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Study of Compaction, Preheating and Strength in Shock Compressed Porous Silica

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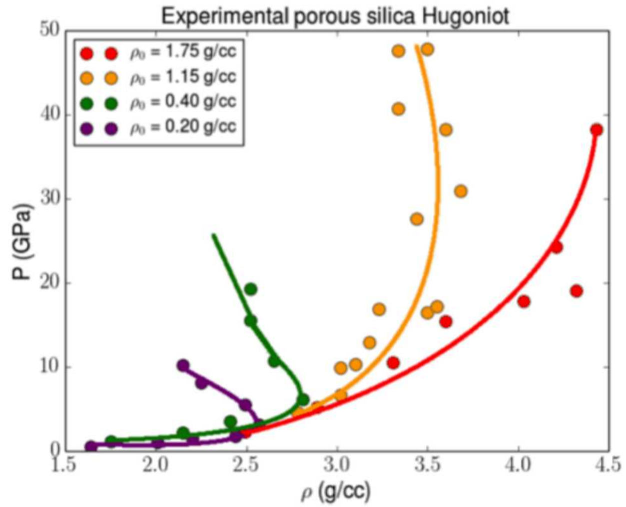
Motivation for Studying Porous Silica (SiO_2)

Trunin et al., *Experimental data on shock compression and adiabatic expansion of condensed matter* (2001)



Exhibits anomalous density dependence with respect to pressure

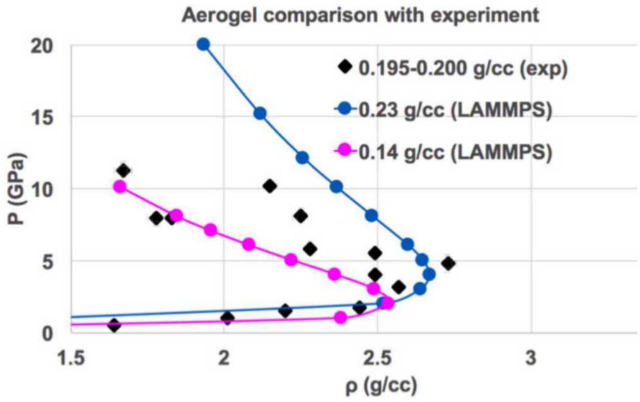
- In porous silica, density can decrease with increasing pressure
- Common in porous materials
  - Shock energy converted into kinetic energy from particles ejected into void space. Results in high temperature.

Parameter ⟶ Structure/ Dynamics ⟶ Property

- The structure and dynamics of a material dictates its macroscale properties and its equation of state
- What experimentally relevant parameters influence the structure and dynamics in the material?

Molecular dynamics (MD) gives direct control of experimentally tunable parameters, access to microscopic structure, and characterization of macroscale properties

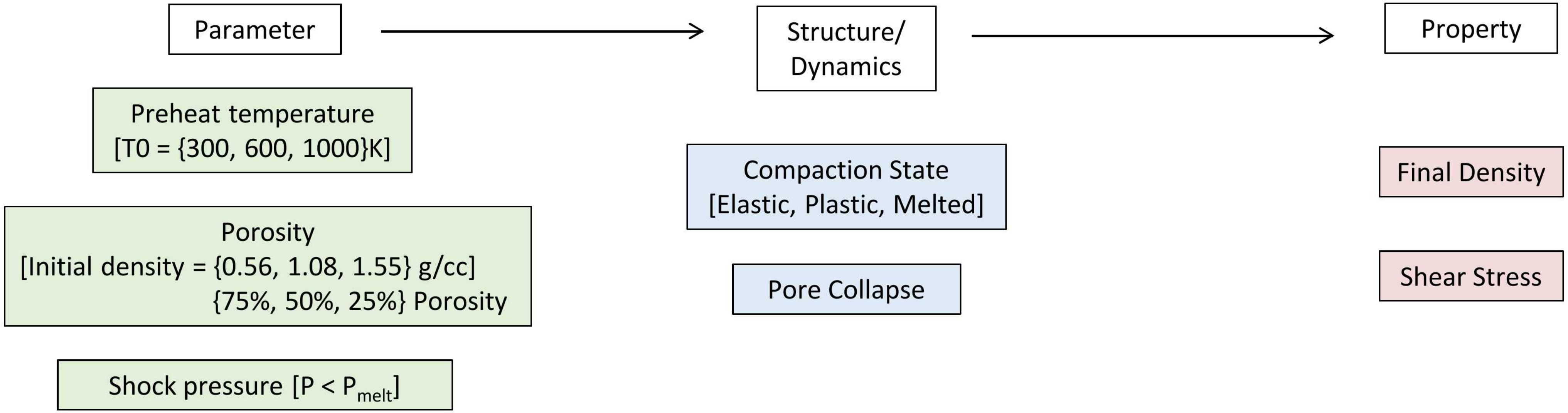
- Previously shown to capture anomalous density dependence in high porosity silica
  - LAMMPS is Sandia's MD package used to run shock compression simulations shown on the right (Blue, Pink)



Jones, Lane, and Vogler, *Shock Compression in Condensed Matter, AIP Conf. Proc.*, **1979**, 090007 (2018)

Goal of this Work

Using molecular dynamics, we will elucidate the local mechanisms that dictate the macroscale density and shear stress as a function of preheat temperature, initial porosity, and shock compression



Parameter

Preheat temperature
[T0 = {300, 600, 1000}K]

Porosity
[Initial density = {0.56, 1.08, 1.55} g/cc]
{75%, 50%, 25%} Porosity

Shock pressure [P < P_{melt}]

Structure/ Dynamics

Compaction State
[Elastic, Plastic, Melted]

