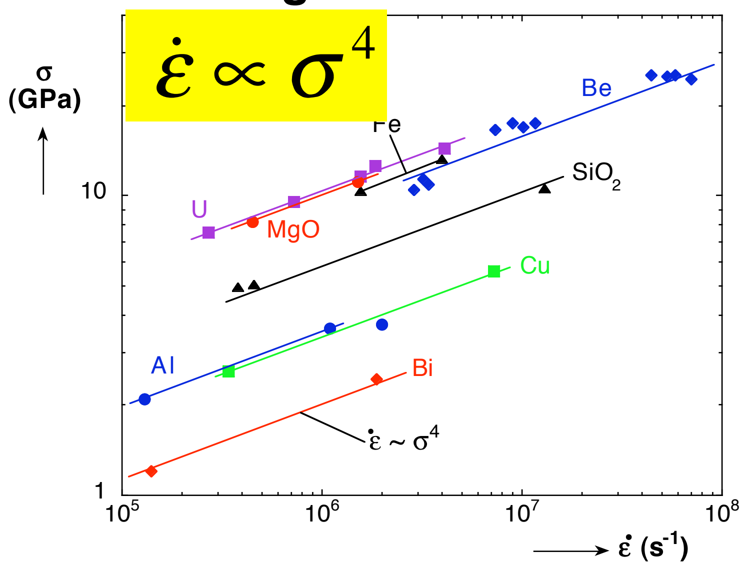


coupled FEM / peridynamics

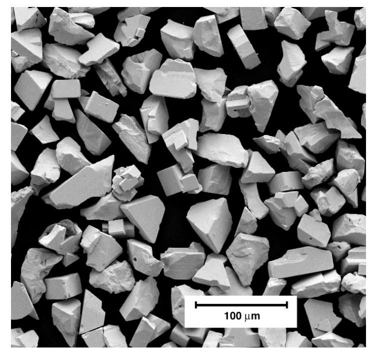
- Introduction to Shock and High-Pressure Physics
- Introduction to Granular Materials
- Planar Impact Experiments
- Mesoscale Modeling
- Scaling Properties of Waves
- Conclusions

