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Dynamic Behavior of Granular Ceramics: Experiments and Simulations

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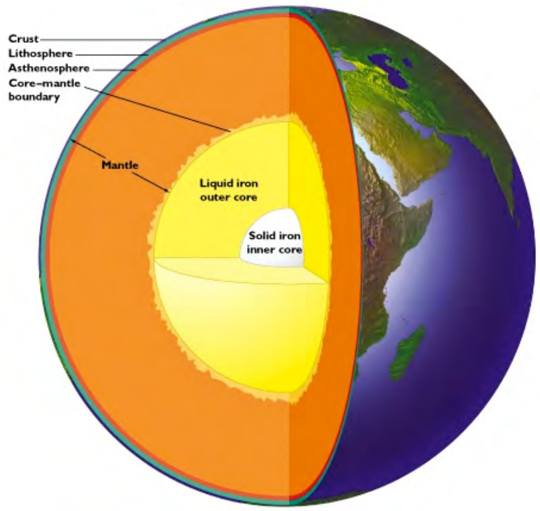
Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

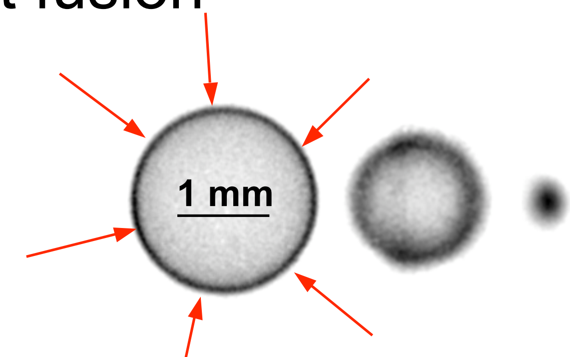
Outline of Talk

- Introduction to shock and high-pressure physics
  - -Motivation
  - -Fundamentals of shock waves
  - -Experimental techniques and applications
- Dynamic behavior of granular materials
- Dynamic behavior of polycrystalline metals
- Conclusions

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

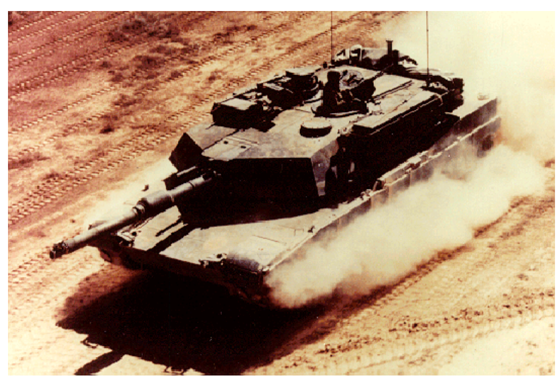


- planetary science applications (P~360 GPa, T~7000 K)
- materials synthesis (diamond, boron nitride, powder metallurgy, etc.)
- blasting for oil and mineral extraction
- inertial confinement fusion



X-ray driven capsule implosion

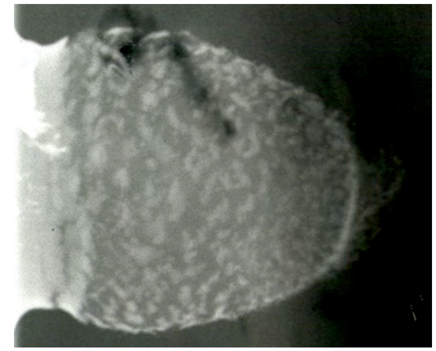
- weapons applications (armor, energetics, warheads, penetrators, etc.)
- exobiology (panspermia)



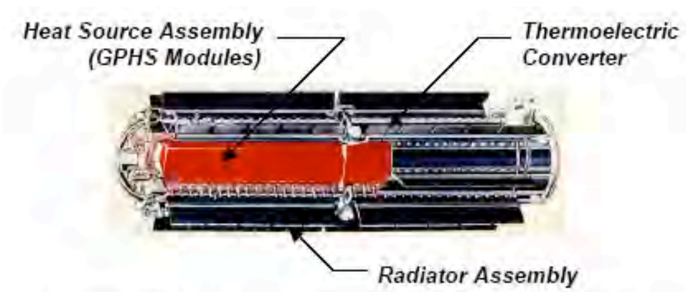
Applications of Shock and Impact Physic

Pluto New Horizons

- impact of asteroids or orbital debris (V=8-15 km/s)
- launch debris (foam, ice, etc.)
- launch safety for radiological materials (RTG’s) or reactors (Prometheus mission)



hypervelocity impact

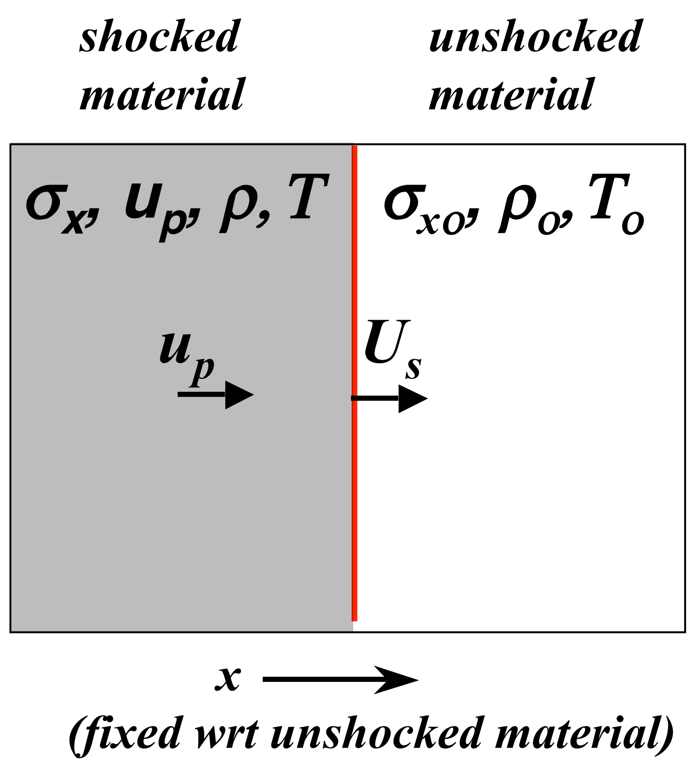


- internal blast
- runway debris & small arms fire
- military aviation and weapons design

SWRI foam impact expt.

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 Hugoniot

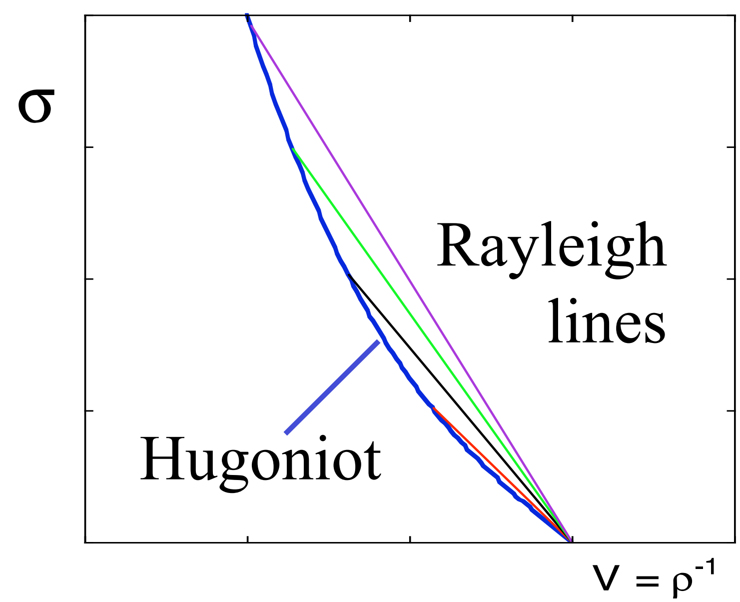
- Five variables: $\boldsymbol{\sigma}_x$, $\boldsymbol{u}_p$, $\boldsymbol{U}_s$, $\boldsymbol{\rho}$, and $\boldsymbol{E}$
- Three conservation relationships (Rankine-Hugoniot jump conditions)
  - By measuring two variables (typically $\boldsymbol{\sigma}_x$, $\boldsymbol{u}_p$, or $\boldsymbol{U}_s$), 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: $E - E_o = 0.5\sigma_x (V_o - V)$

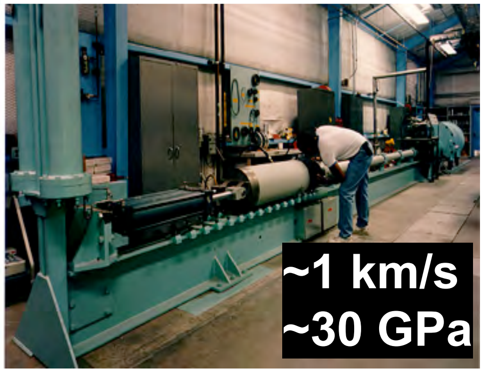


material loads along the Rayleigh line, so the Hugoniot is a <u>collection of end states</u>, not a material response curve

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

How Are Shock Waves Generated?

Single Stage Gun 100mm



Propellant Gun 89mm

Two-Stage Gun 29mm

<u>gas guns</u>

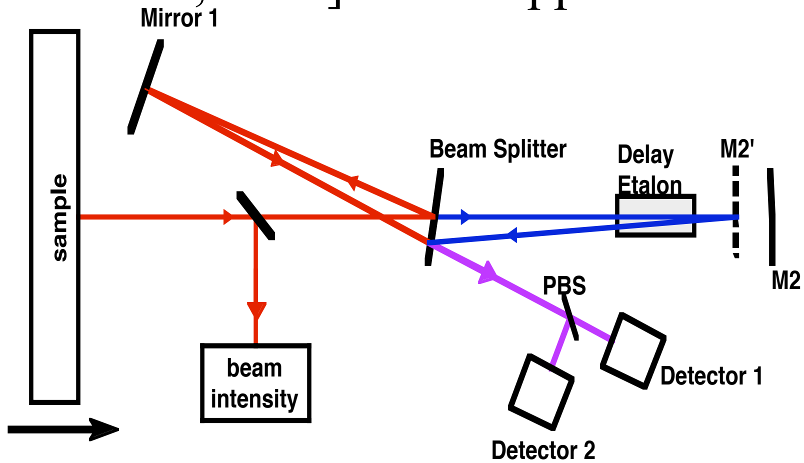
- launch thin plates (mm’s) at high velocities
- well-posed, repeatable initial conditions
- sample is in uniaxial ***<u>strain</u>***
- used to study material behavior at high pressures and strain rates
- usable in laboratory setting

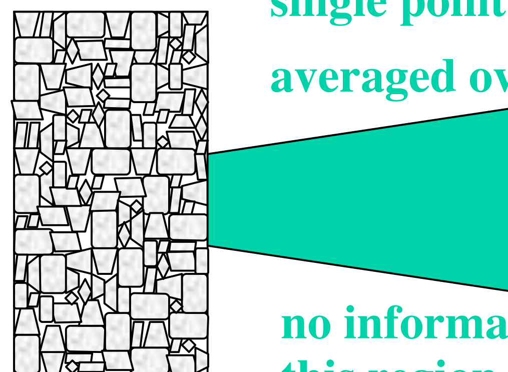
Three-Stage Gun 17mm

also: explosives, lasers, magnetic loading (Z)

Example: Using the Line-VISAR to Probe Material Heterogeneity

Velocity Interferometer System for Any Reflector (VISAR) [Barker & Hollenbach, 1972] uses Doppler shift to measure velocity history

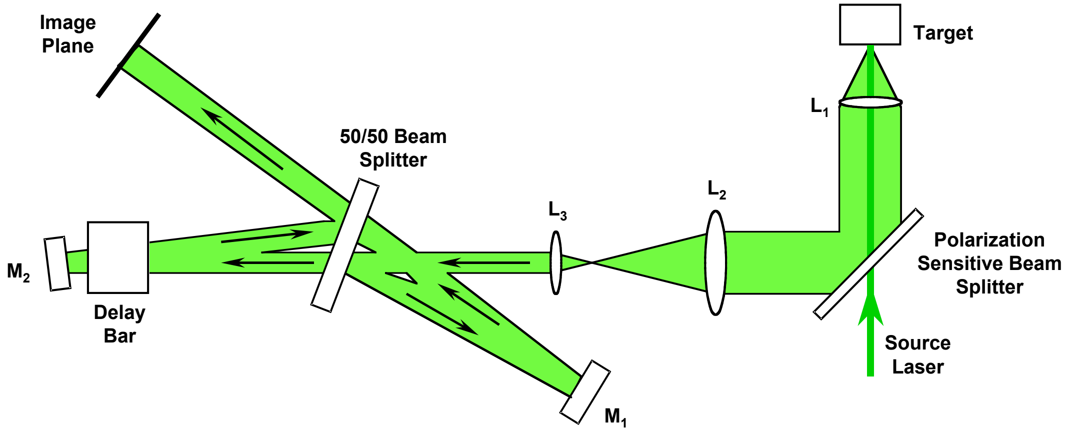




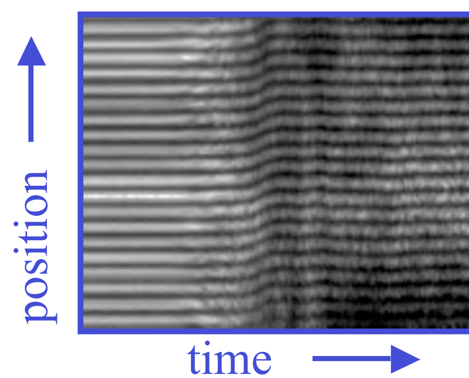
single point measurement

averaged over 50-200 μm

no information outside this region



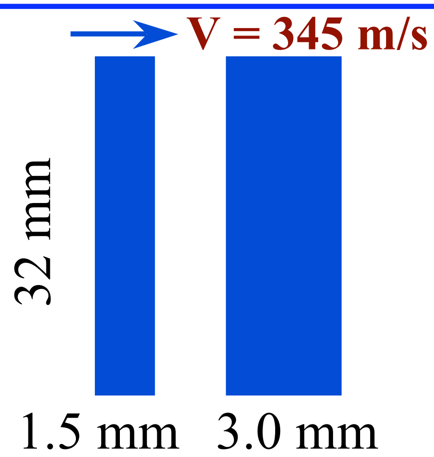
streak camera image

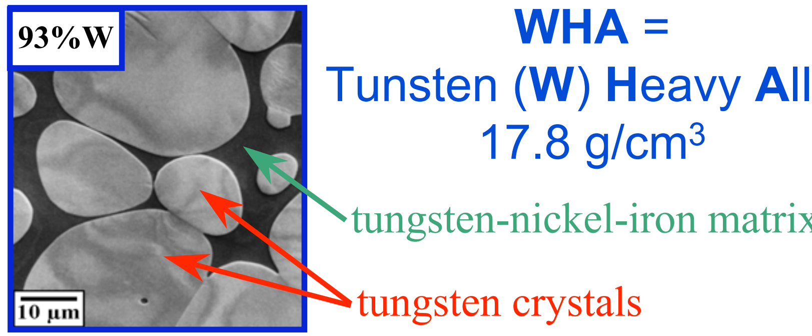


resolution as high as ~10 µm can be achieved along the line

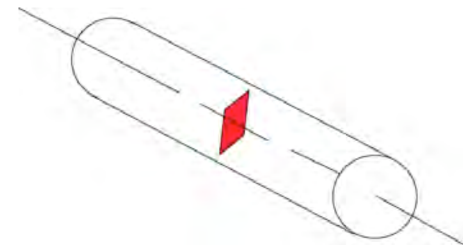
only practical way to resolve this scale in dynamic experiments