Pore Collapse

Property

Final Density

Shear Stress

Methodology

Beest, Kramer, van Santen, PRL, (1990)
Vollmayr *et al.*, Phys. Rev. B (1996)
Lane, Phys. Rev. E. (2015)

$$\Phi_{ij} = \frac{q_i q_j}{r_{ij}} + A_{ij}\exp(-b_{ij} r_{ij}) - \frac{c_{ij}}{r_{ij}^6} \qquad r_{ij} \geq R_c$$

$$\Phi_{ij} = \frac{1}{2} K r_{ij}^2 - F_{ij}^0 r_{ij} + V_{ij}^0 \qquad r_{ij} < R_c$$

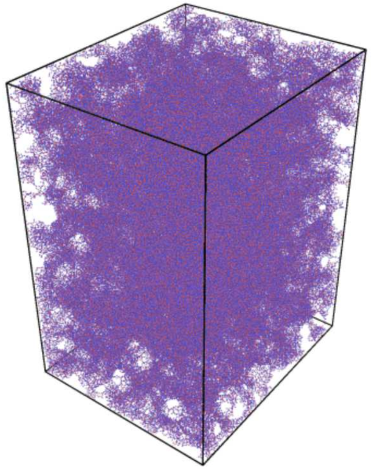
van Beest-Kramer-van Santen (BKS) Potential:

- Shown to reproduce anomalous density dependence on temperature for silica (SiO_2)
- Particles assigned partial charges
- Coulomb interactions calculated based on Ewald summation

Initializing System:

- Spherical voids grown at 2500K to introduce target porosity
- Cooled to 300K
- NVT/NPT simulations to equilibrate the pressure/density at target initial temperature (T_0)

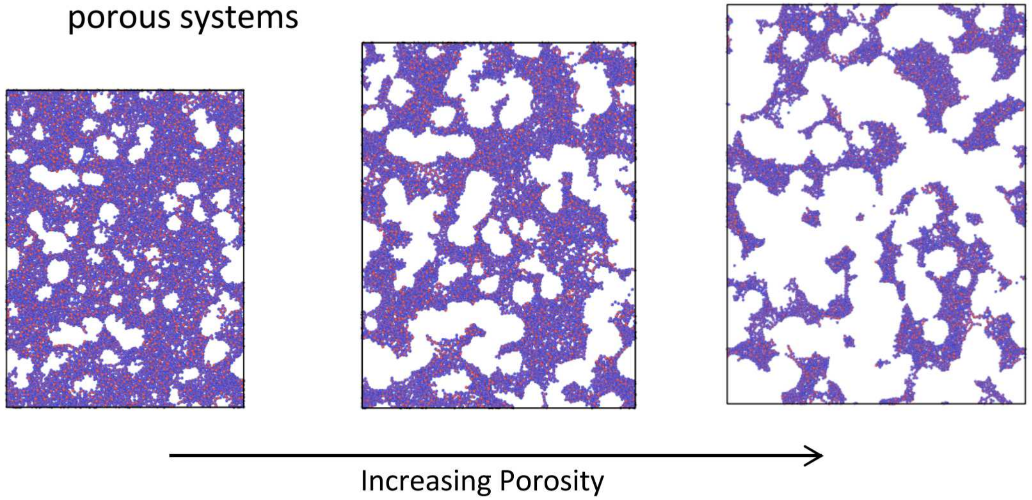
Visual of
50% porous
system



Hugoniostat method in Molecular Dynamics (MD)*:

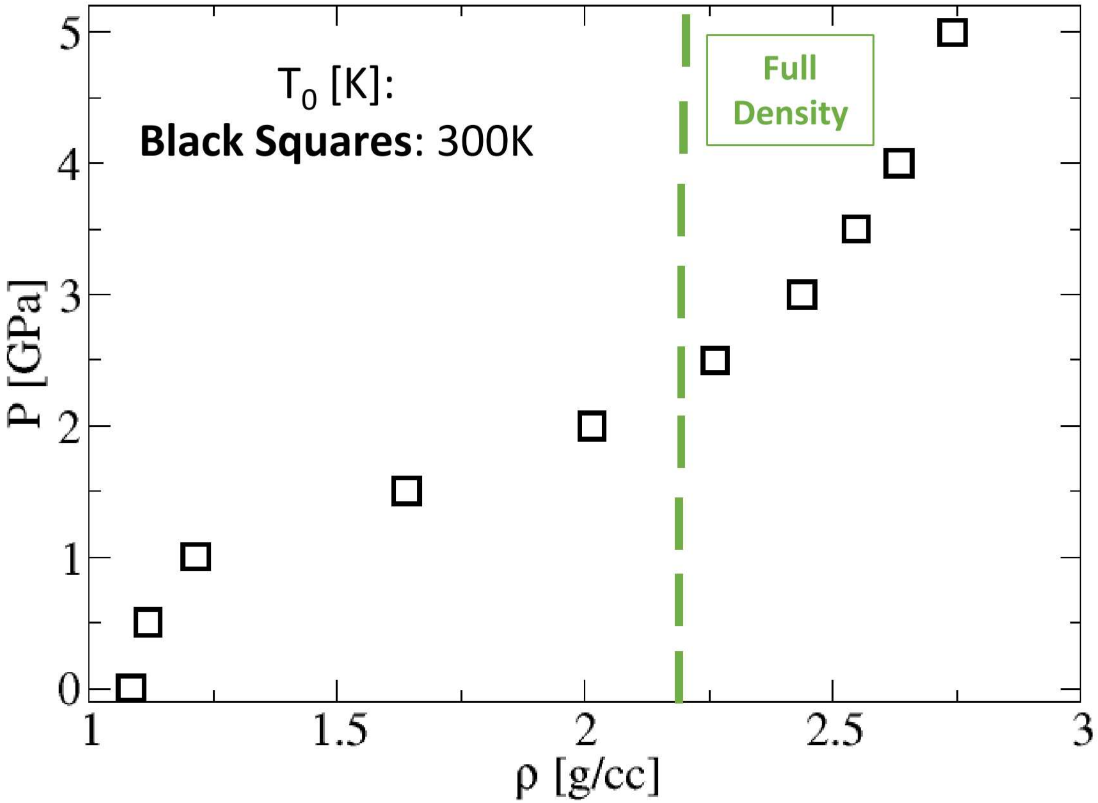
- Constant stress, non-propagating
- Uniaxially compressed until target pressure is reached and jump conditions met
- Less expensive than Non-Equilibrium Molecular Dynamics (NEMD) shock compression
- Does not necessarily evolve across Rayleigh line
  - Can produce fictitious dynamics