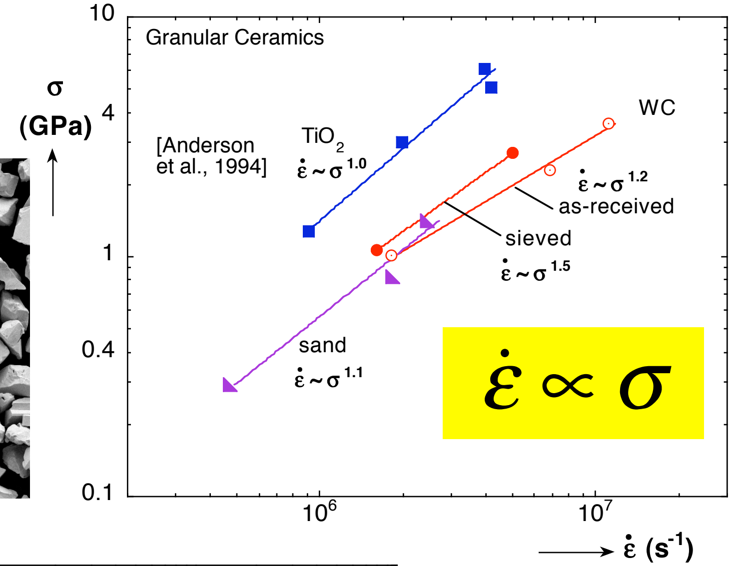
Scaling of Waves in Materials

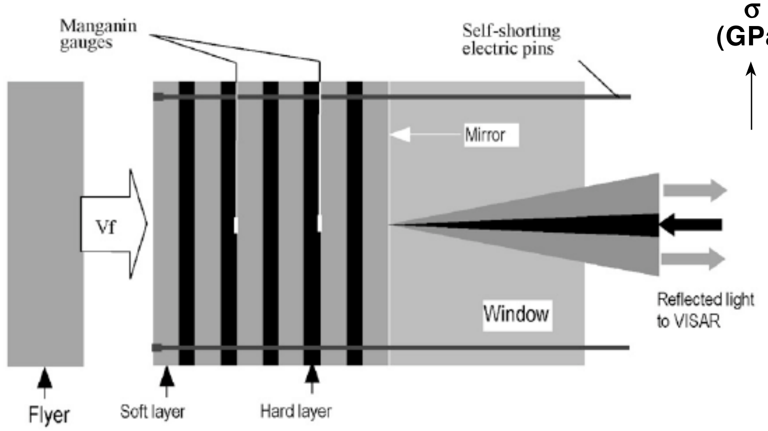
"Homogeneous" Materials

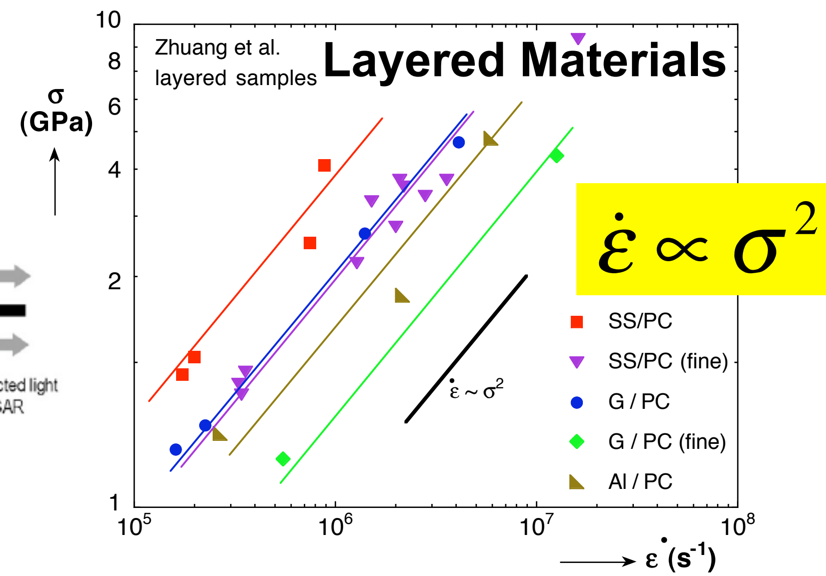


Granular Materials



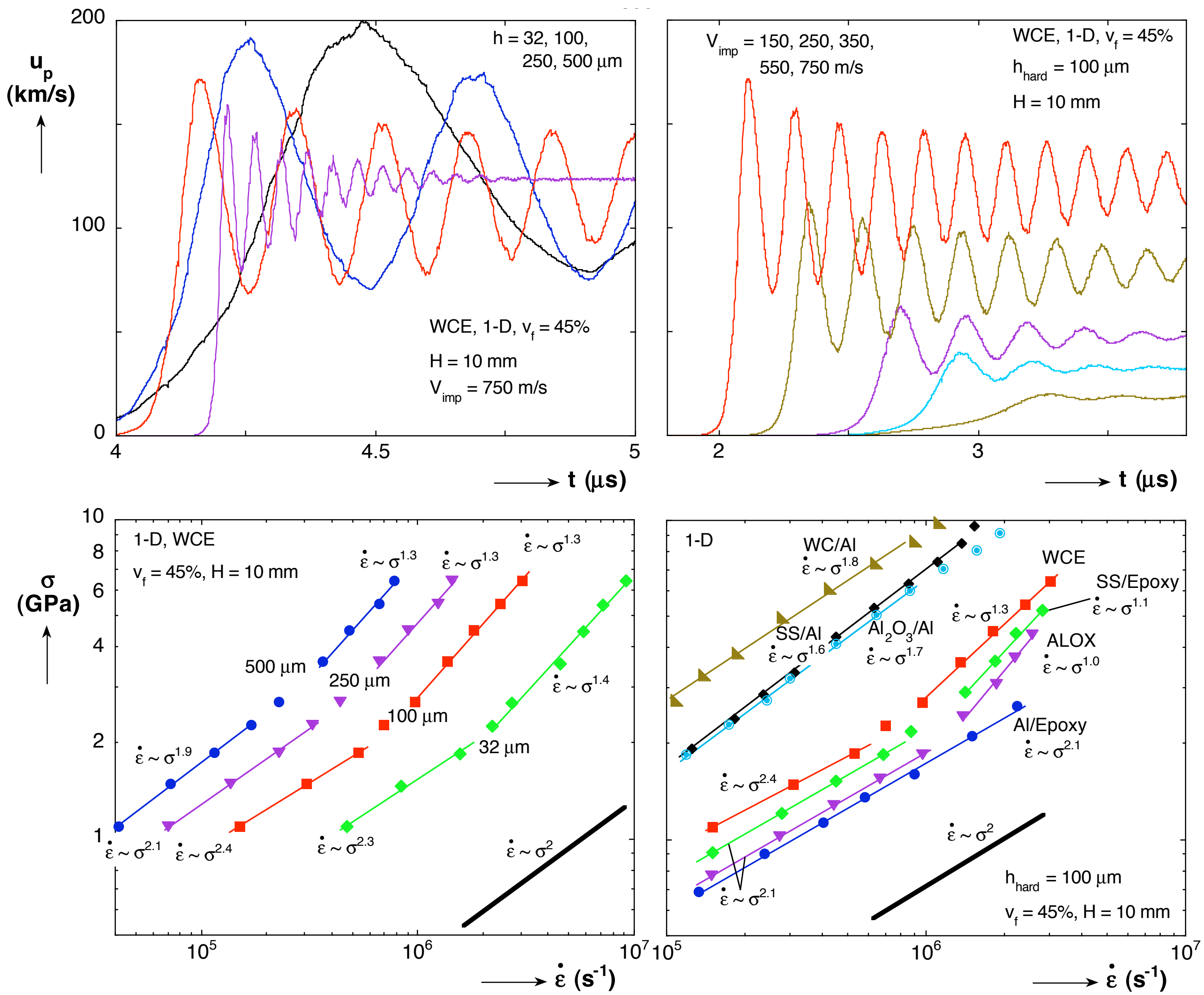






particulate composites (e.g. WC/epoxy, ALOX, PBX) show 4th power scaling

Simulations for Layered Materials
1-D CTH Calculations



h ↑ $\dot{\varepsilon}$ ↓

V,σ ↑ $\dot{\varepsilon}$ ↑

also a function of material parameters of layers

Dimensional Analysis for Layered Materials

variables of problem:

σ, $\dot{\varepsilon}$, h, v_f, C, (ρ_s,ρ_h) or (z_s,z_h)