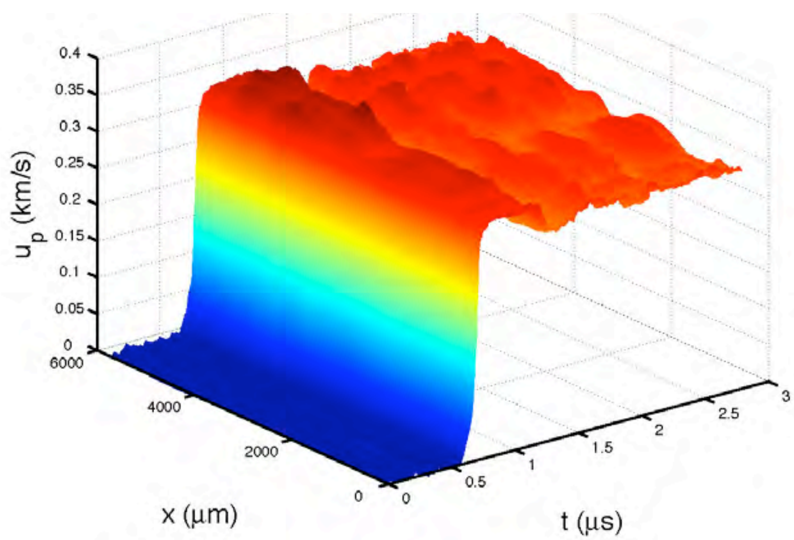
WHA Impact Experiment

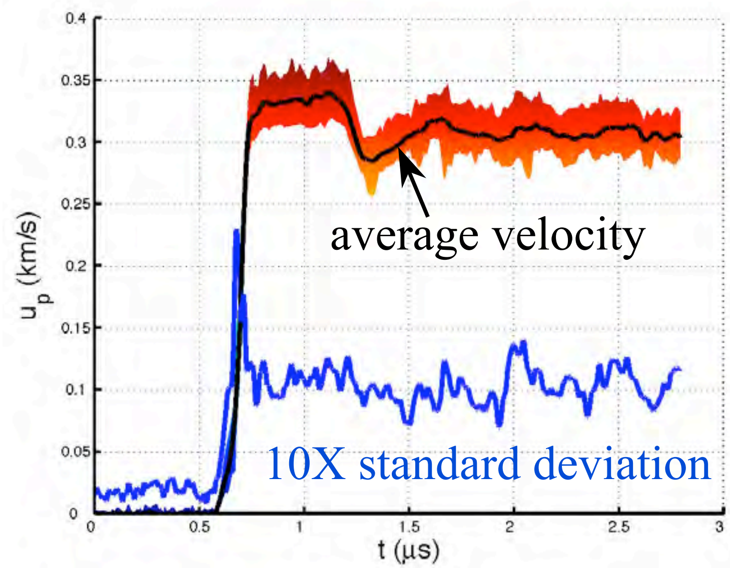




WHA =
Tunsten (**W**) **H**eavy **A**lloy
17.8 g/cm^3



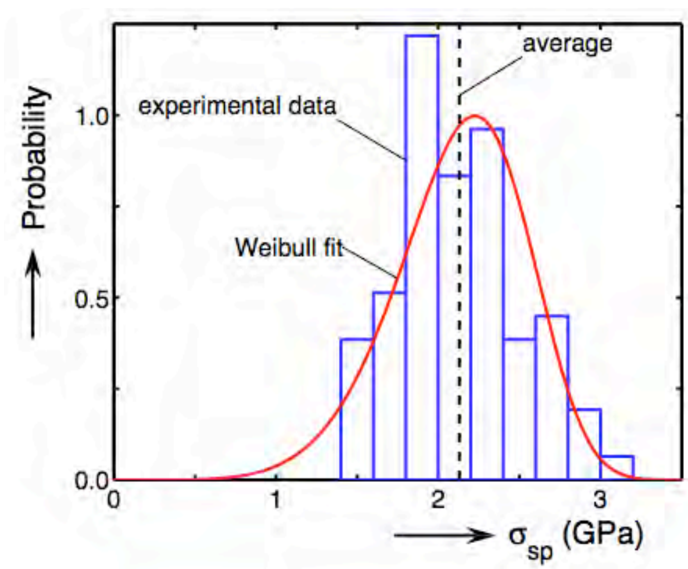




Vogler, T.J., and Clayton, J.D., “Heterogeneous deformation and spall of an extruded tungsten alloy: plate impact experiments and crystal plasticity modeling,” *J. Mech. Phys. Solids* (submitted).

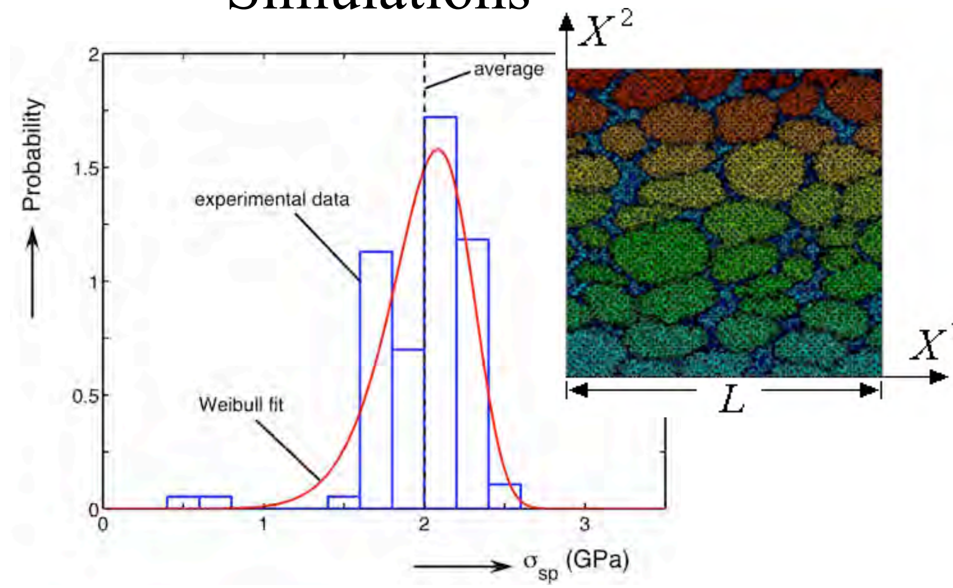
Distributions of Spall Strengths

Experiments



- significant variation observed in spall strength distributions
- Weibull distribution fits data well
- Weibull modulus, $\beta = 6.7$

Simulations

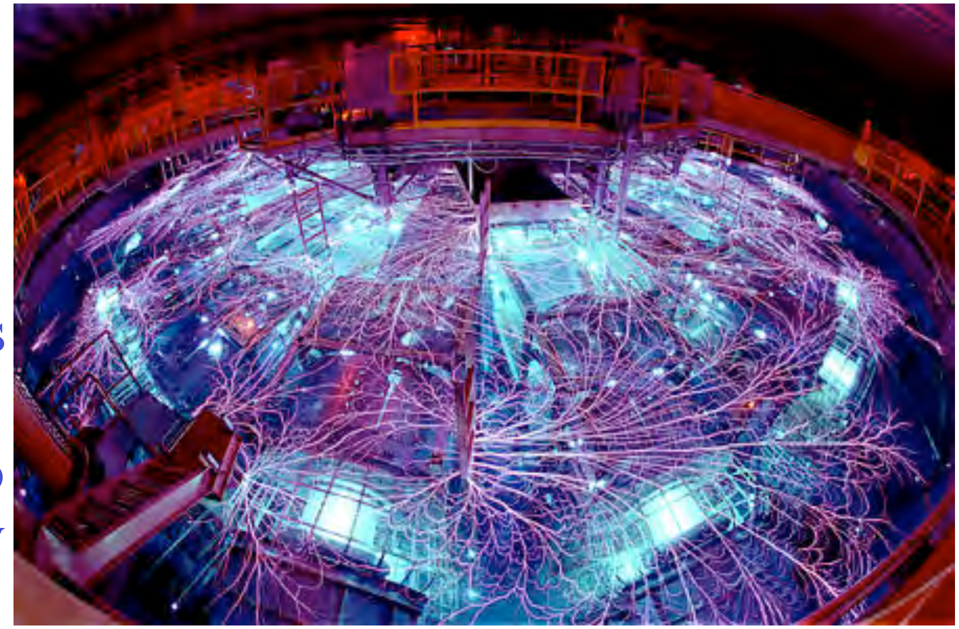


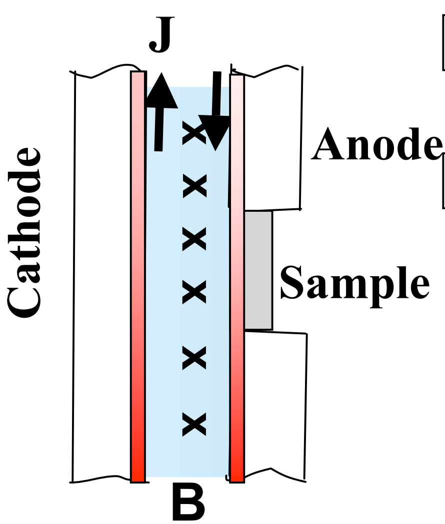
- 2-D crystal plasticity model with cohesive zone elements at W grain boundaries
- no variability in cohesive zone elements, but $\beta = 8.7$

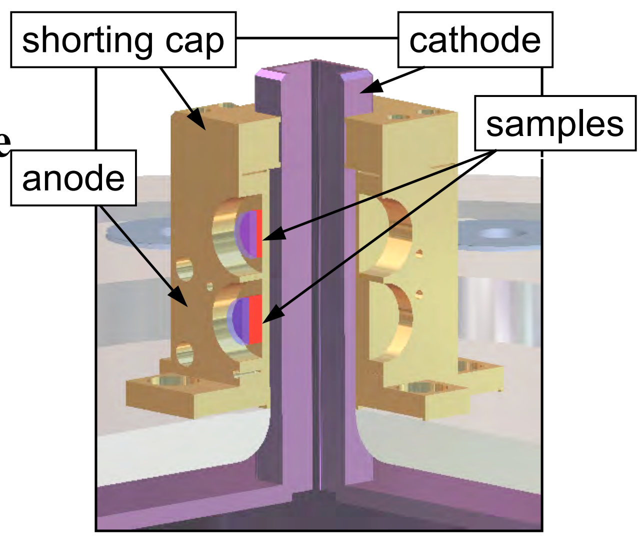
Clayton, J.D., *J. Mech. Phys. Solids* **53**, 2005.
Clayton, J.D., *Int. J. Solids Structures* **42**, 2005.

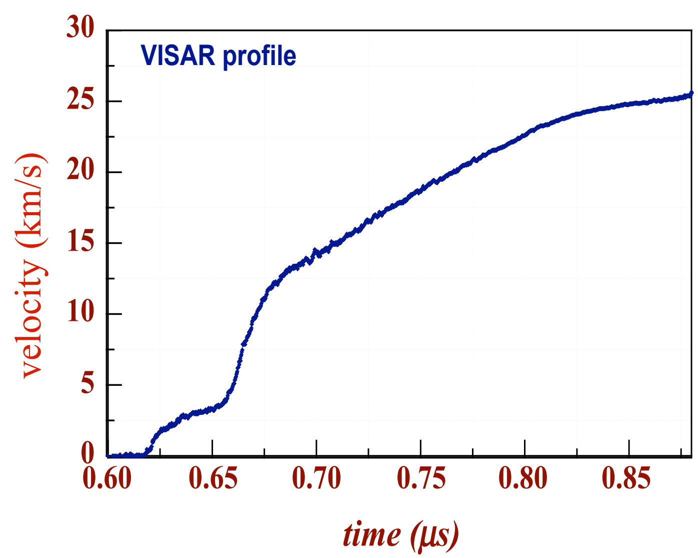
Z Machine Provides New Capabilities for High Pressure Experiments

- Designed for ICF applications
- Generates >20 MA over 100’s of ns, 11.5 MJ of stored energy
- Current generate magnetic forces
- Magnetic forces create smooth waves in materials
- Waves used for isentropic loading (to 250 GPa) and to launch high-velocity flyer plates (to 34 km/s = 1.2 TPa)