1nm slices to show
porous systems



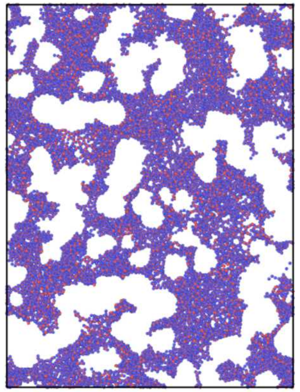
*Ravelo *et al., Phys. Rev. E*, (2004)

Compaction of Porous Silica



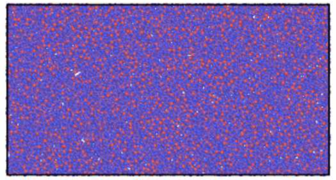
*Full Density: Vitreous Silica

50% porosity
(initial density = 1.08 g/cc)

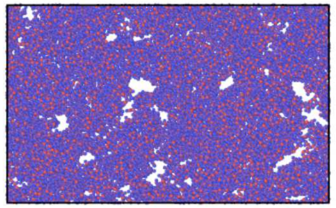


P = 0 GPa
(Pre-Shock)

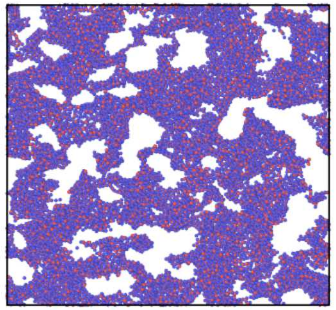
P = 5 GPa
(Fully Compact)



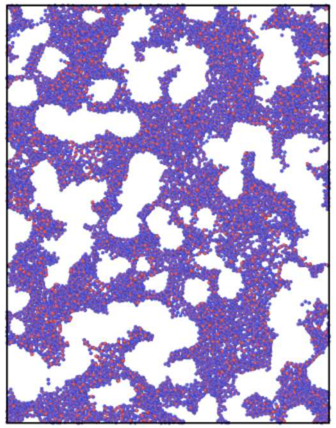
P = 3 GPa
(Plastic)



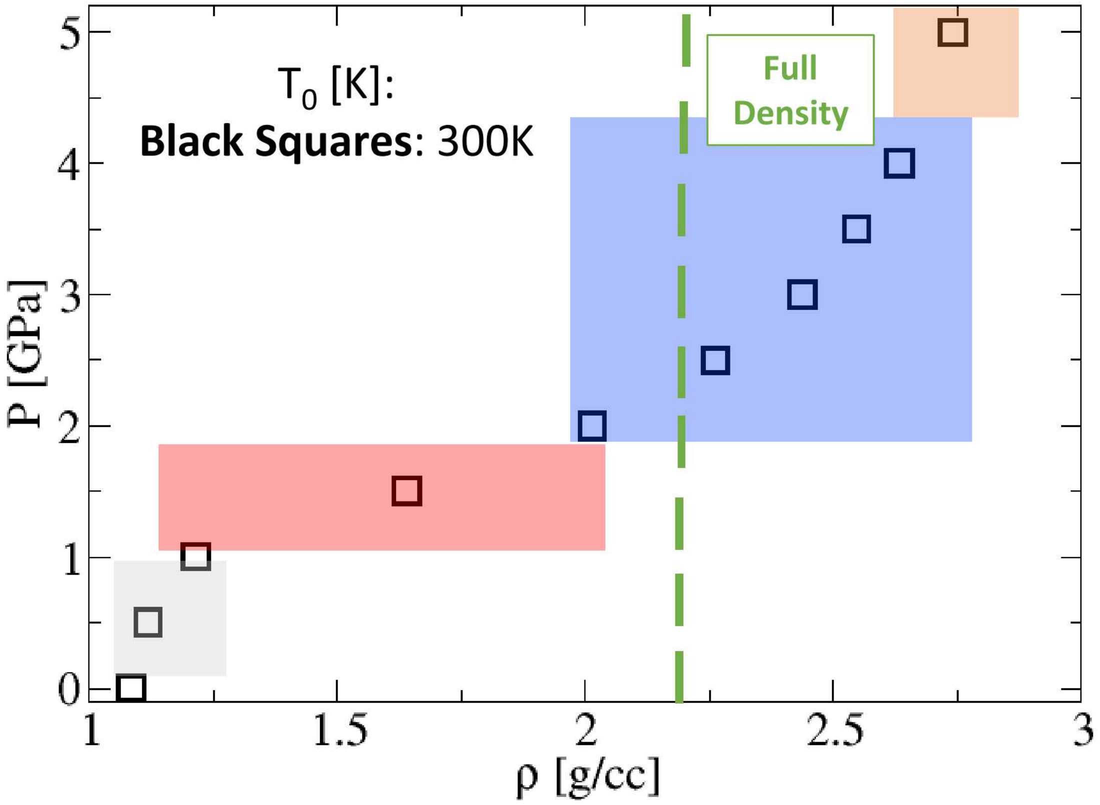
P = 1.5 GPa
(Near HEL)