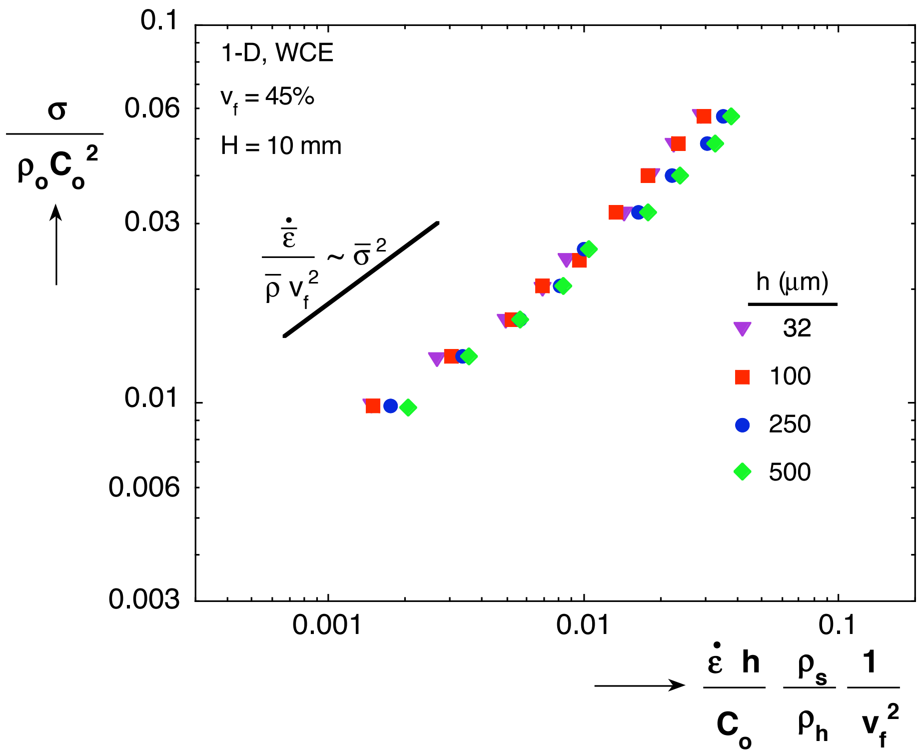
construct non-dimensional groups:

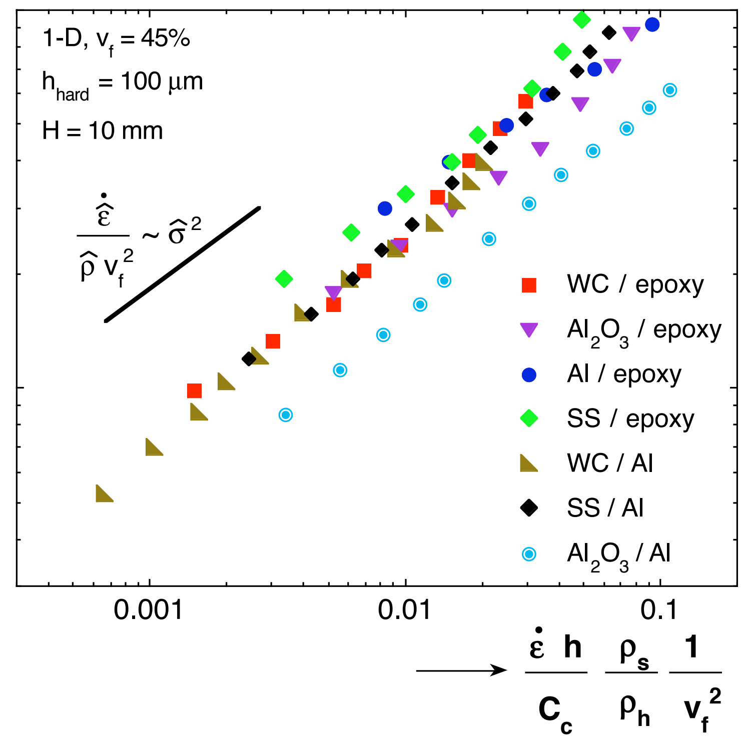
$$\bar{\dot{\varepsilon}} = \left(\frac{\dot{\varepsilon}\, h}{C_o}\right) \qquad \bar{\sigma} = \left(\frac{\sigma}{\rho_o\, C_o^2}\right) \qquad \left(v_f\right) \qquad \bar{\rho} = \left(\frac{\rho_s}{\rho_h}\right)$$