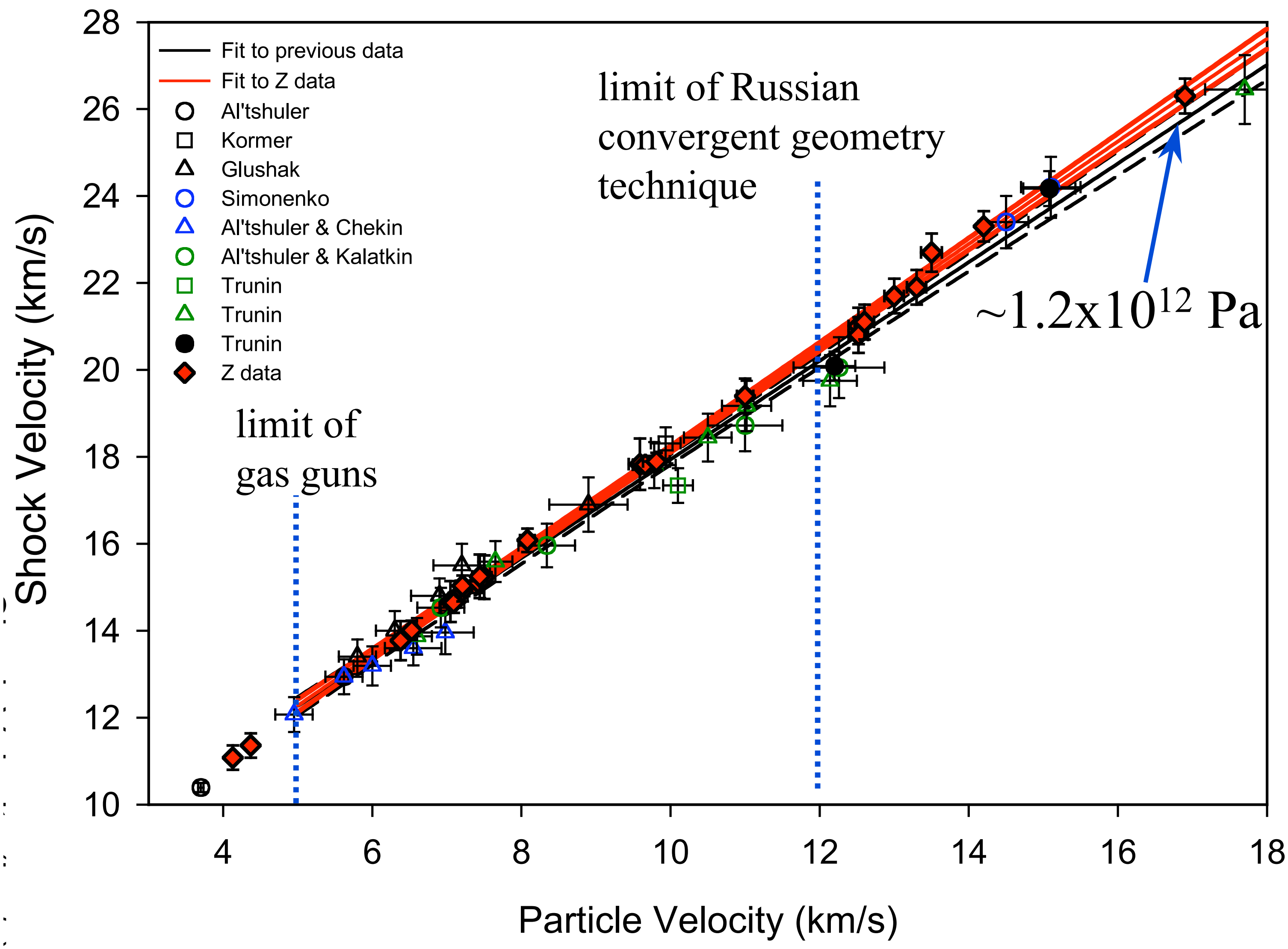








Example: Shock Hugoniot of Aluminum



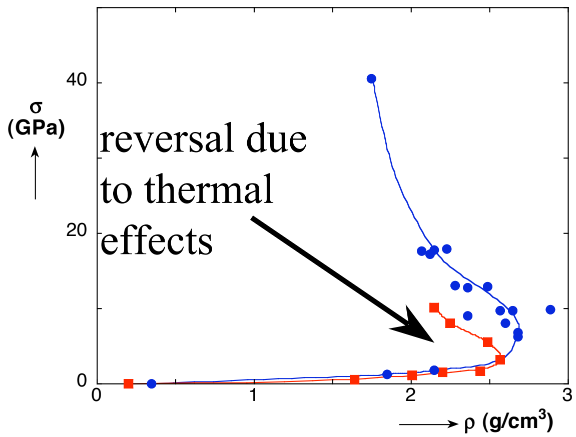
Outline of Talk

- **Introduction to shock and high-pressure physics**
- **Dynamic behavior of granular materials: experiments**
  - **Background**
  - **Static compaction results**
  - **Plate impact experiments on tungsten carbide (WC) powder**
  - **Validation experiments**
- **Mesoscale simulations of granular materials**
- **Conclusions**

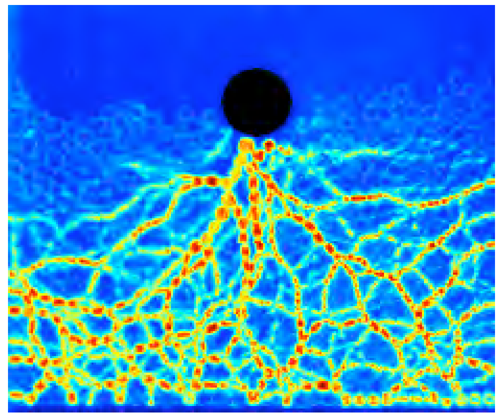
Vogler, T.J., Lee, M.Y., and Grady, D. E. (2007). “Static and dynamic compaction of ceramic powders,” *Int. J. of Solids & Structures* **44**, 636-658.

Background on Dynamic Behavior of Granular Materials

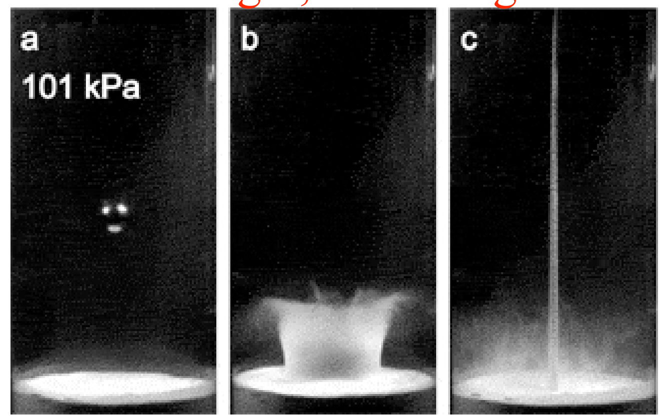
porous SiO_2, Trunin et al.



B. Behringer, Duke



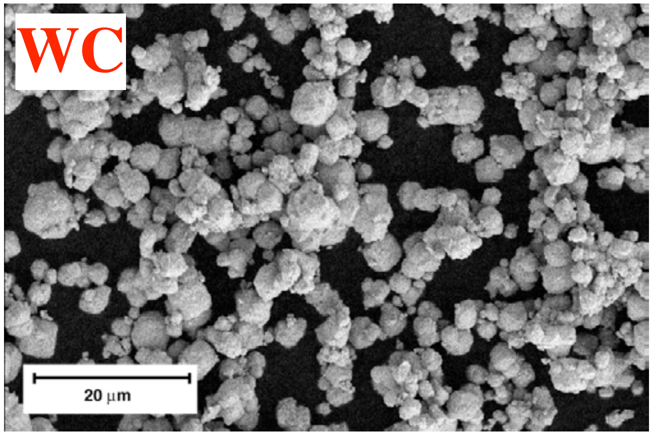
H. Jaeger, U. Chicago



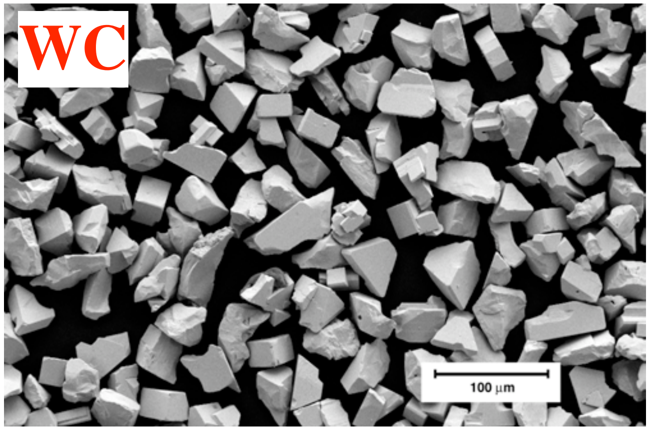
- granular materials display a rich variety of behaviors
- significant experimental and modeling challenges
- extensive quasi-static and low-velocity impact work
- determine thermal behavior through P-V work (Trunin, 2004)
- consolidation studied extensively to optimize loading, etc.
- partial compaction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

Investigation of Dynamic Behavior of Granular Ceramics

- investigate dynamic compaction behavior of ceramic powders (primarily tungsten carbide and sand to-date)
- 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

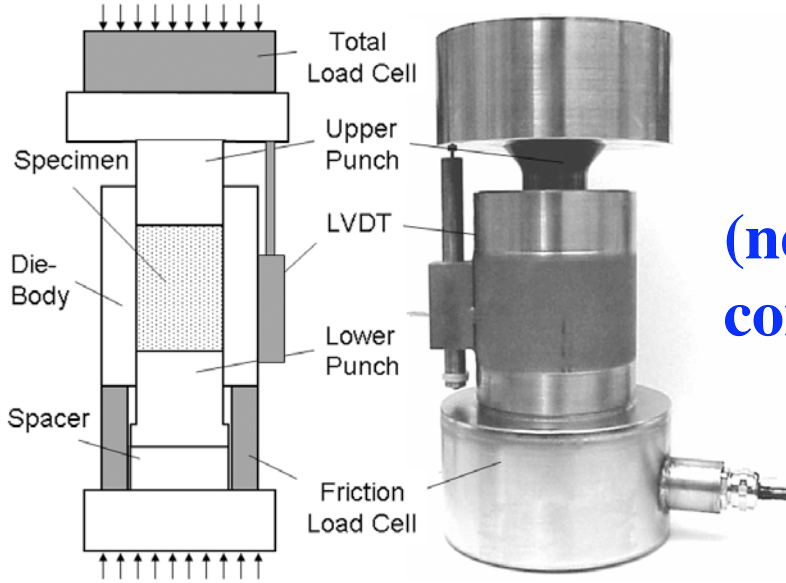


diffusion process yields agglomerations of smaller particles



Kennametal melt process yields individual single crystals

Static Die Compaction Experiments



(nearly) uniaxial strain compaction to ~1.6 GPa

<u>Objectives</u>

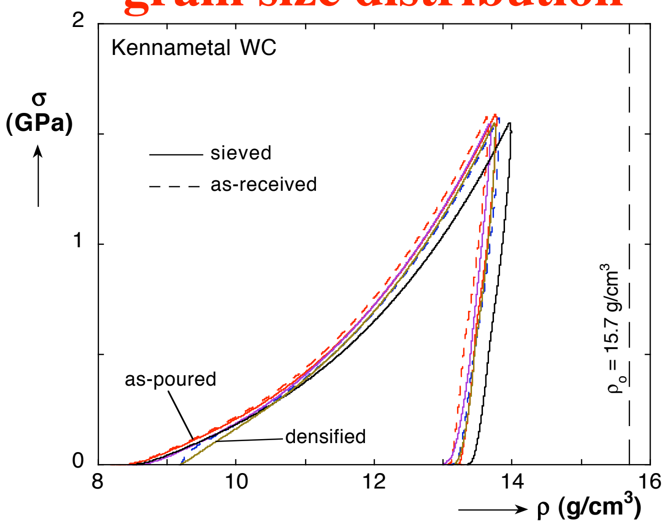
- **Determine compaction curve functional form**
- **Examine effects of experimental parameters (grain size, grain size distribution, grain shape, initial density, loading path, etc.)**
- **Correlate with dynamic results**

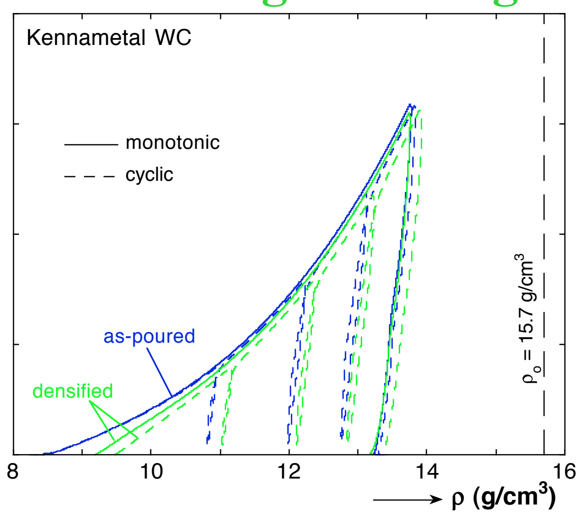
M. Lee, 06117

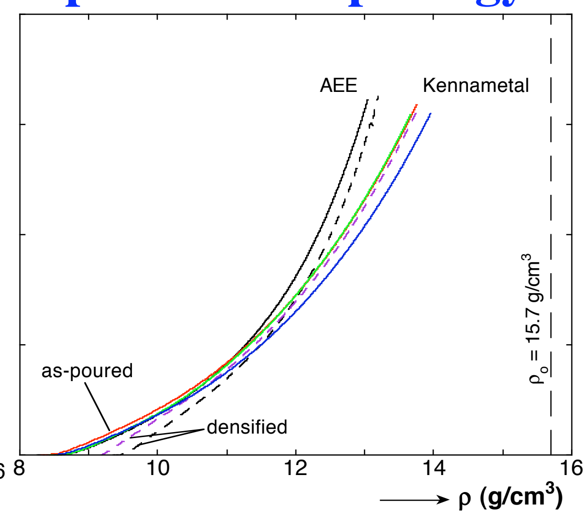
Static Compaction Results for WC

evaluate effects of important variables on loading response

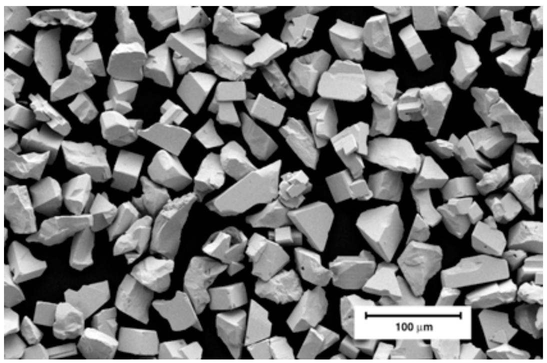
grain size distribution | **unloading/reloading** | **particle morphology**