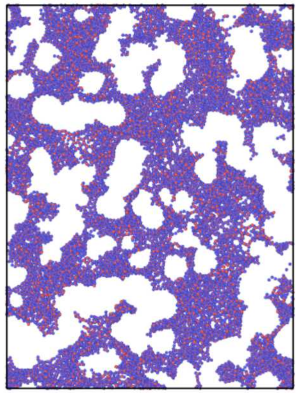
P = 0.5 GPa
(Elastic)



Compaction of Porous Silica



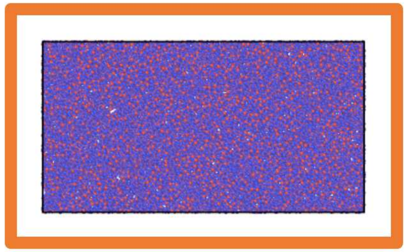
50% porosity
(initial density = 1.08 g/cc)



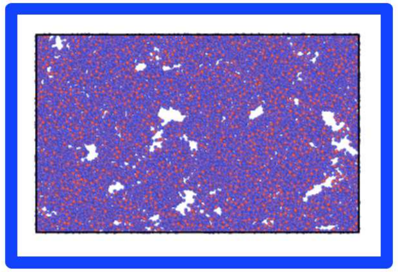
P = 0 GPa
(Pre-Shock)

- Enhanced densification at relatively low pressures
- Pores are still present at densities greater than “full density”
- Compaction regime directly linked to system properties

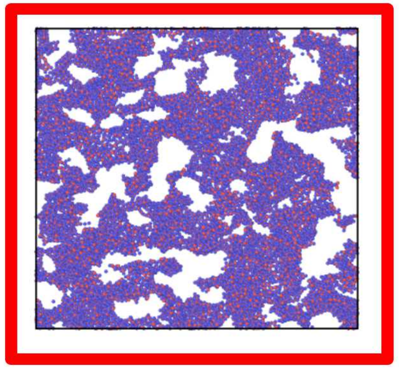
P = 5 GPa
(Fully Compact)



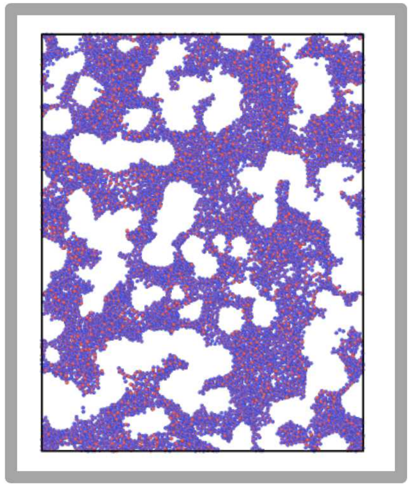
P = 3 GPa
(Plastic)



P = 1.5 GPa
(Near HEL)



P = 0.5 GPa
(Elastic)



Visual Indications of Preheat Temperature Effect

$$D^2_{i,min} = \sum_{\alpha} \{ r^{\alpha}_{ij}(t) - \sum_{\beta} [\delta_{\alpha\beta} + \epsilon_{\alpha\beta}] \times [r^{\beta}_{ih}(t - \Delta t)] \}$$

$D^2_{i,min}$ [Å^2] 0 – 100

t = 1ns

P = 0.5 GPa (Elastic)

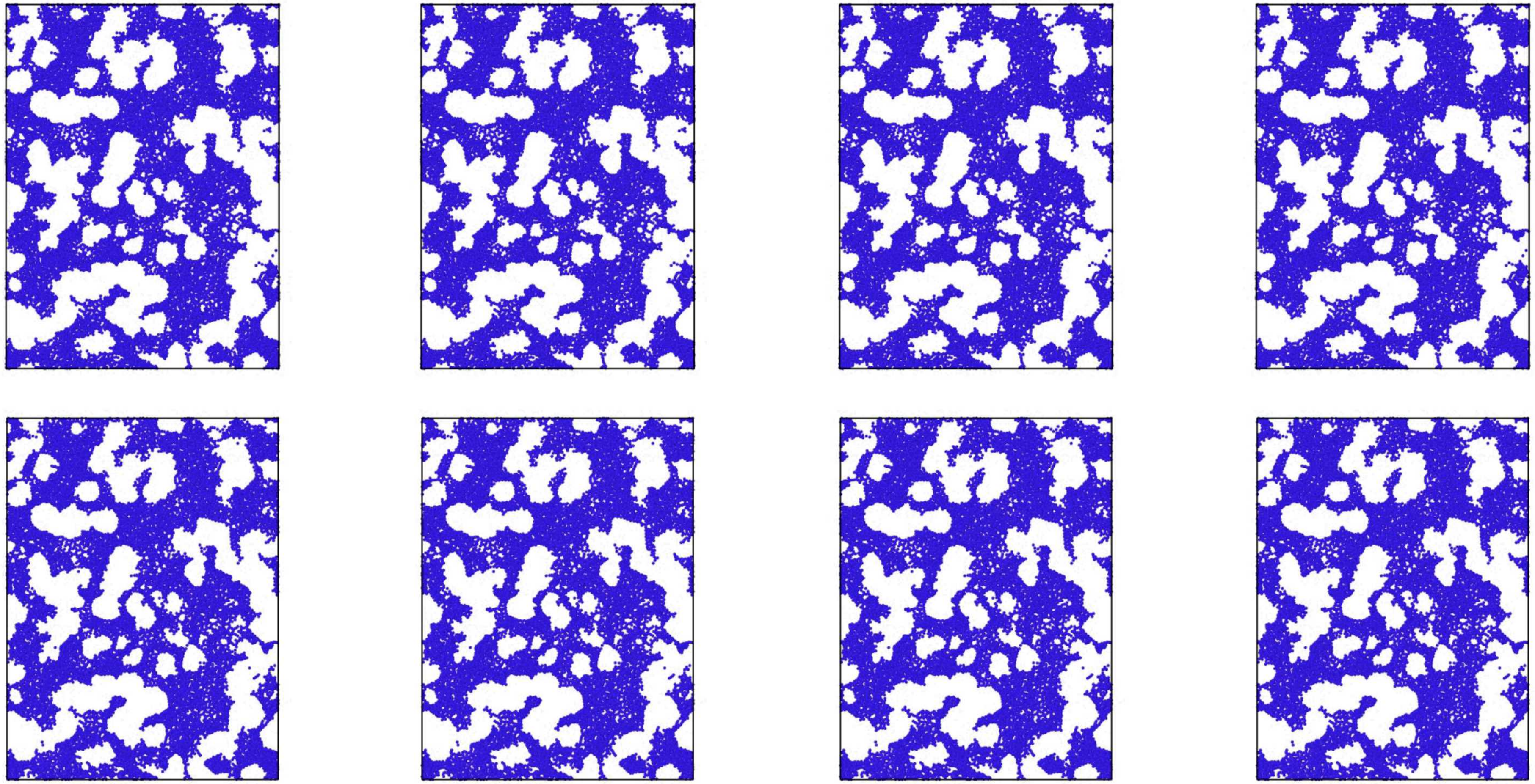
P = 1.5 GPa (Near HEL)