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

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

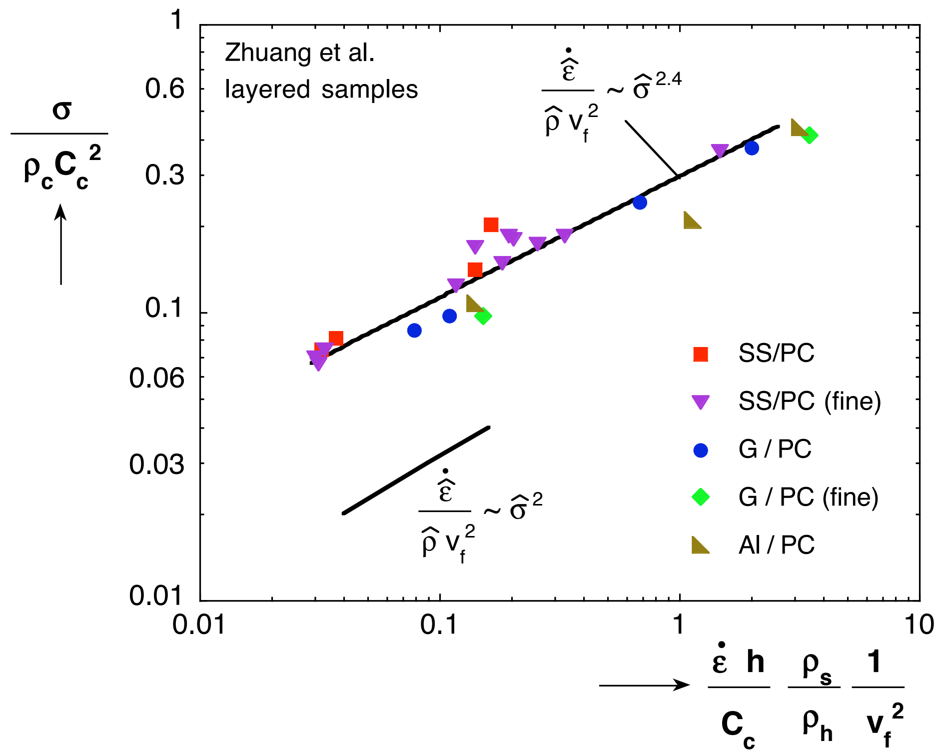
Non-Dimensional Simulation Results





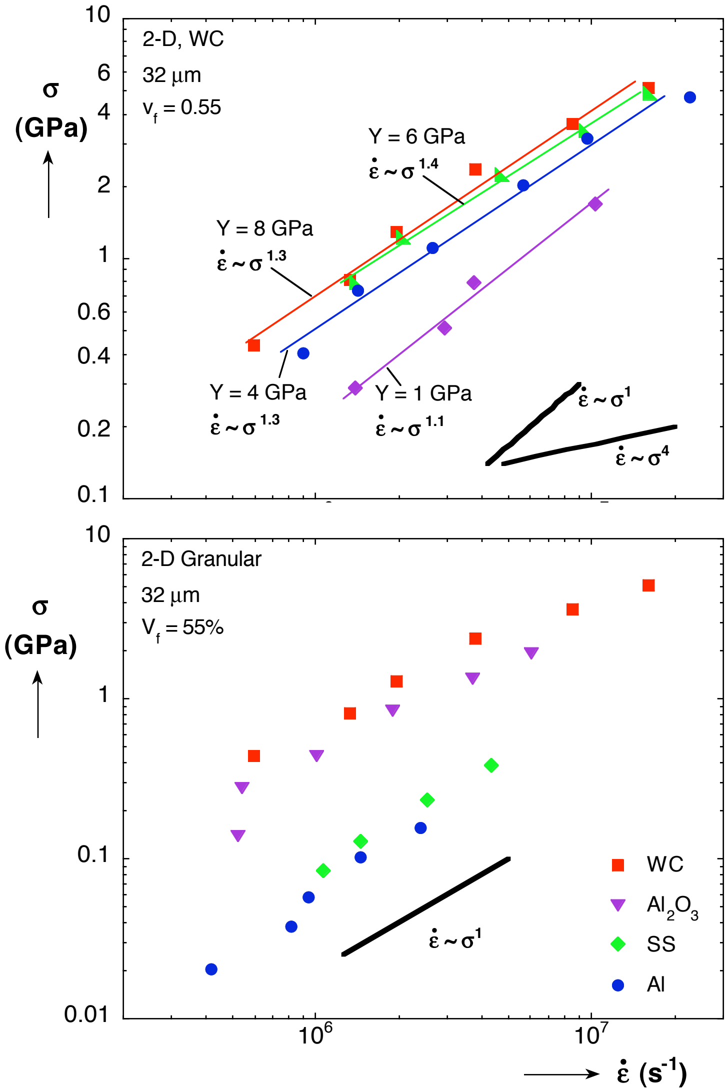
- non-dimensionalization collapses data for different layer thicknesses
- data for different material combinations collapse well using density ratio (with one exception)

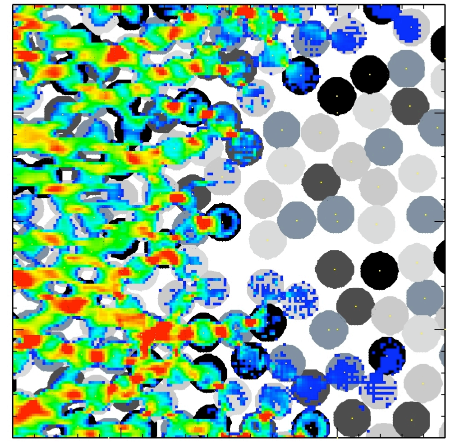
Non-Dimensionalized Experimental Results