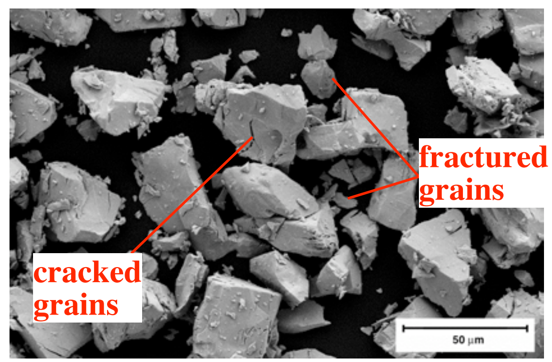




pre-compaction

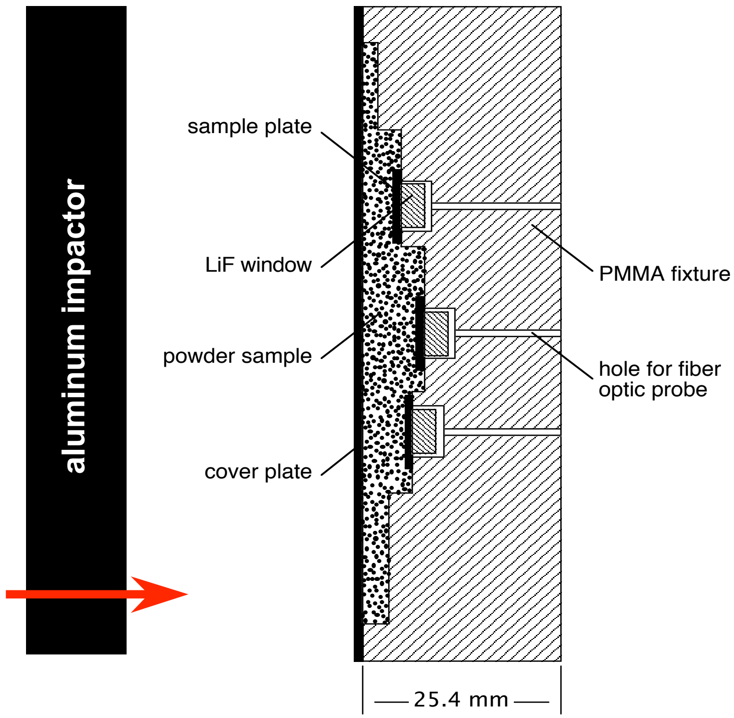


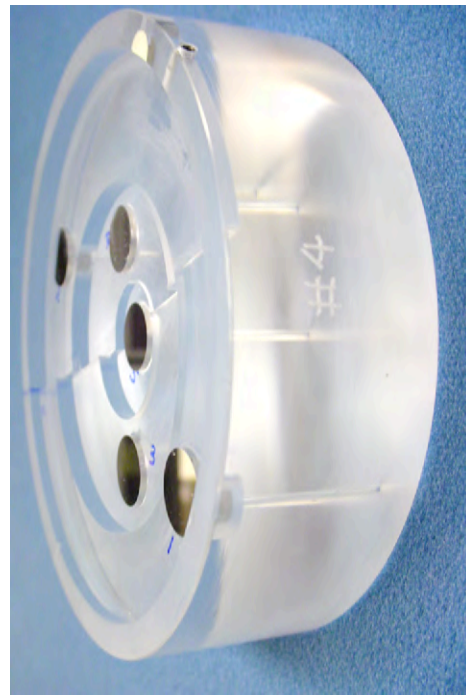
post-compaction



M. Lee, 06117

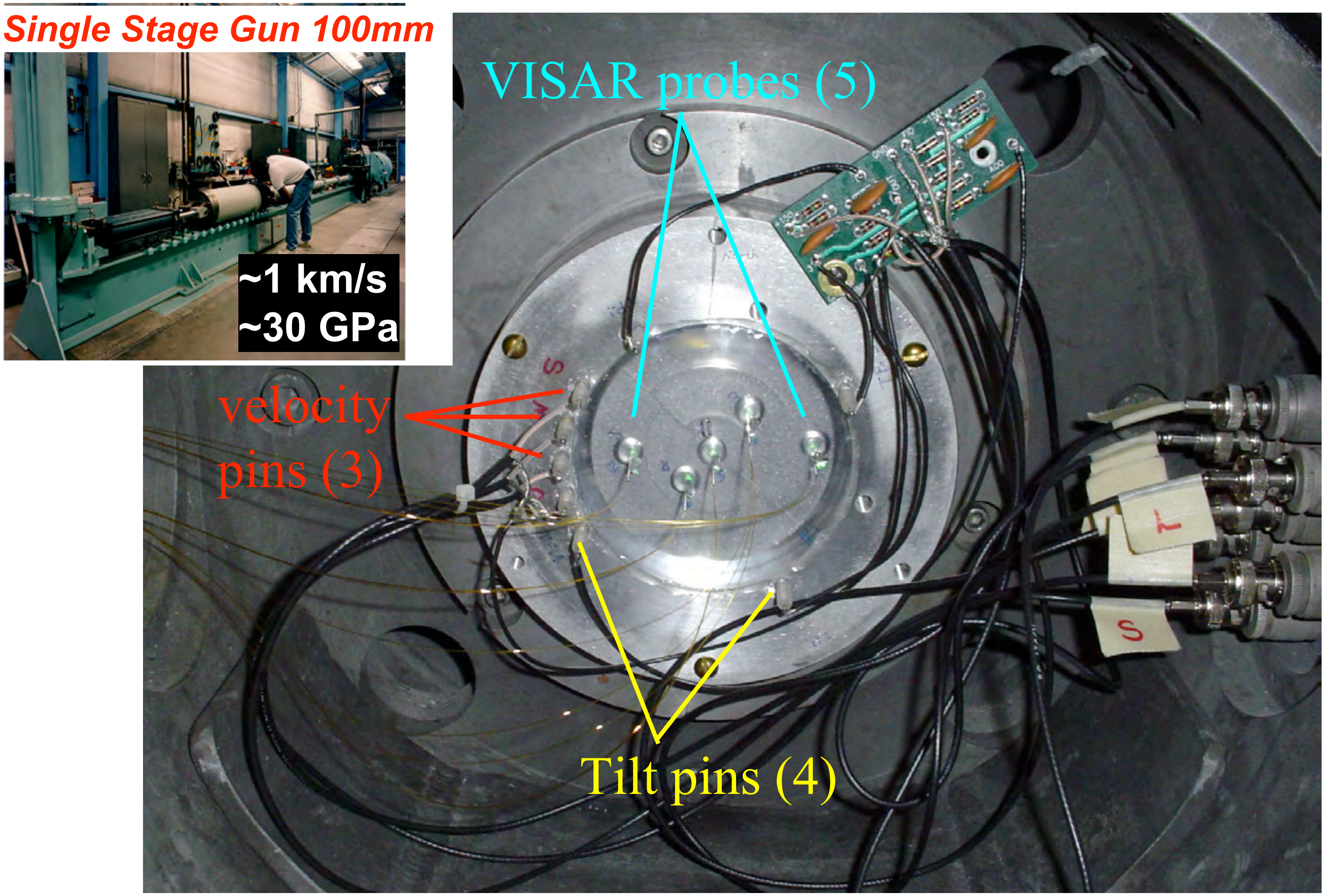
Gas Gun Experiments on WC



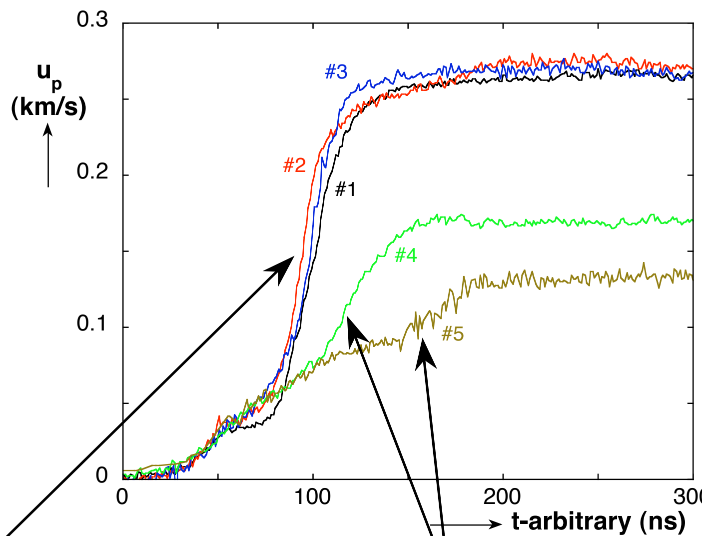


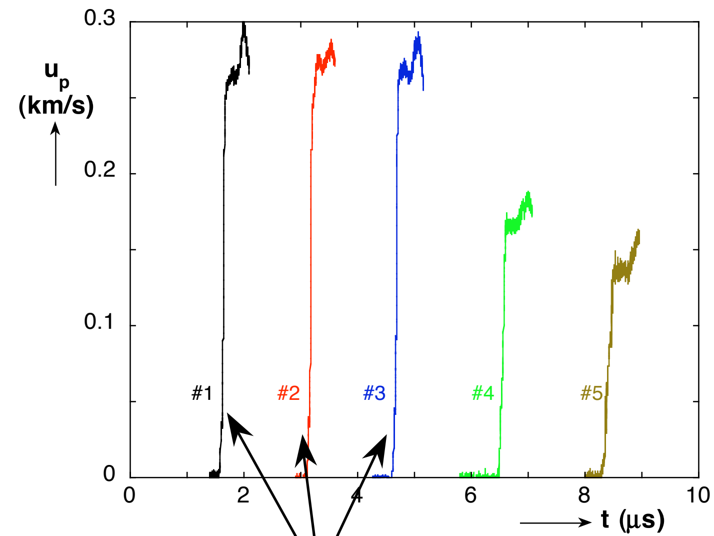
stepped impactor design gives multiple sample thicknesses on the same experiment for accurate determination of shock velocity as well as uniform powder density