P = 3 GPa (Plastic)

P = 5 GPa (Fully Compact)

T_0 = 300K

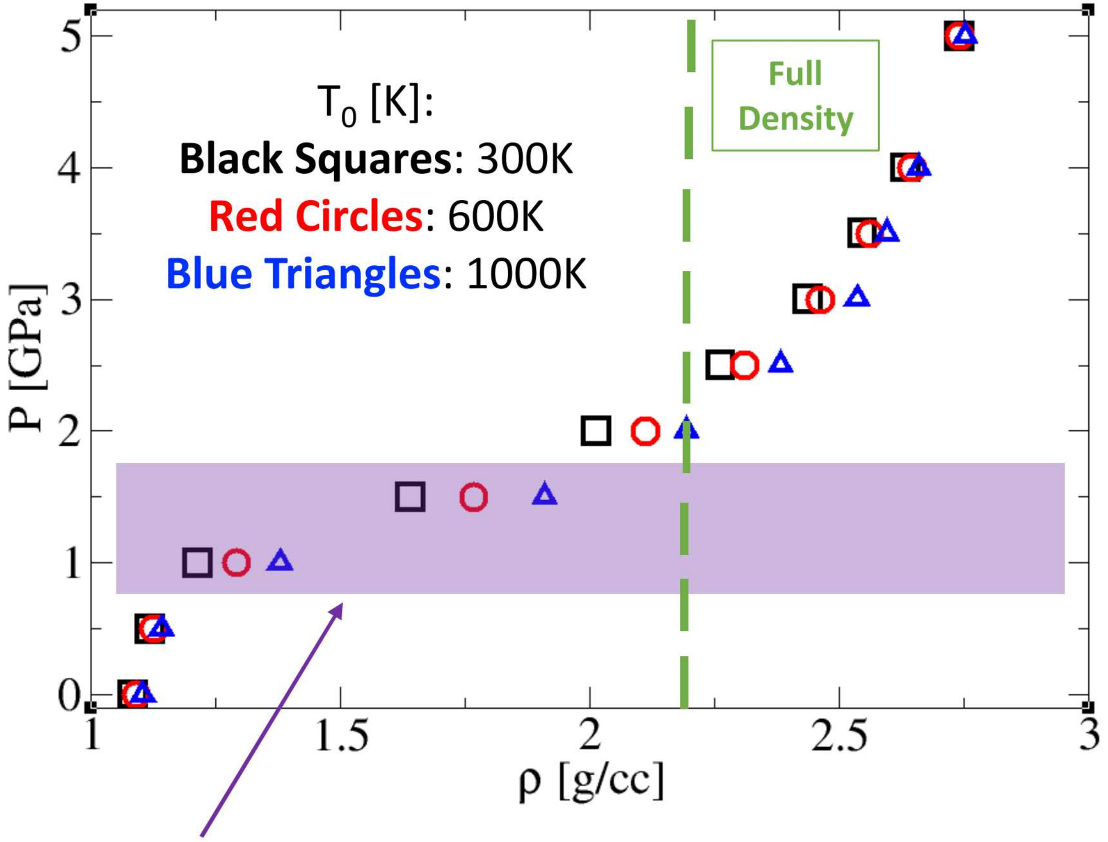
T_0 = 1000K



Preheat Temperature Effect on the Hugoniot

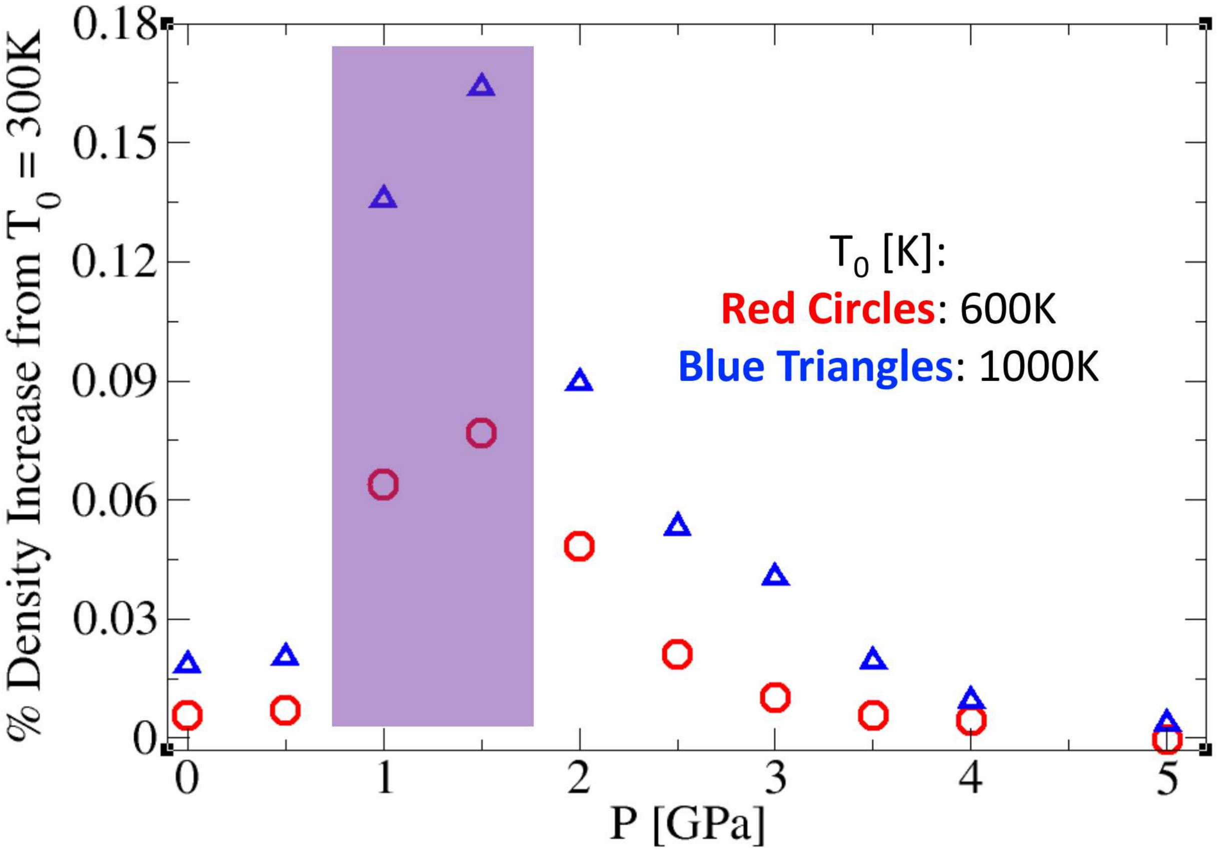
50% porosity (initial density = 1.08 g/cc)

Hugoniot