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

2-D CTH Simulations of Granular Materials

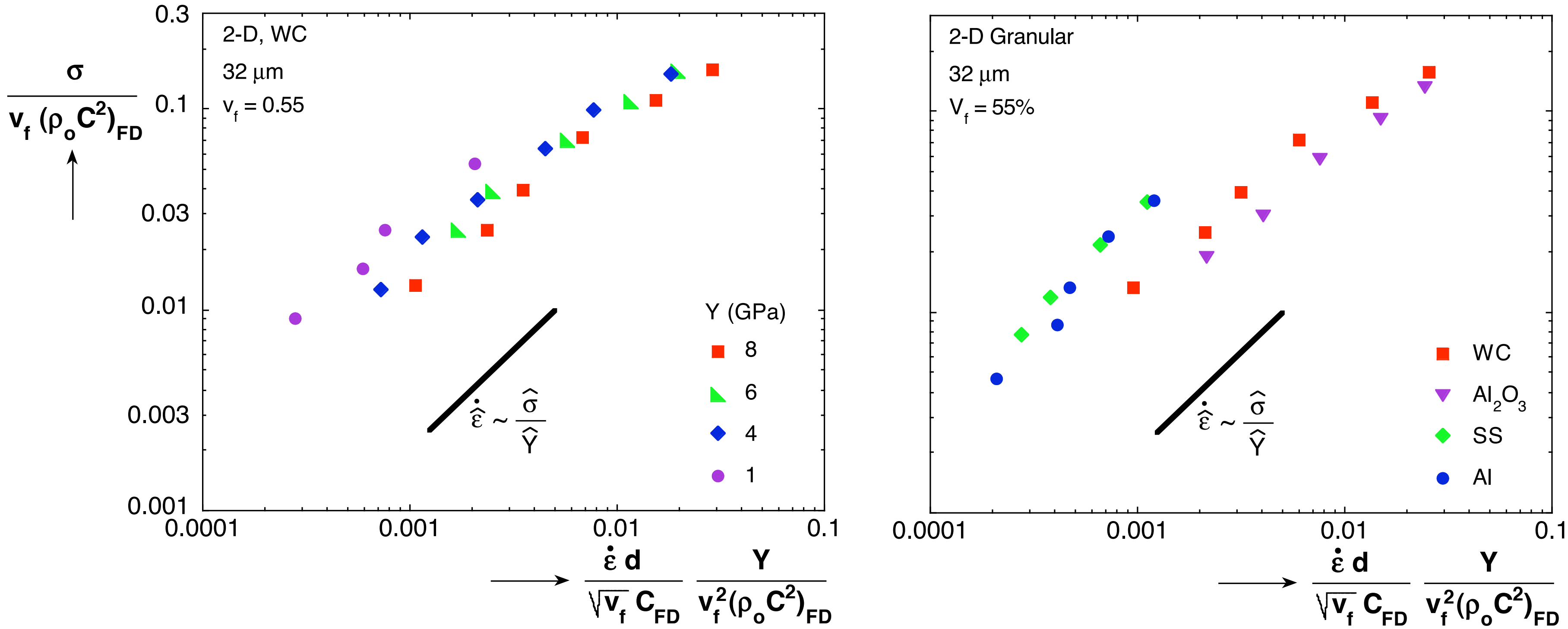




- non-planar shock structure
- CTH simulations reproduce first power scaling
- some dependence on Y, strong material dependence
- non-dimensionalization suggested by Grady (2010):

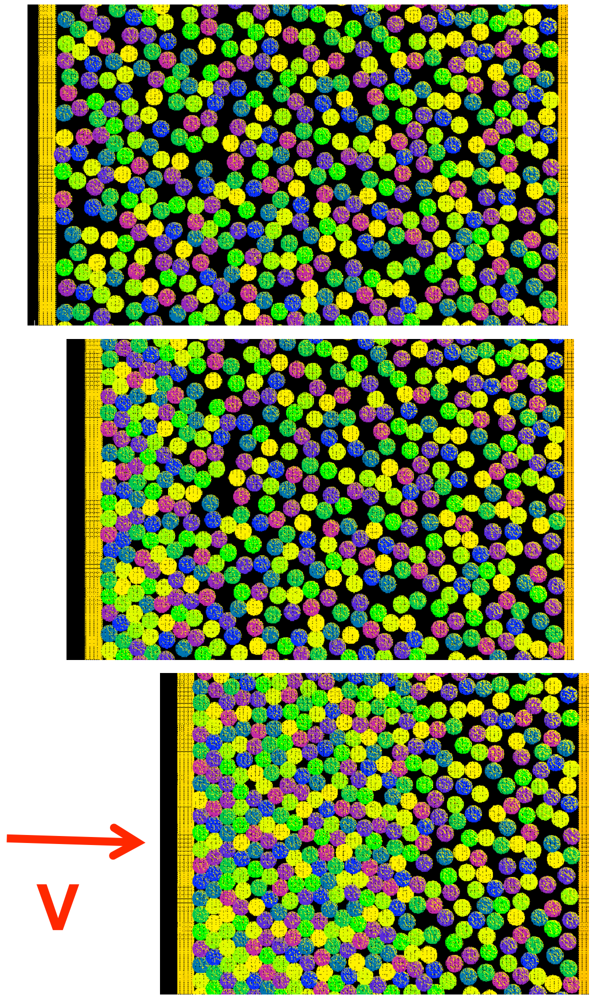
$$\frac{\sigma}{\dot{\varepsilon}} \propto \left(\frac{\rho_o}{\rho_s}\right)^m \sqrt{\rho_o\, d^2\, \sigma_c}$$

Non-Dimensionalization of CTH Results

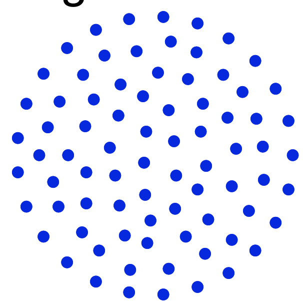


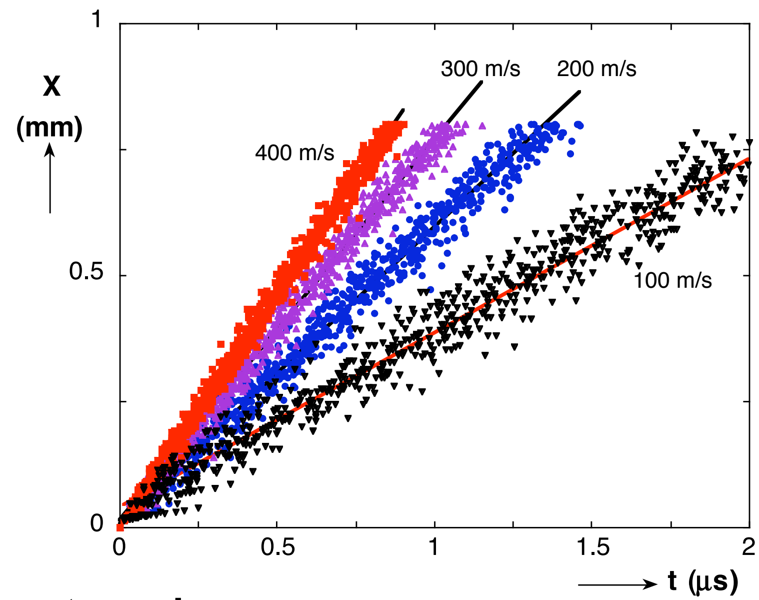
- scale wave speeds by square root of volume fraction (suggested by Steinberg, some validation by Bless)
- Y needed to collapse data, though metals and ceramics separated somewhat