Target Mounted in Gas Gun



Measured Steady Waves





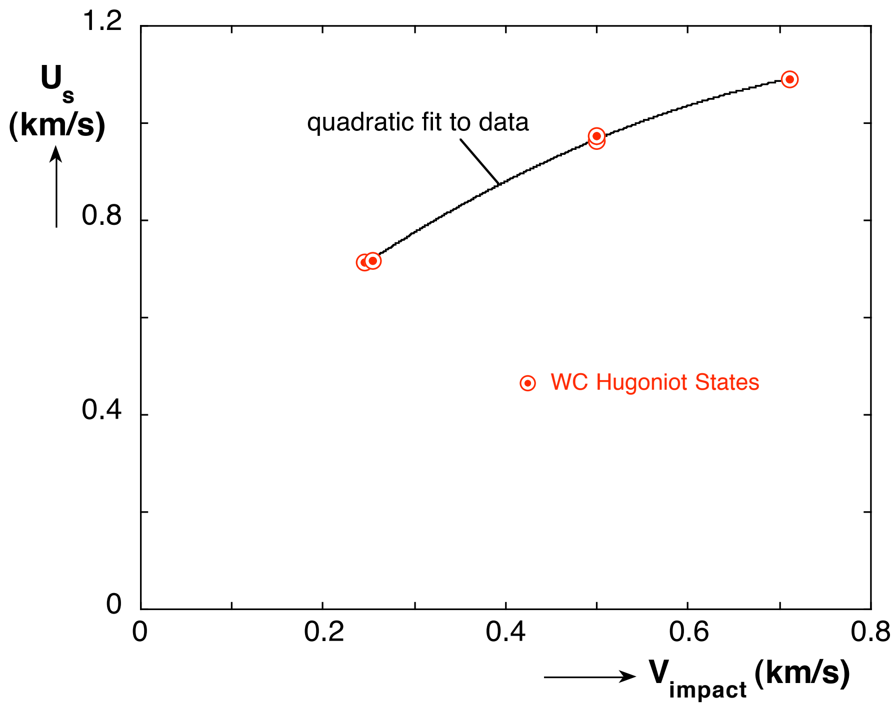
steady, structured waves

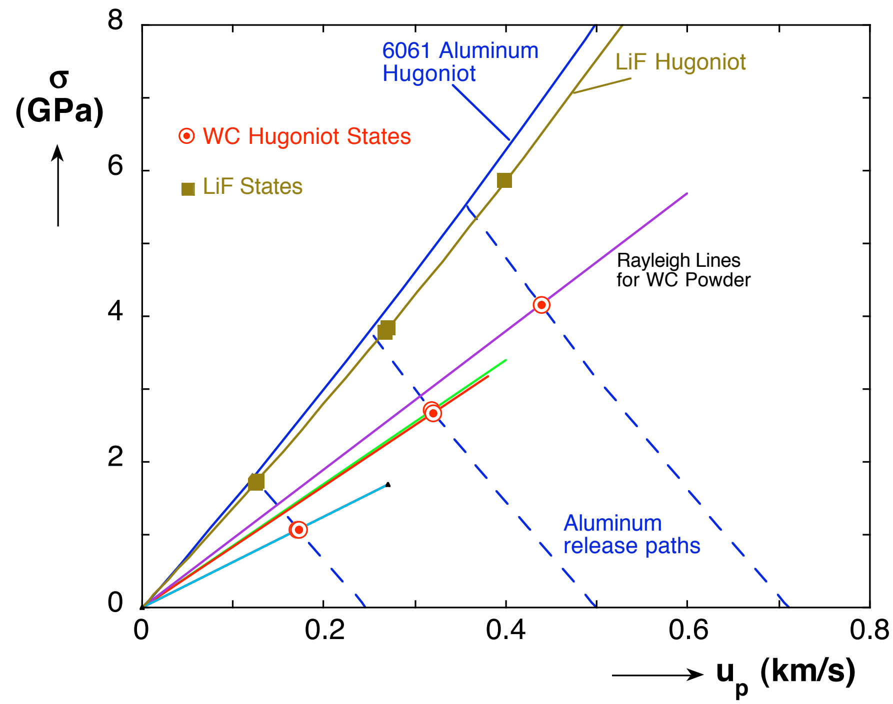
attenuated waves

shock velocity calculated based on powder thicknesses and arrival times

- 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

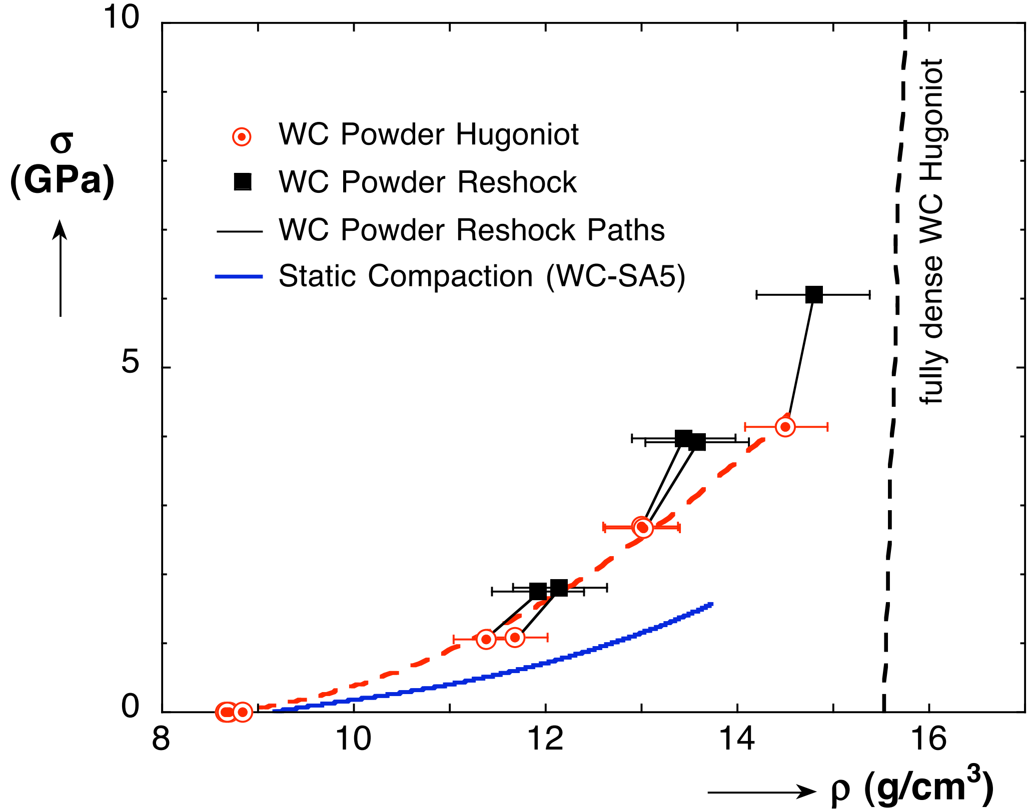
Shock Velocities and Hugoniot States





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

Compaction Response for WC

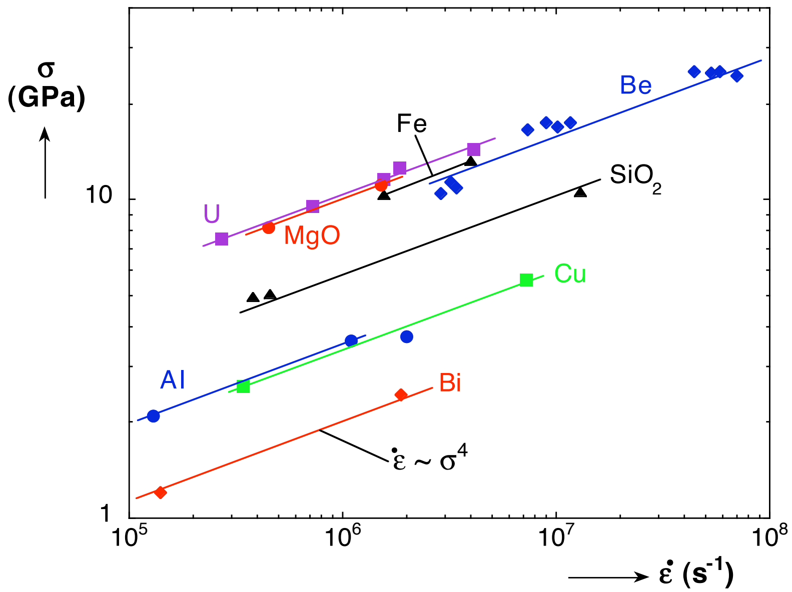


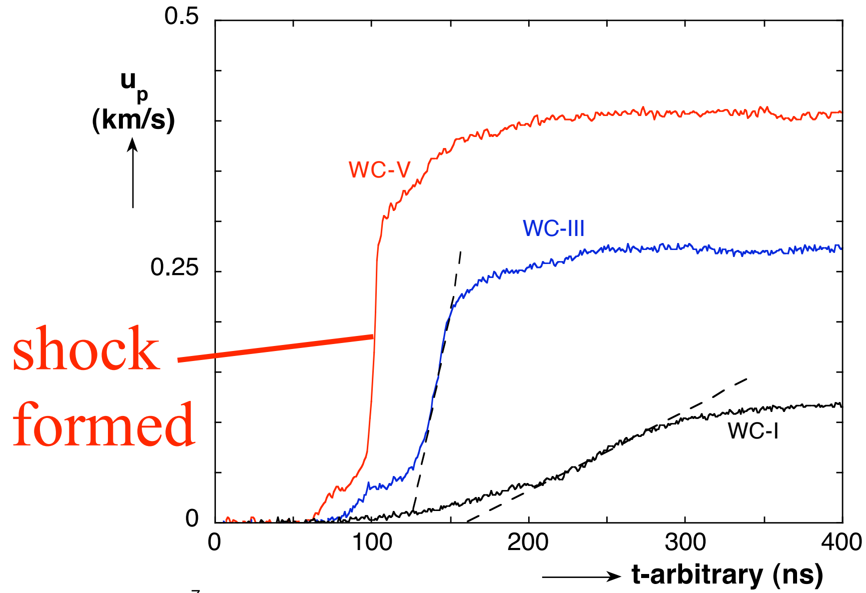
- **dynamic compaction response of WC significantly stiffer than static response**

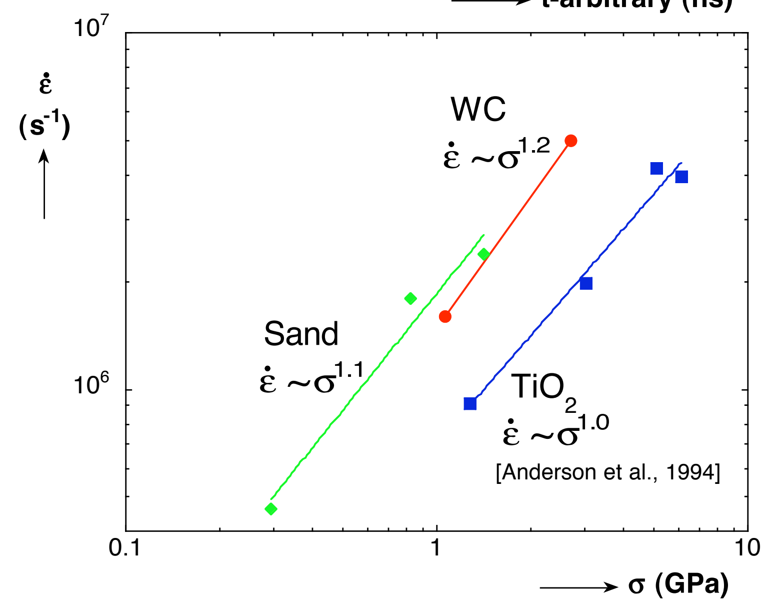
- **first reshock state lies above Hugoniot suggesting elastic response of compacted material**
- **the difference between static and dynamic responses appears to be due to the relatively thin compaction front over which deformation occurs**

Scaling Between Rise Time of Wave and Stress

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



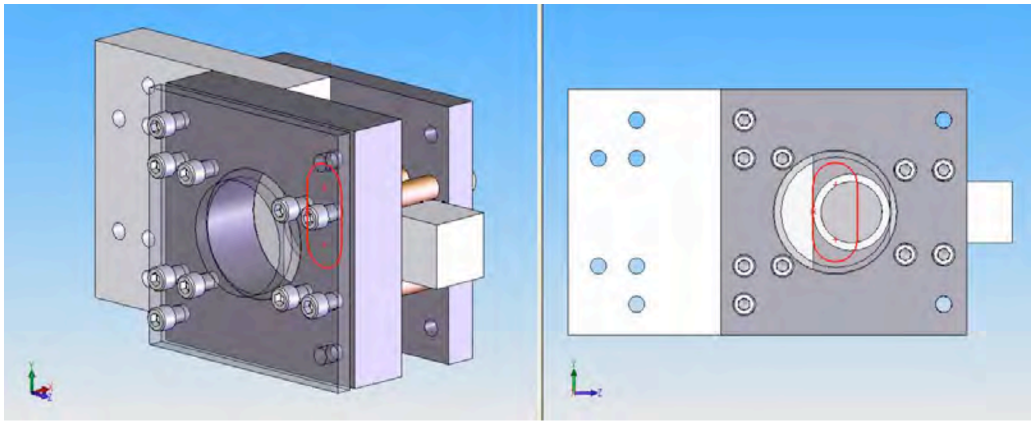


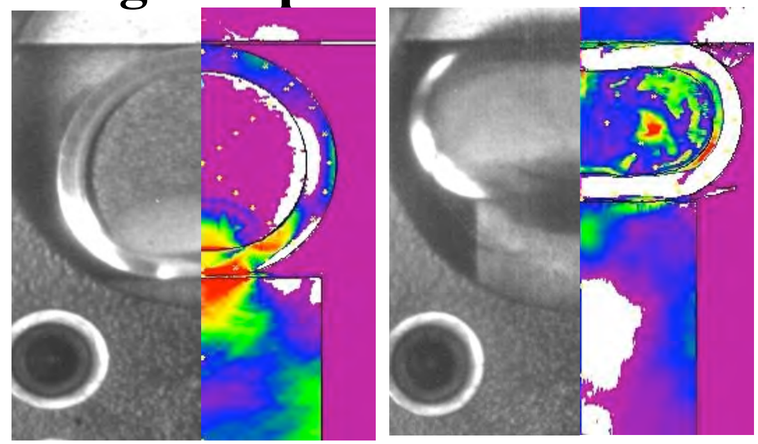


data on three granular ceramics suggest a linear scaling between stress and strain rate

Validation Experiments for Granular Materials

simple, well-controlled experiments providing non-planar data





- explosively compacted cylinders allow comparison with simulations and analytic solutions
- tomographic analysis of compaction underway

challenge is to obtain results that are sensetive to the relevant material behavior and can be accurately measured

Outline of Talk

- **Introduction to shock and high-pressure physics**
- **Dynamic behavior of granular materials: experiments**
- **Mesoscale simulations of granular materials**
  - **Background**
  - **Model set-up and results**
  - **Sensitivity study**
  - **Statistical aspects of mesoscal modeling**
  - **System level results**
- **Conclusions**

Borg, J.P., and Vogler, T.J., "Mesoscale calculations of the dynamic behavior of a granular ceramic," *Int. J. Solids & Structures* (in preparation).

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 compation 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

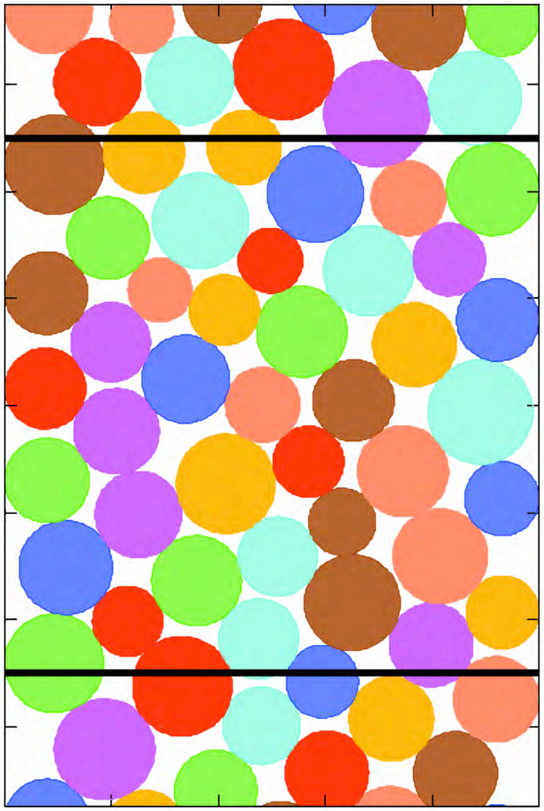
Mesoscale Modeling of Granular Materials (with J. Borg, Marquette University)

- follow approach of Benson et al. for 2-D simulations
- particles idealized as circles (rods) for initial work
- duplicate geometry of experiments except constant velocity boundary condition applied
- run in CTH (explicit Eulerian finite difference code) on 16 processors for ~12 hours with 10-15 cells across particle
- WC modeled with Mie-Gruneisen EOS, elastic-perfectly plastic strength, and failure at a specified tensile stress

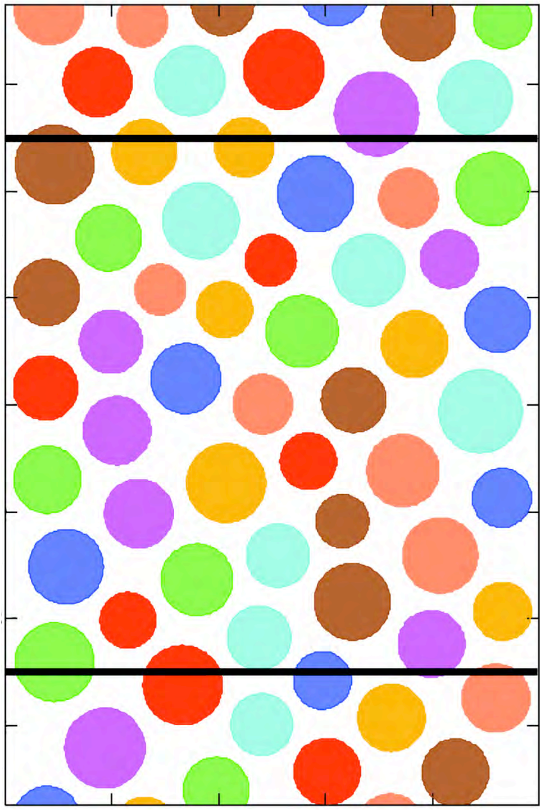
get at underlying physics of granular materials

Generation of Initial 2-D Microstructure

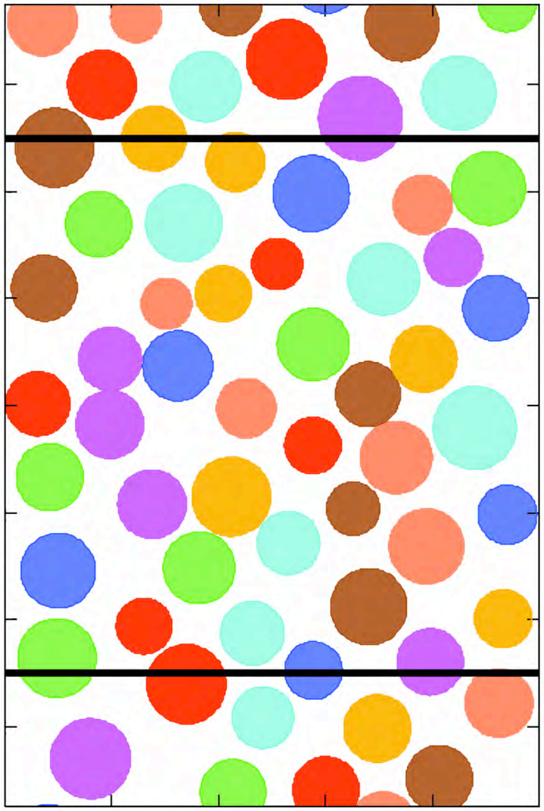
fill domain with circles with Gaussian distribution of sizes using hard elastic circles in gravity field



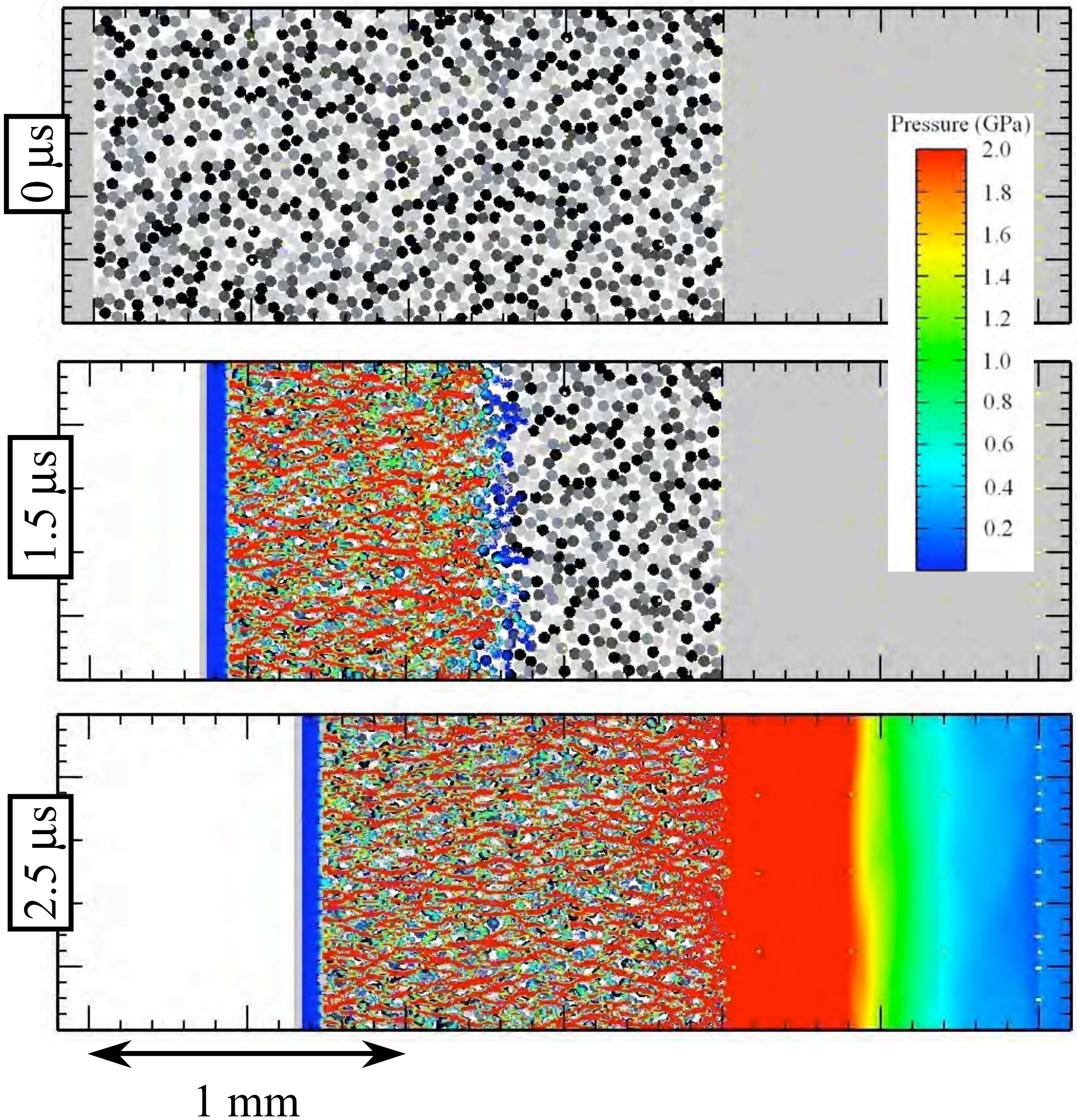
scale diameters to give proper volume fraction (~55%) as suggested by Benson