Evidence of softening indicating Hugoniot Elastic Limit (HEL) is in this pressure range

% Density Increase w.r.t. T_0 = 300K

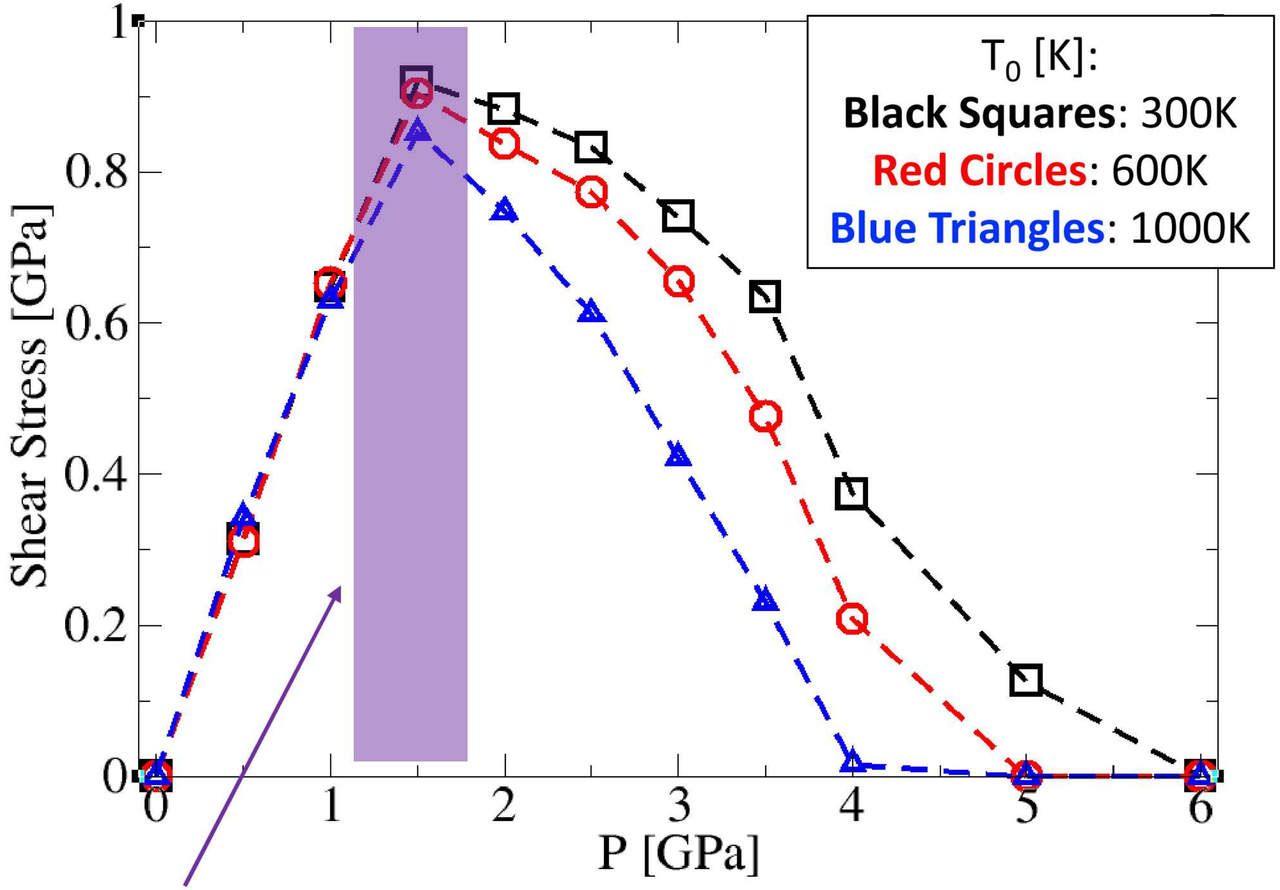


1.) Preheating increases density up to “fully compact” regime
2.) Maximum density difference near elastic to plastic transition (or the HEL)