Results from a Particle-Based Peridynamics Code



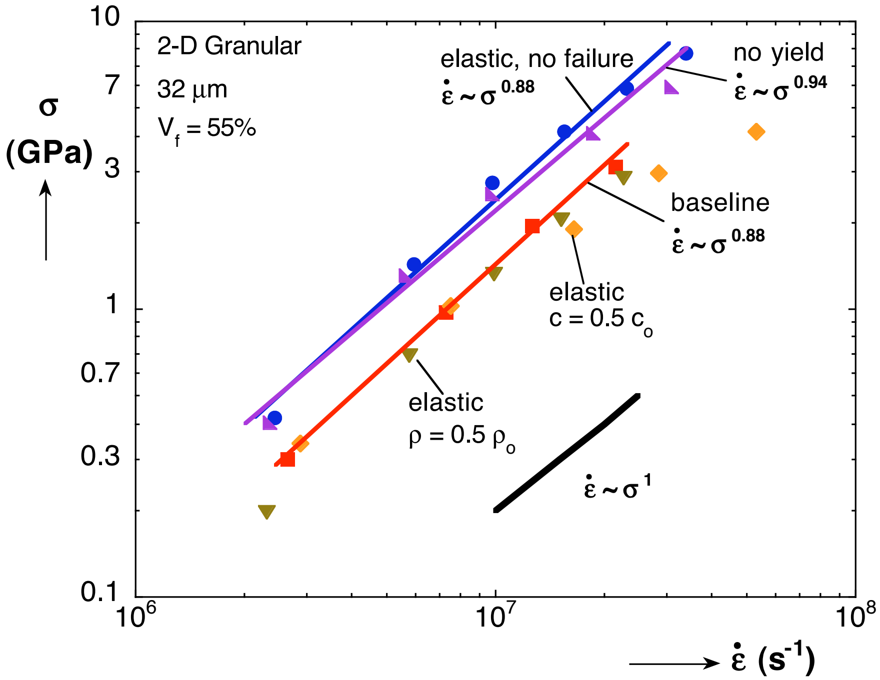
discretization of grains

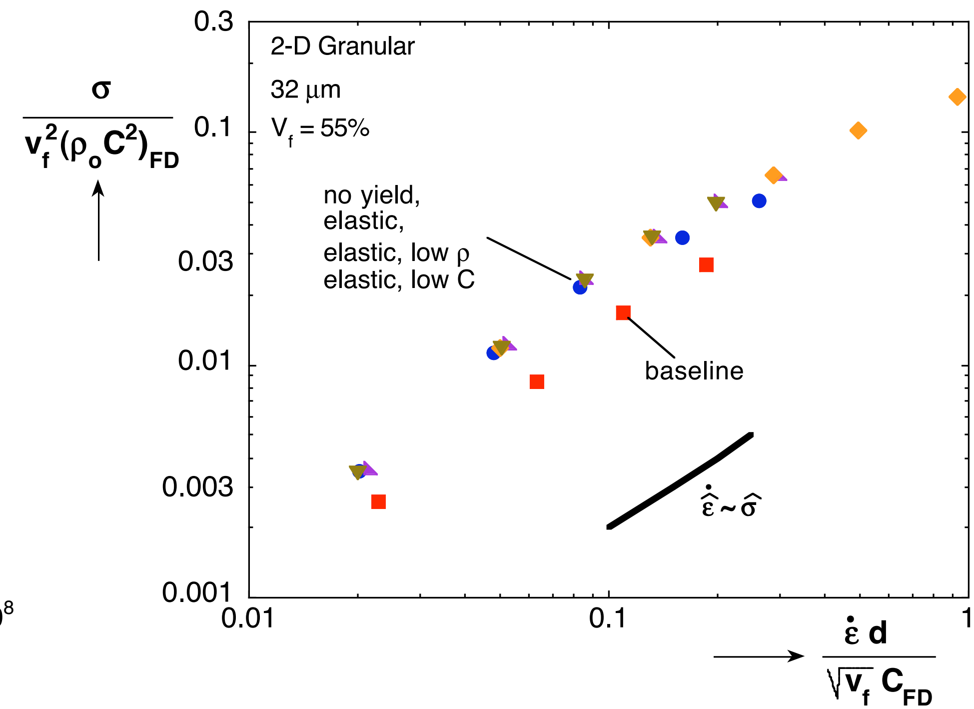




- waves are steady
- wave speed increases with V
- width of band decreases with V
- elastic simulations yield same scaling
  - Grady's scaling doesn't work