perturb positions to give less “regular” distribution

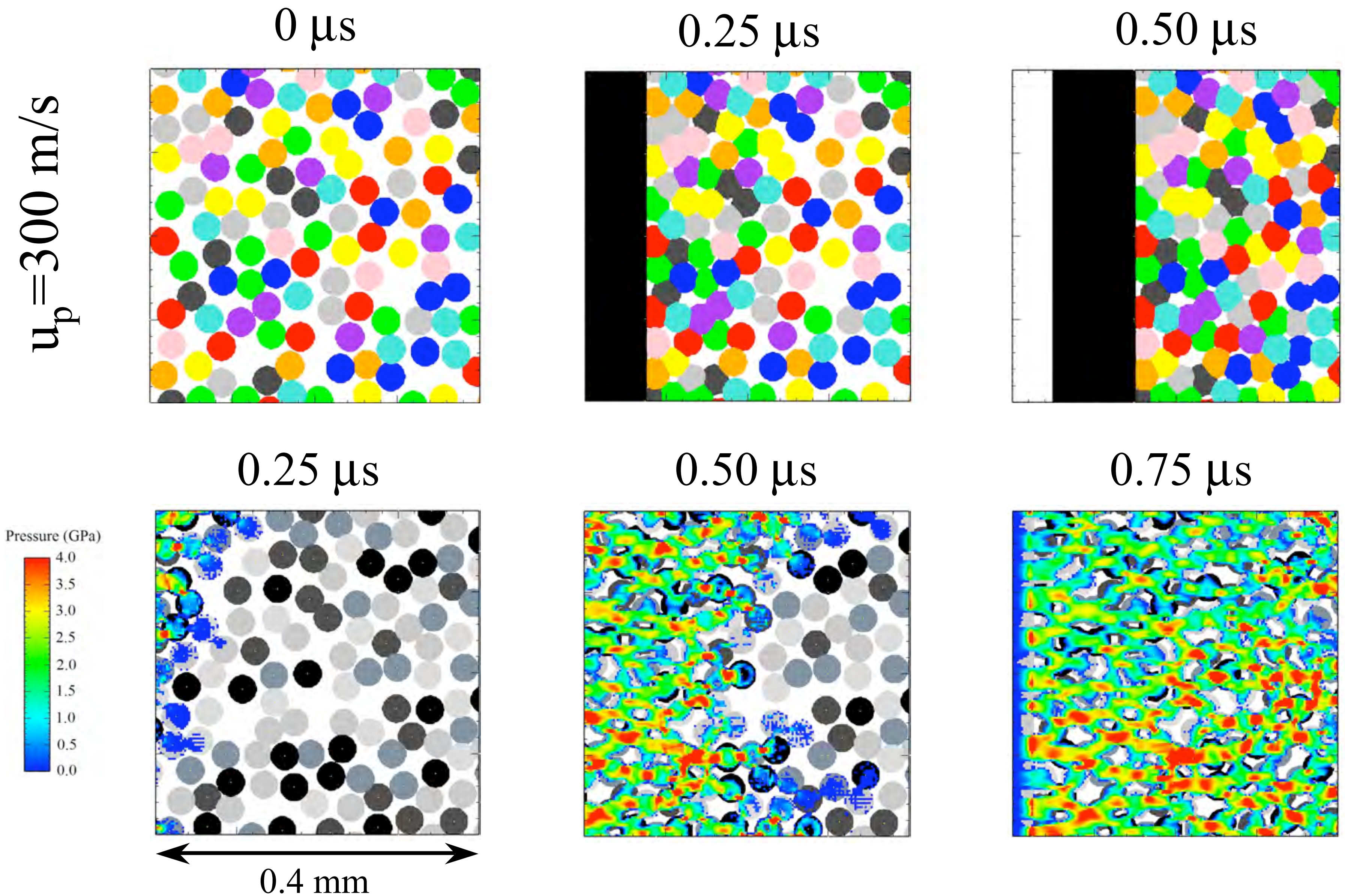


Computational Dynamic Compaction

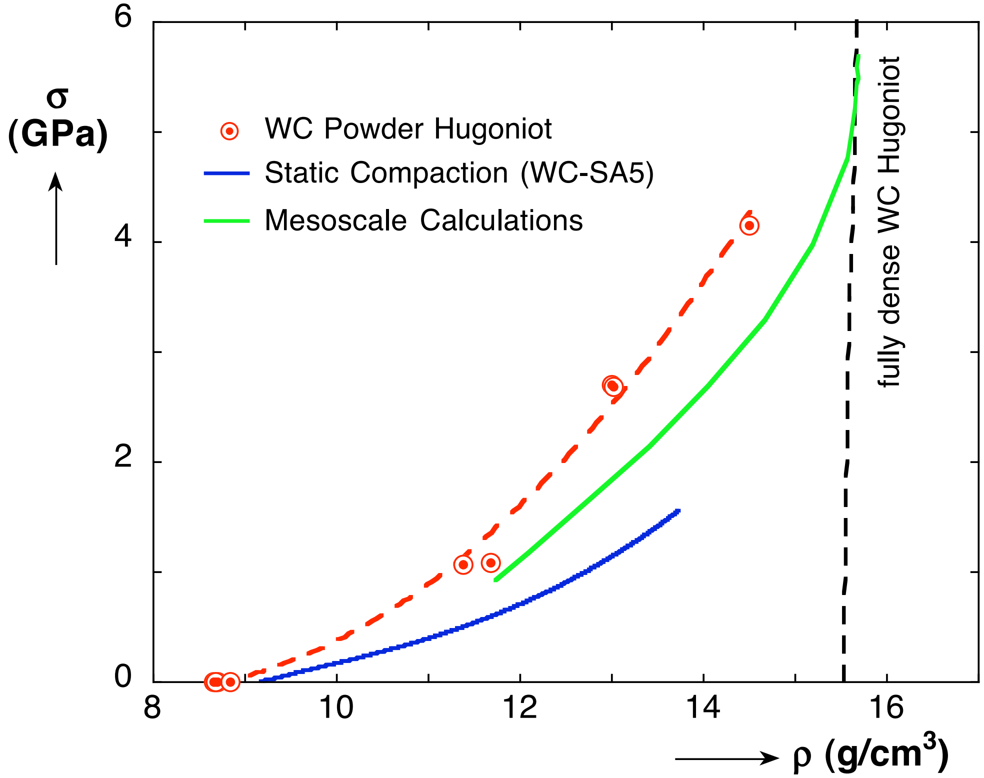


- driver plate velocity u_p=300 m/s
- shock thickness on the order of ~2-5 particles
- strong force chains observed
- wave smooths in aluminum buffer

Close-Up of Compaction Process



Calculated Hugoniot

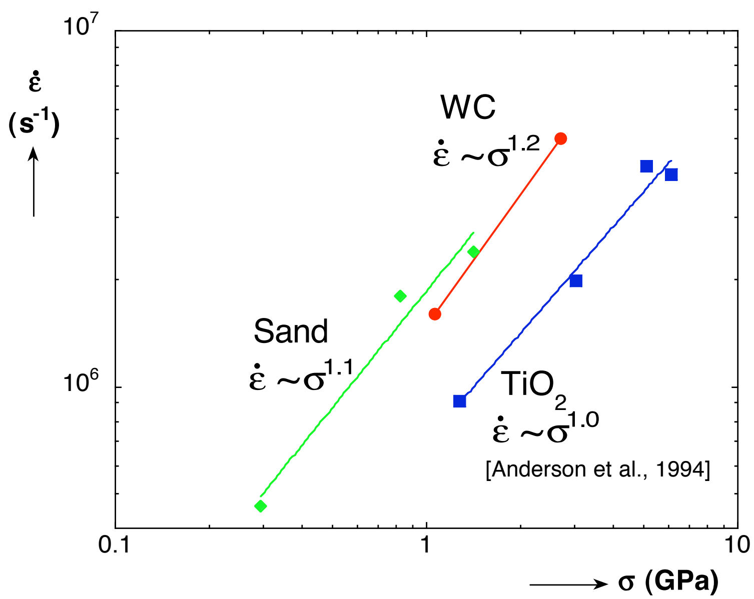


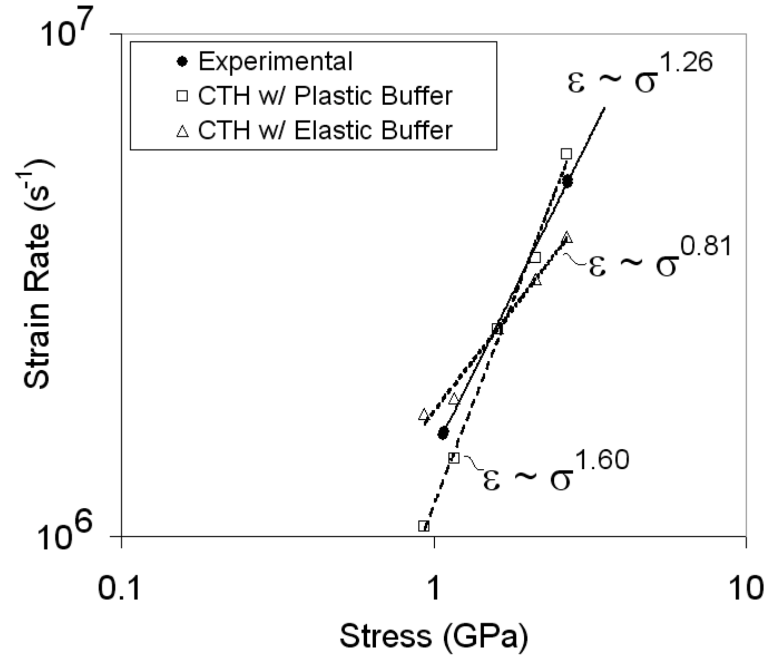
$$\sigma = \rho_o U_s u_p$$

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

- simulations provide reasonable estimate for Hugoniot
- shortcomings of model:
  - missing physics of granular contact and fracture
  - wrong connectivity in 2-D
  - spherical particles unrealistic
  - inaccurate strength for small particles

Scaling Between Rise Time of Wave and Stress





scaling between stress and strain rate is similar to that in experiments

Sensitivity to Simulation Parameters

Material Properties

- Particle size distribution (negligible effect)
- Dynamic yield strength (strong effect)
- Material EOS (negligible effect)

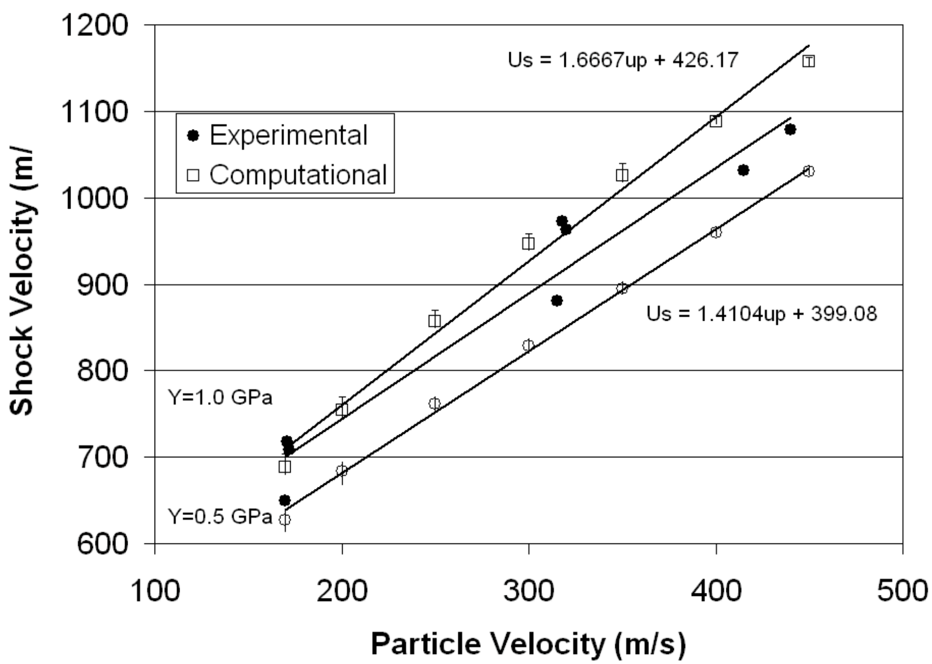
Two-Dimensional Properties

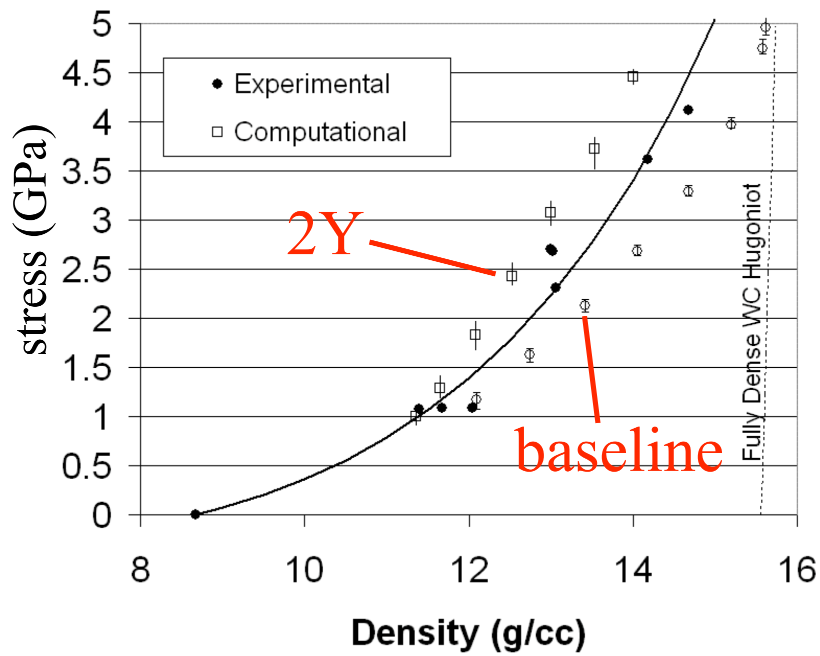
- Material distribution (strong effect)
- Variations in boundary conditions (small effect)