Preheat Temperature Effect on Shear Stress

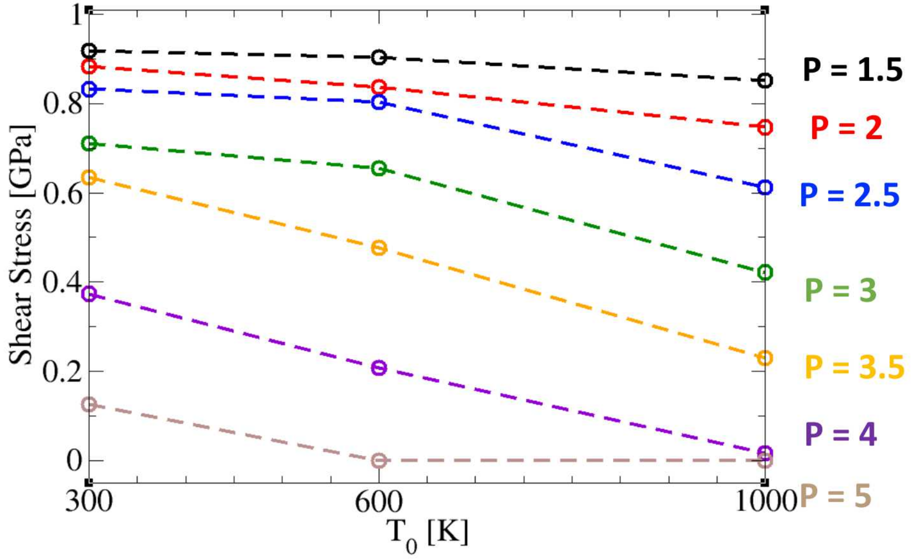
50% porosity (initial density = 1.08 g/cc)

Shear Stress versus Pressure for different Preheat Temperatures



HEL is in this pressure range indicated from maximum shear stress

Shear Stress versus Preheat Temperature for different Pressures



1.) The shear stress is a very weak function of preheating in the elastic regime
2.) The shear stress decreases with preheating in the plastic regime.

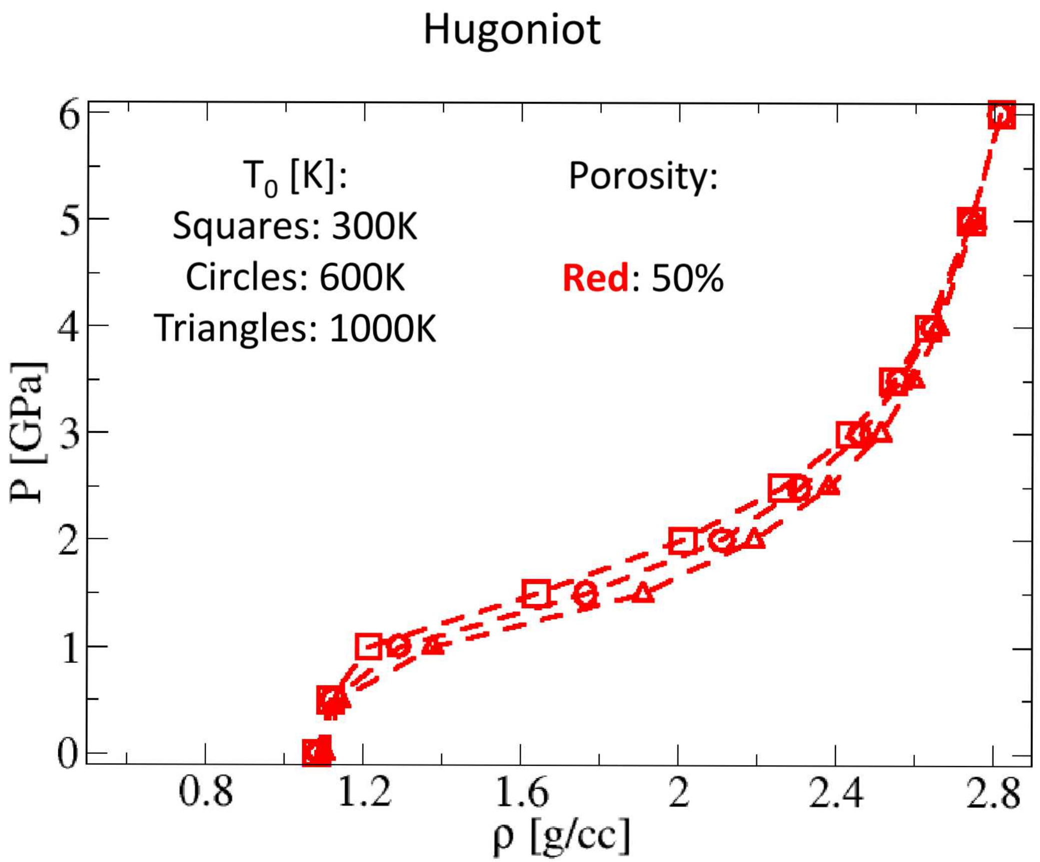
Take Home Messages: Part 1

- The final density and shear stress are directly related to the compaction regime
    - Density and shear stress increase until the HEL
    - At pressures just past the HEL, large increases in density are observed corresponding to major pore collapse.
    - Shear stress decreases past HEL until it gets to 0 denoted by the melt regime
- Generally, the preheat temperature increases the density but lowers the shear stress