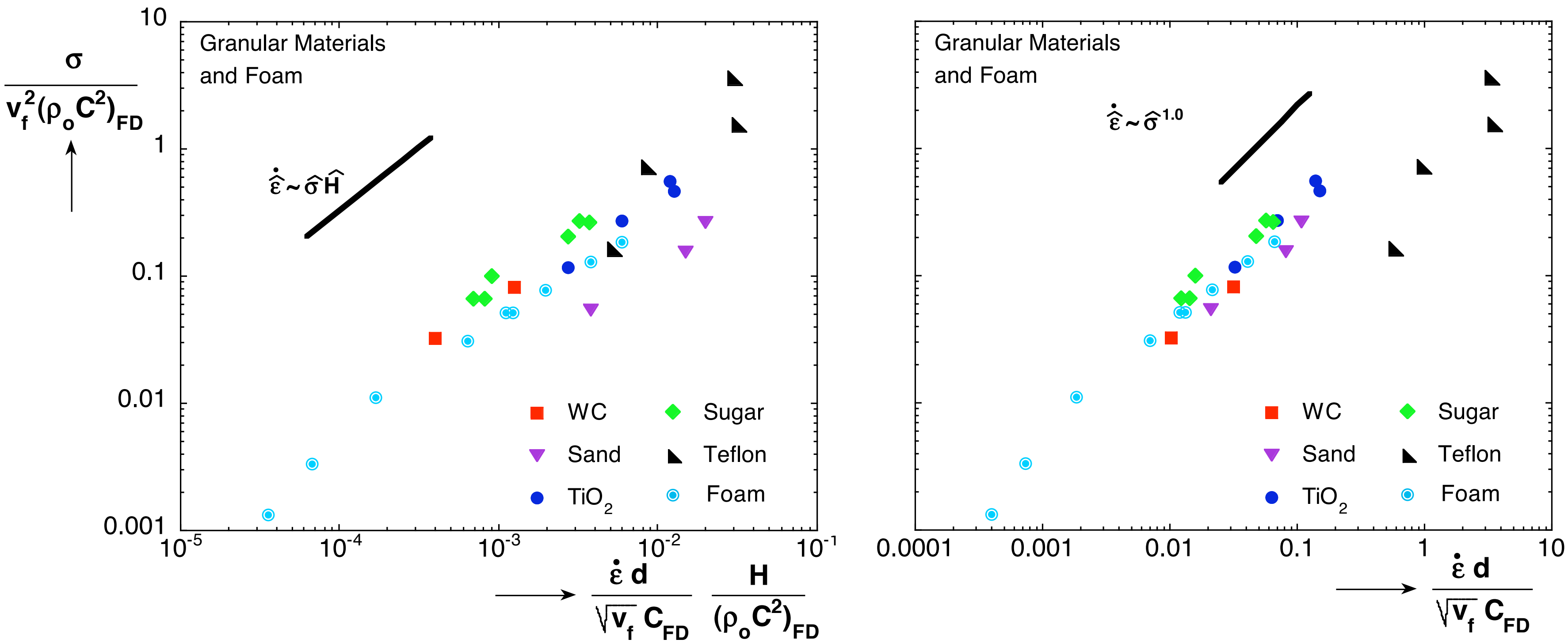
Non-Dimensionalization of Peridynamics Results





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

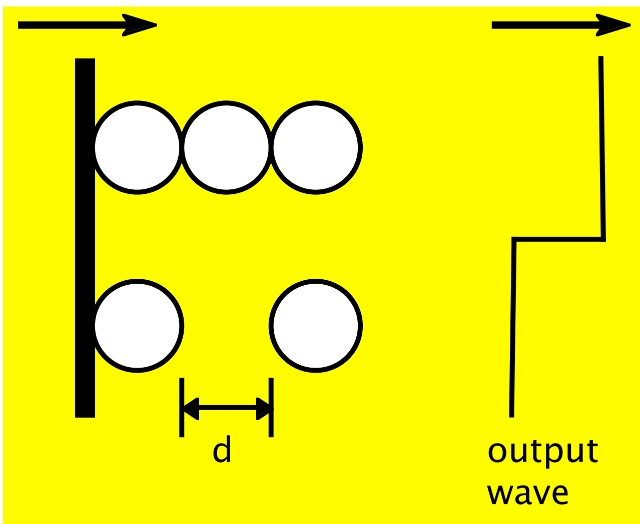
Non-Dimensionalization of Experimental Results



- use hardness (H) as characteristic strength
- does volume fraction enter in separately?
- ceramics collapsed better without H, teflon collapsed better with 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)



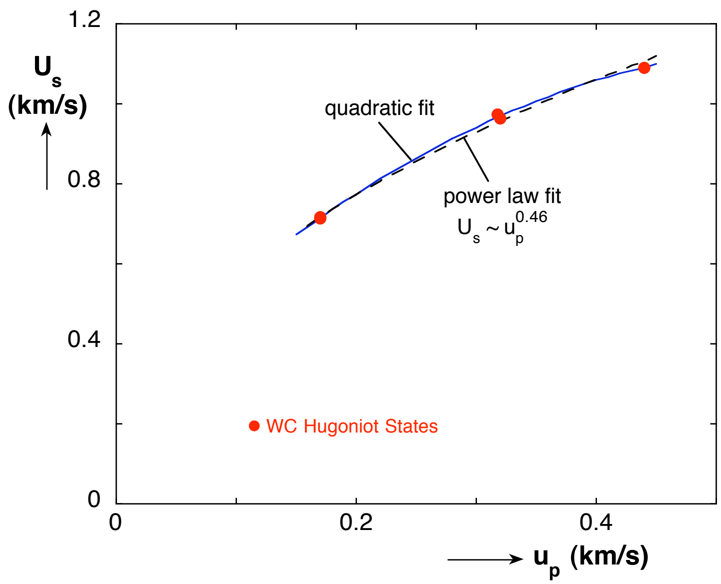
$$\dot{\varepsilon} \propto \frac{\varepsilon}{\Delta t} \propto \frac{u_p / U_s}{d / u_p}$$