Hydrocode Behavior

- Mixed cell strength (very strong effect)

Effect of Dynamic Strength

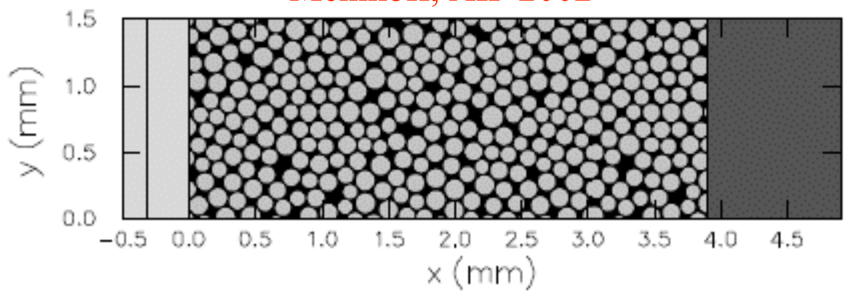


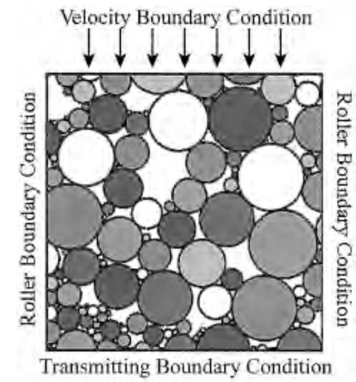


- increasing *Y* by factor of 2, i.e. from 5 GPa to 10 GPa, results in significant increase in model stiffness
- strength from macroscopic plate impact experiments on WC too low for 30 µm particles

2-D Material Distribution

Menikoff, AIP 2002

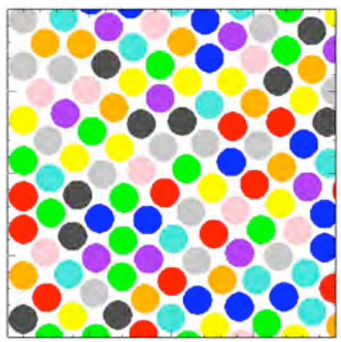




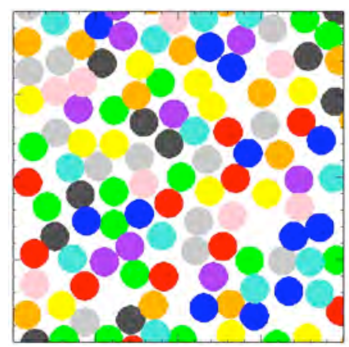
Meyers et al., 1999

- two-dimensional mesoscale studies have been performed with various material distributions.
- how does this choice affect the results?

Quasi-Crystalline



Baseline

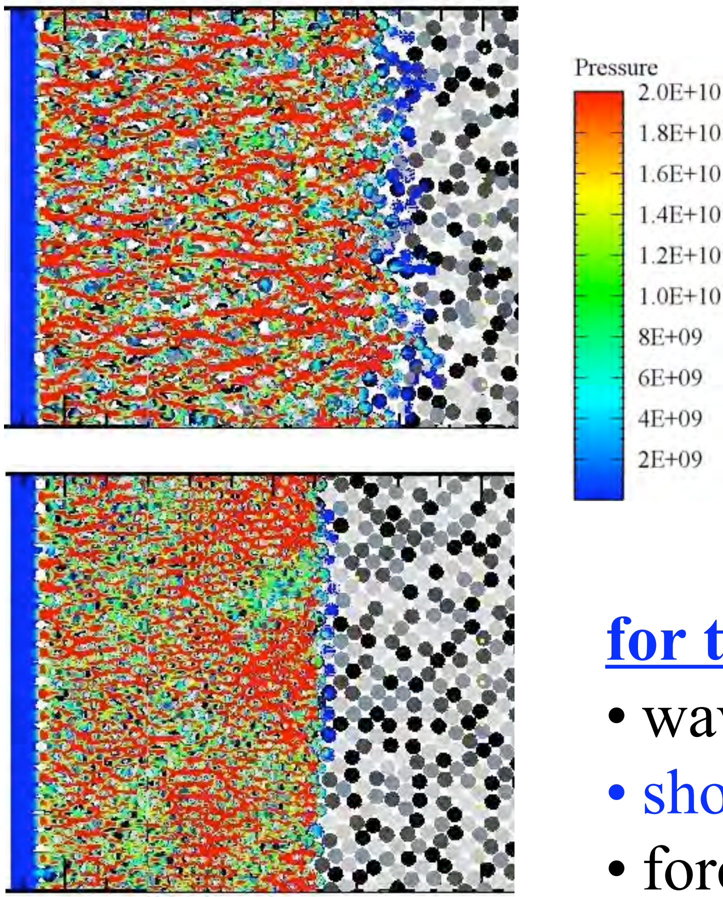


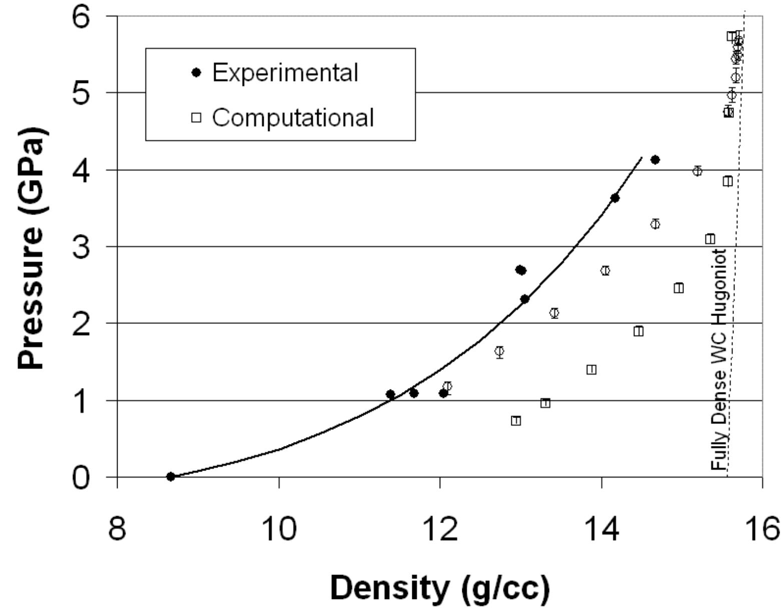
- highly ordered arrangement arises when particle diameter reduced to obtain correct volume fraction
- perturbation step produces disordered particles with some contact

Effect of Order on Shock Structure

Baseline

Quasi-Crystalline





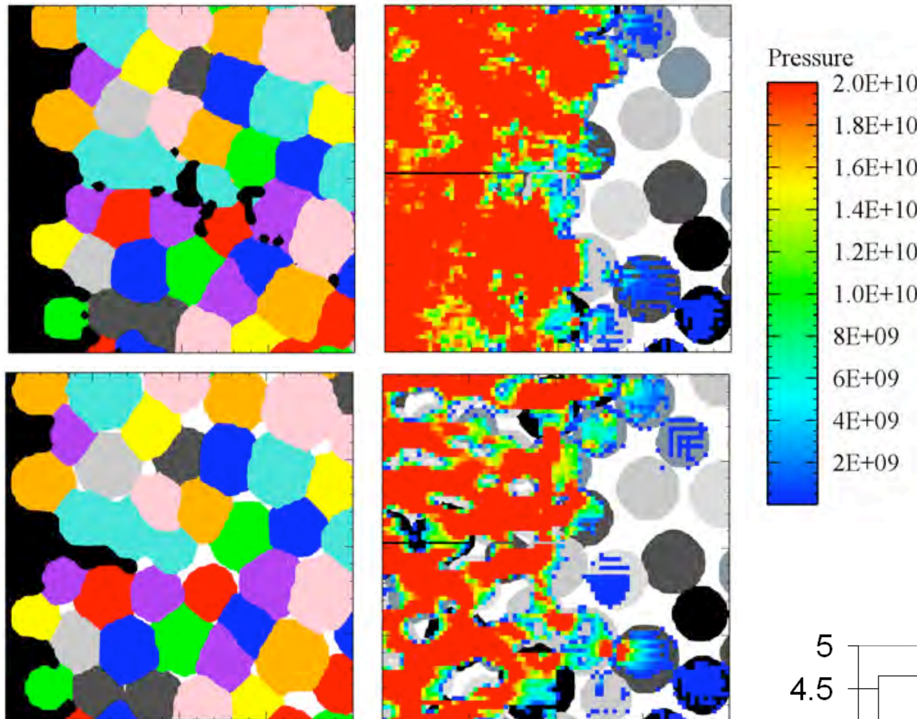
for the quasi-crystalline case:

- wave much slower
- shock front less diffuse
- force chains less pronounced
- shock propagation must rely on momentum (i.e. particle motion) to transport shock information
- lateral motion minimized
- material becomes anisotropic (slow and fast directions)

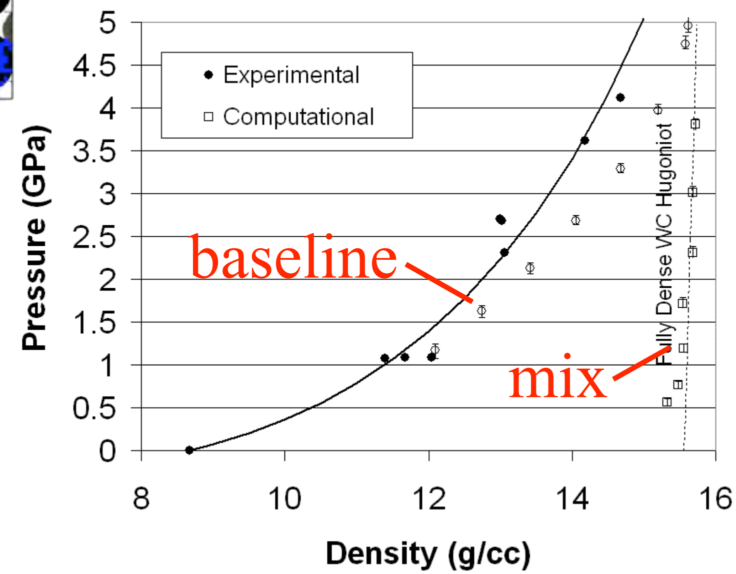
Effect of Mixing Laws for Strength

mixed cells have no strength

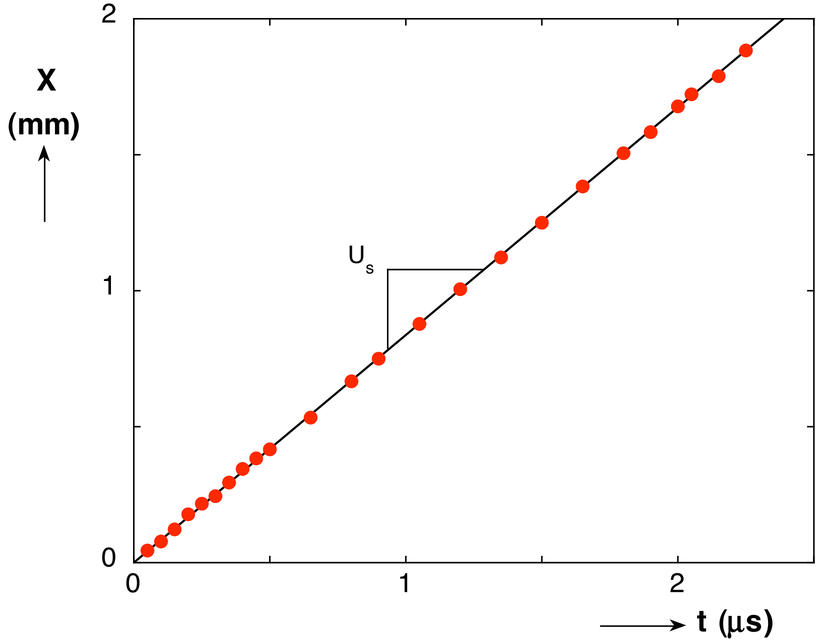
mixed cells have volume fraction weighted strength

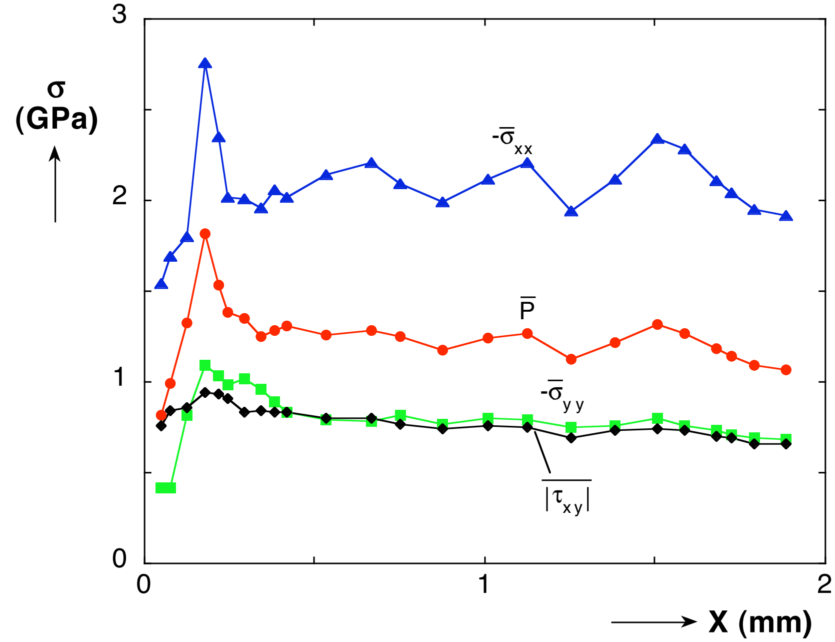


when mixed cells have no strength, material behaves in "snowplow" manner

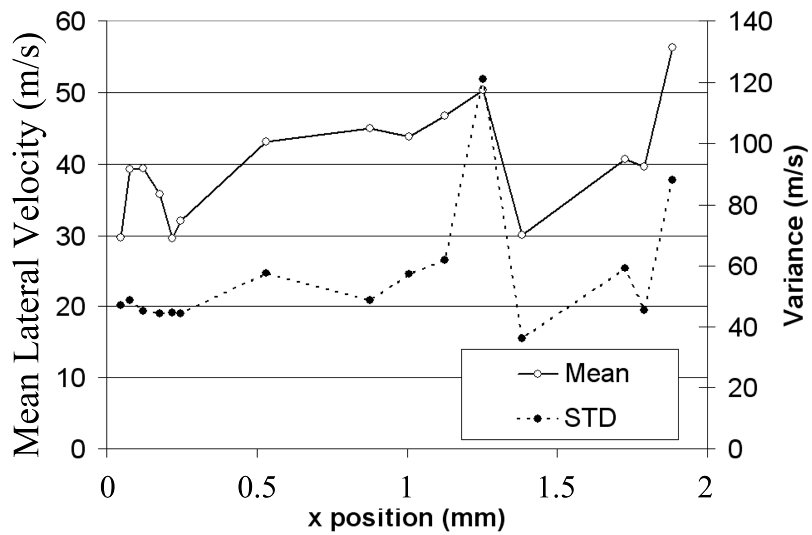


Properties of Propagating Wave

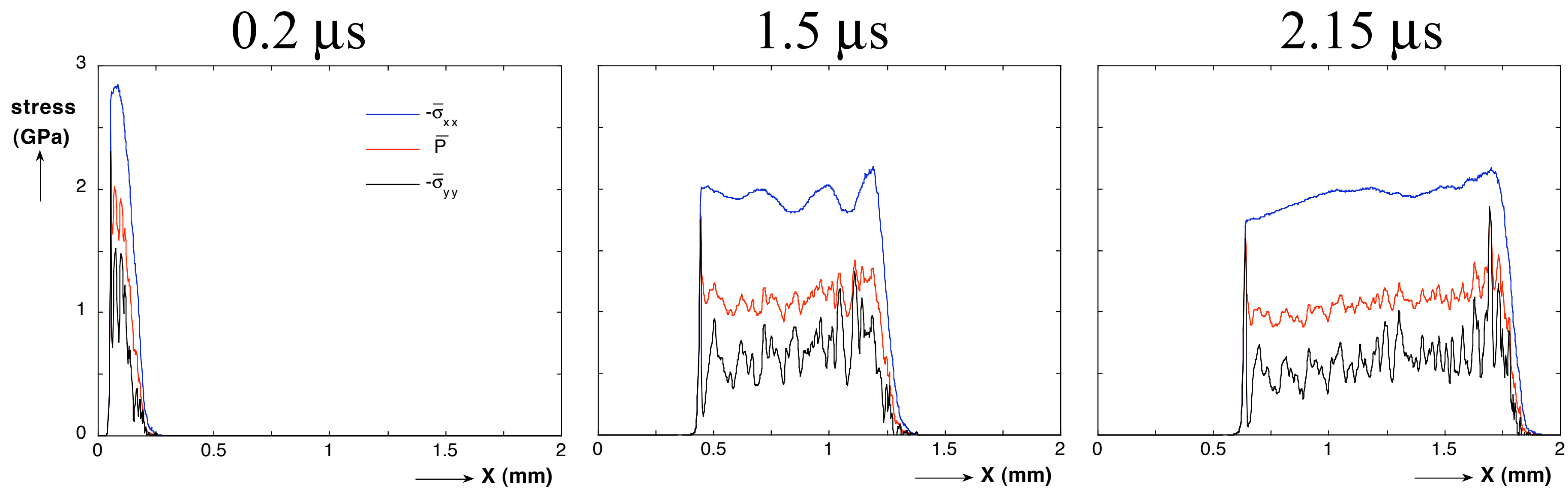




- arrival time of wave suggests steadiness at all times
- stresses in wave front indicate nearly 0.5 mm required to reach steady state
- lateral motion >10% of longitudinal velocity

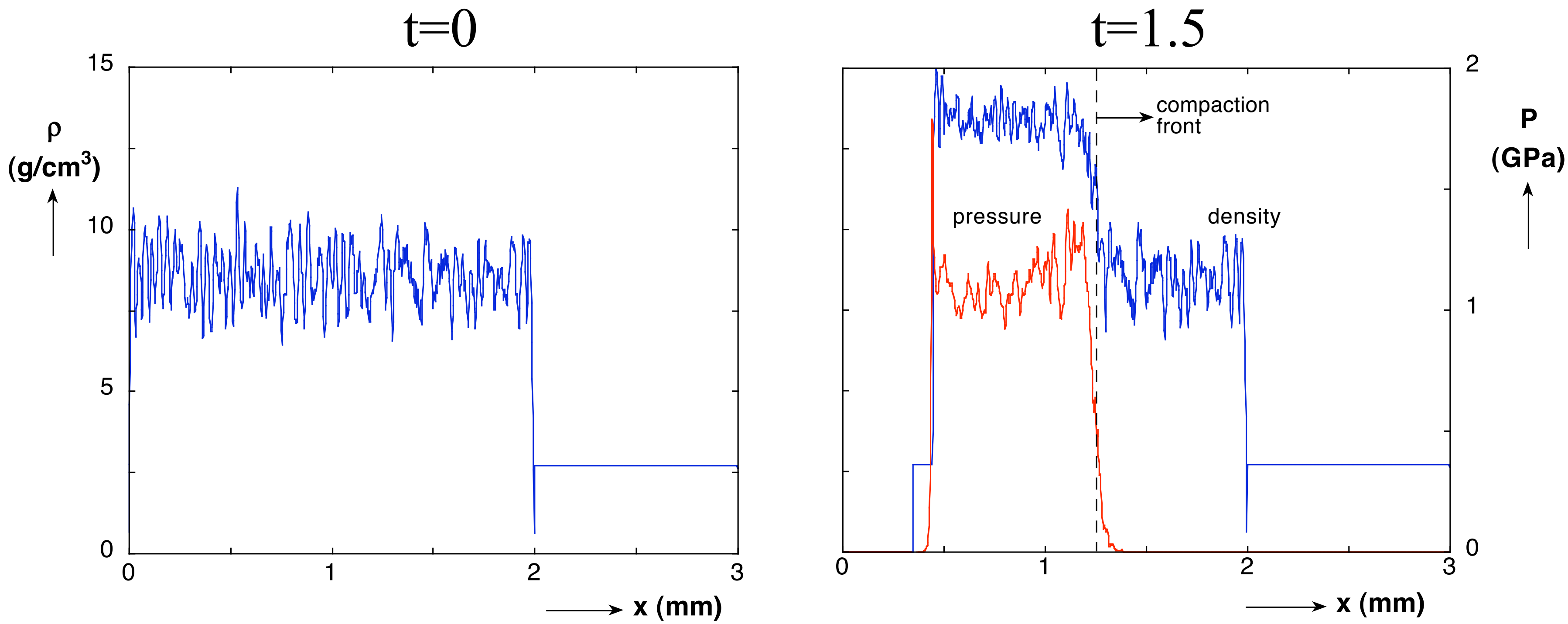


Spatially Averaged Stresses in Propagating Wave



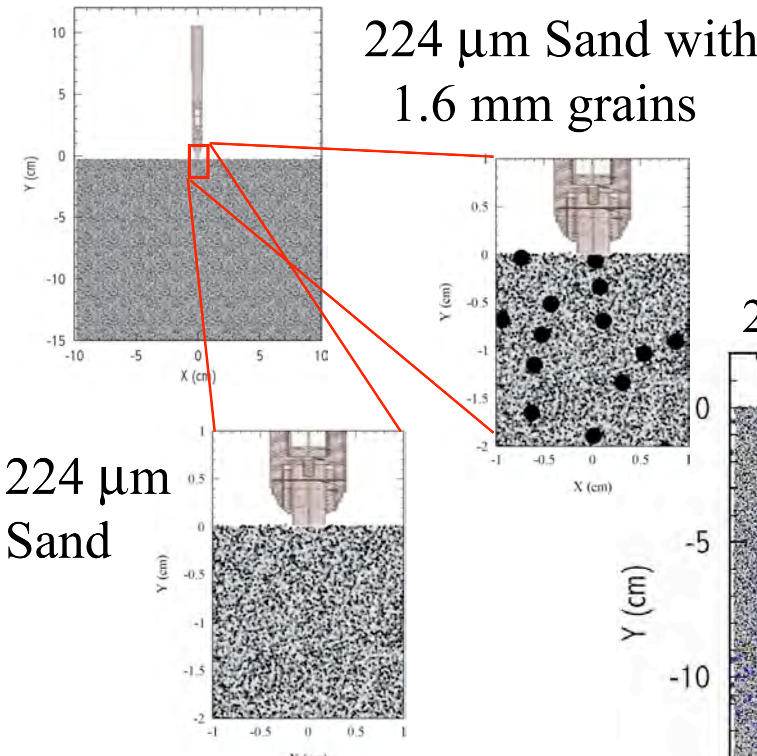
- strong transient in initial loading
- stresses stabilize after some distance but significant fluctuations still seen

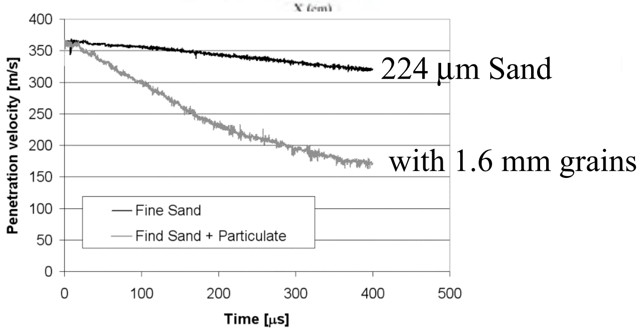
Spatially Averaged Density and Pressure



System Level Results

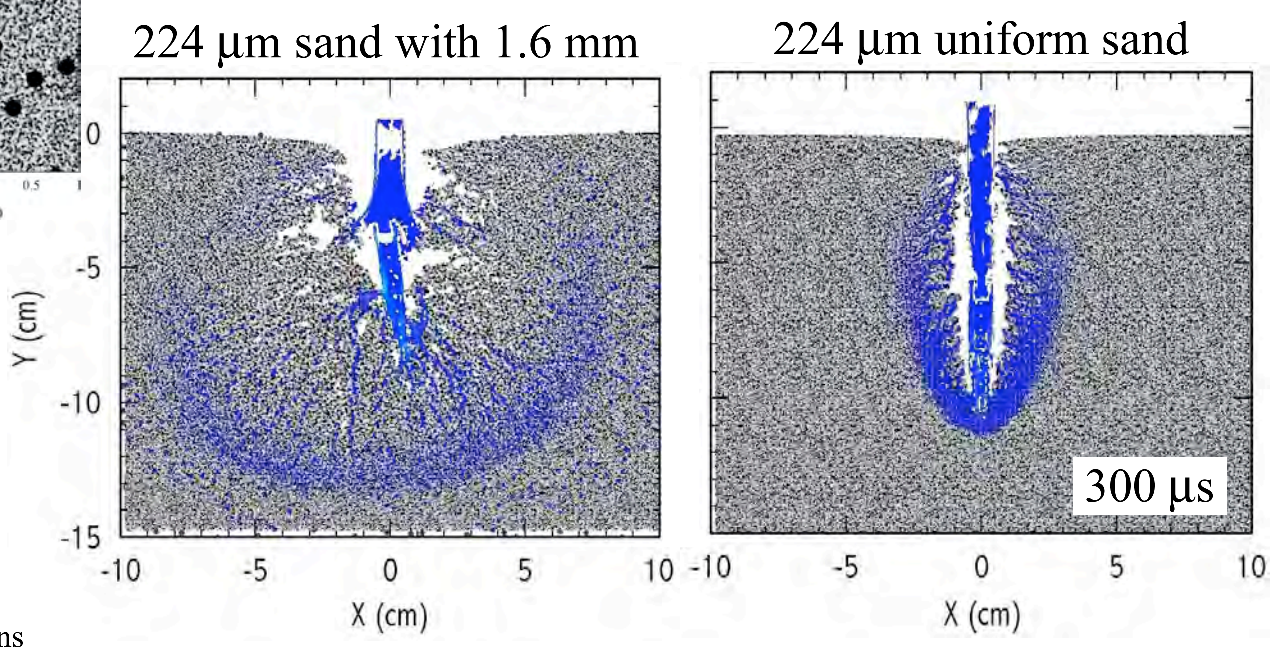
mesoscale simulations demonstrate the effect of material heterogeneity





__Computational Horsepower__

- 128 Processors
- 2.5 days
- adequate resolution is challenging



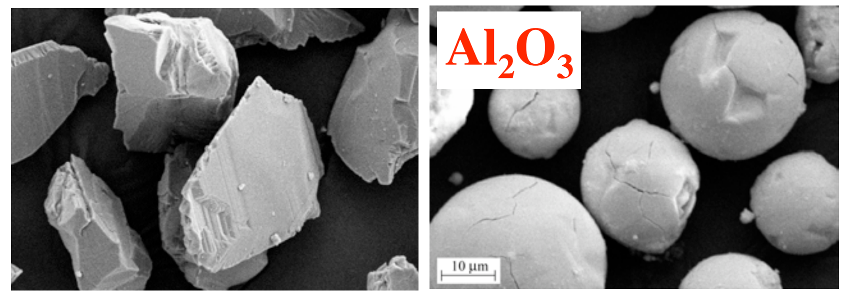
Mesoscale simulations demonstrate performance variations that continuous modeling cannot capture

Conclusions

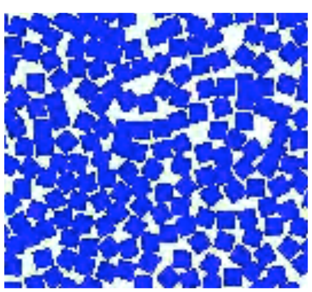
- waves in WC (and granular ceramics in general) have interesting characteristics:
  - very slow wave speeds
  - steady waves observed for several sample thicknesses, perhaps the first time-resolved observation of steadiness
  - waves have finite rise times; strain rate scales approximately with stress to the first power
- dynamic response significantly stiffer than static response for WC (also for SiO_2 and sand)
- mesoscale simulations reveal details of compaction process
  - distribution of stresses nonuniform (force chains)
  - significant momentum transfer in lateral direction
  - waves require significant distance to become steady
  - sensitivity of simulations determined - strength, order, cell mixing critical

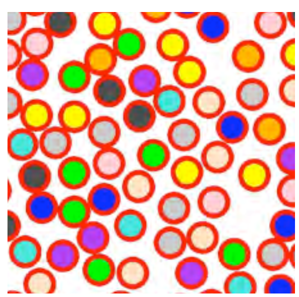
Future Work

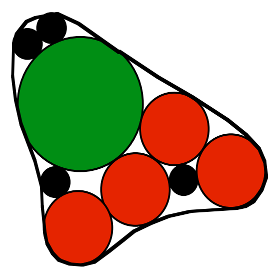
- development of techniques for testing wet sand
- detailed comparison of simulations to validation experiments
- plasma spheridization to study morphology effects
- characterize comminution of grains in recovered material



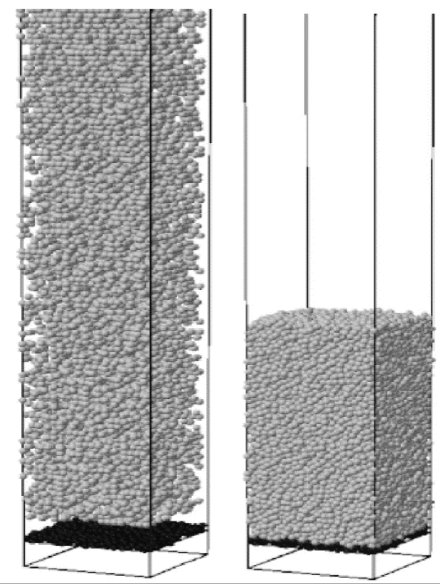
- determine effect of variations in particle shape
- look at surface effects (mimic sliding)
- 3-D simulations with spheres and other shapes
- other simulation techniques (e.g. DEM)







Jensen et al., 2001



Silbert, Ertas, Grest, Halsey and Levine, **Physical Review E, 65**, 031304**,** 2002

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