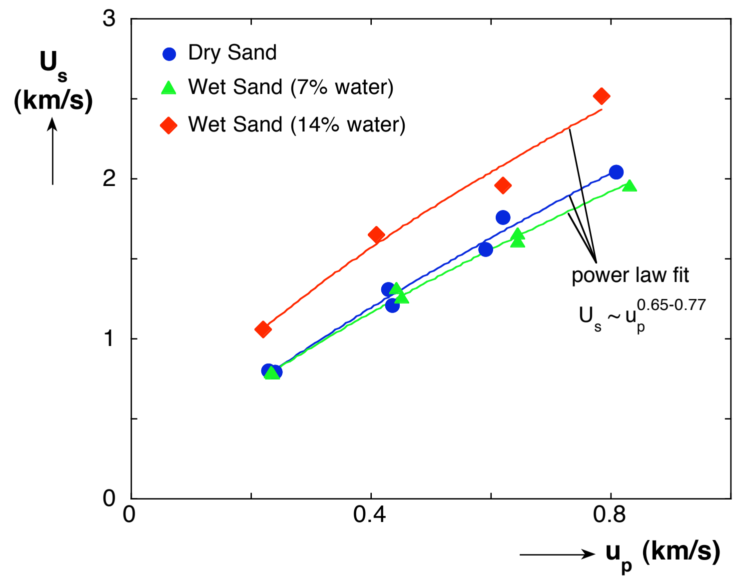
mass traversing pores controls width of shock front

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

A Simple Scaling Argument for Granular Materials (2)

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





$$\text{if} \quad U_s \propto u_p^{0.5}$$

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

$$\text{if} \quad U_s \propto u_p^{0.75}$$

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

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
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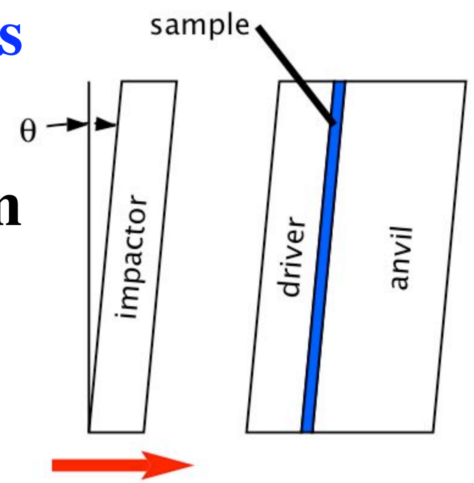
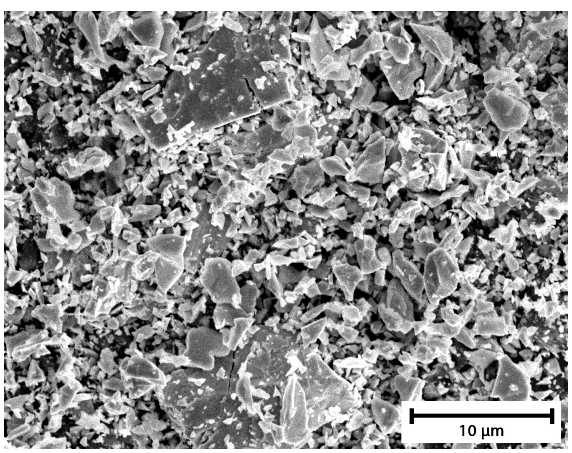
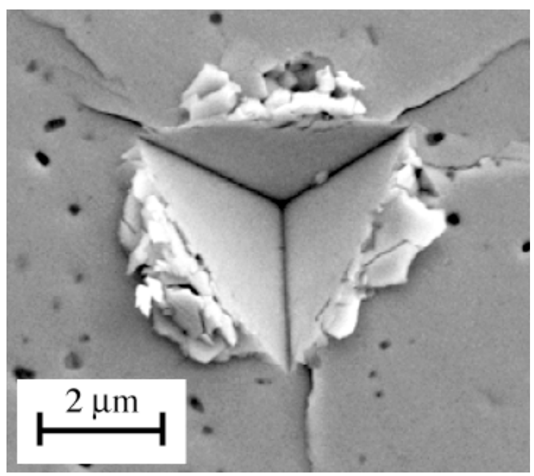
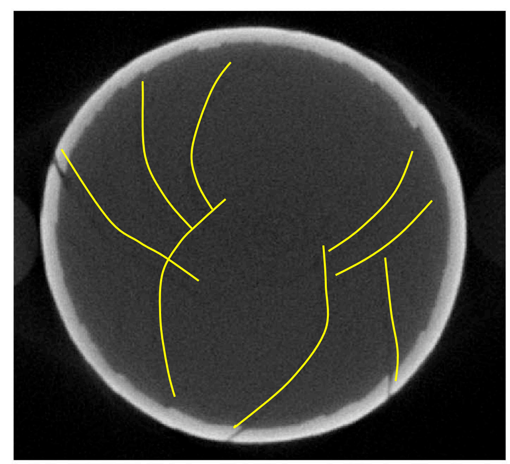
Topics Not Covered

- pressure-shear loading and other approaches for measuring strength
- non-planar and multi-dimensional validation experiments
- nanoindentation of individual grains
- role of particle fracture
- EOS development for granular materials and mixtures in the high-pressure regime









Conclusions

- **planar waves in granular ceramics:**
  - steady waves with very low wave speeds observed
  - dynamic response significantly stiffer than static response for WC; about the same for sand
  - Z machine attains pressures well above those for gas guns
  - shock of porous materials probes thermal behavior of materials
- **mesoscale simulations:**
  - nonuniform stress distribution (force chains) and lateral motion
  - 2-D and 3-D results comparable but differences in distributions
  - particle methods or other techniques needed for missing physics
  - may be suitable for some macroscopic simulations
- **scaling of waves:**
  - strain rate scales with stress to 1^{st} power in granular materials due to mass transport across pores
  - non-dimensional groups identified for heterogeneous materials

Acknowledgements

J.P. Borg - mesoscale modeling

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

numerous technicians and support staff are essential to facility operations