1. The preheat temperature increases the density most greatly near the HEL
2. The shear stress decreases most greatly in the plastic regime
3. Both the density and shear stress are weak functions of preheat temperature in the elastic and fully compact regime

Visualizations and trends in the density and shear stress indicate that the energetic contribution from the preheat temperature contributes to the onset of plasticity and the pore collapse in the system

Porosity effect on the Hugoniot


Hugoniot

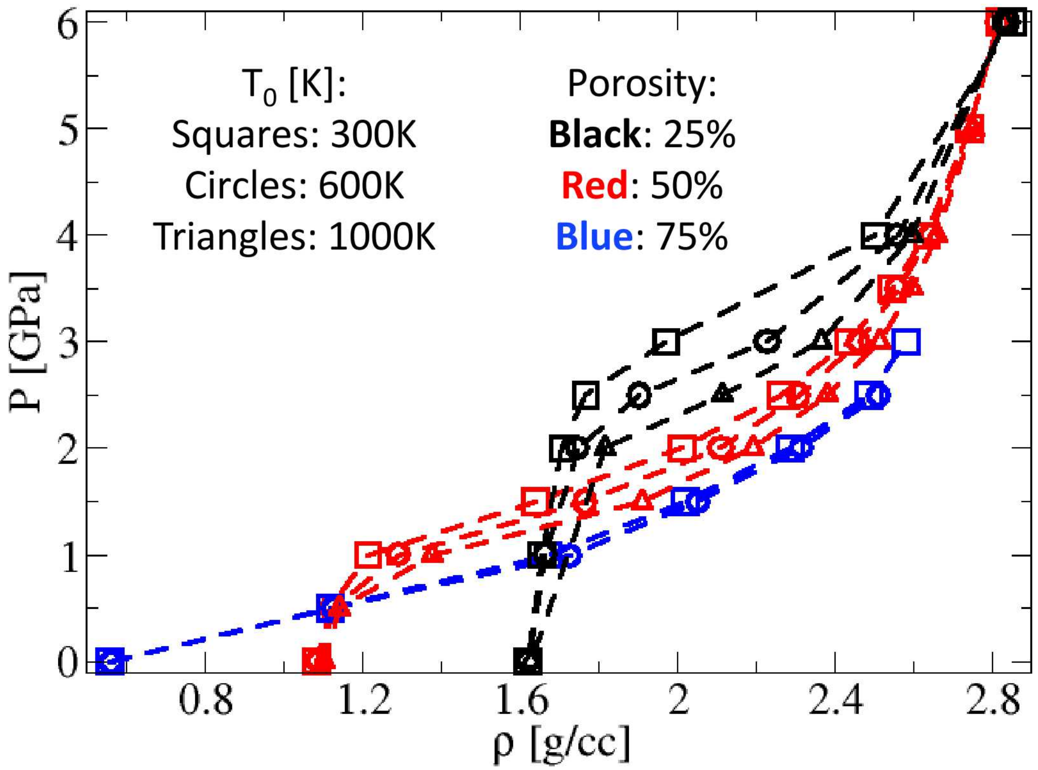
T_0 [K]:
Squares: 300K
Circles: 600K
Triangles: 1000K

Porosity:

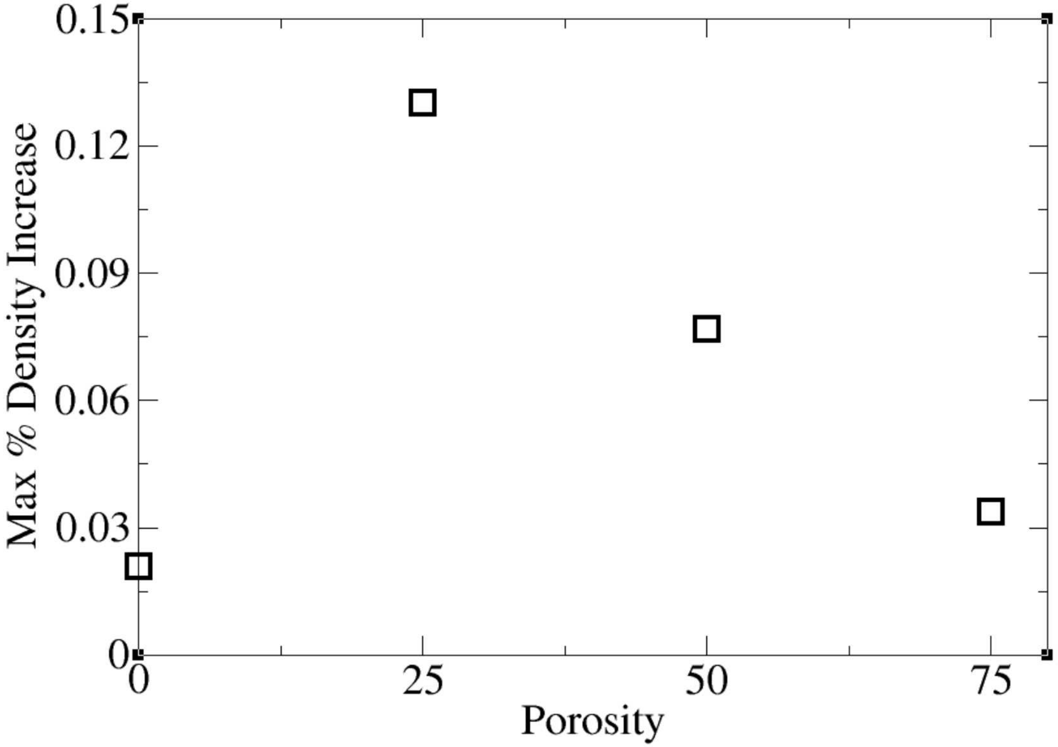
Red: 50%

Porosity effect on the Hugoniot

Hugoniot



Difference between T_0 = 600K and T_0 = 300K

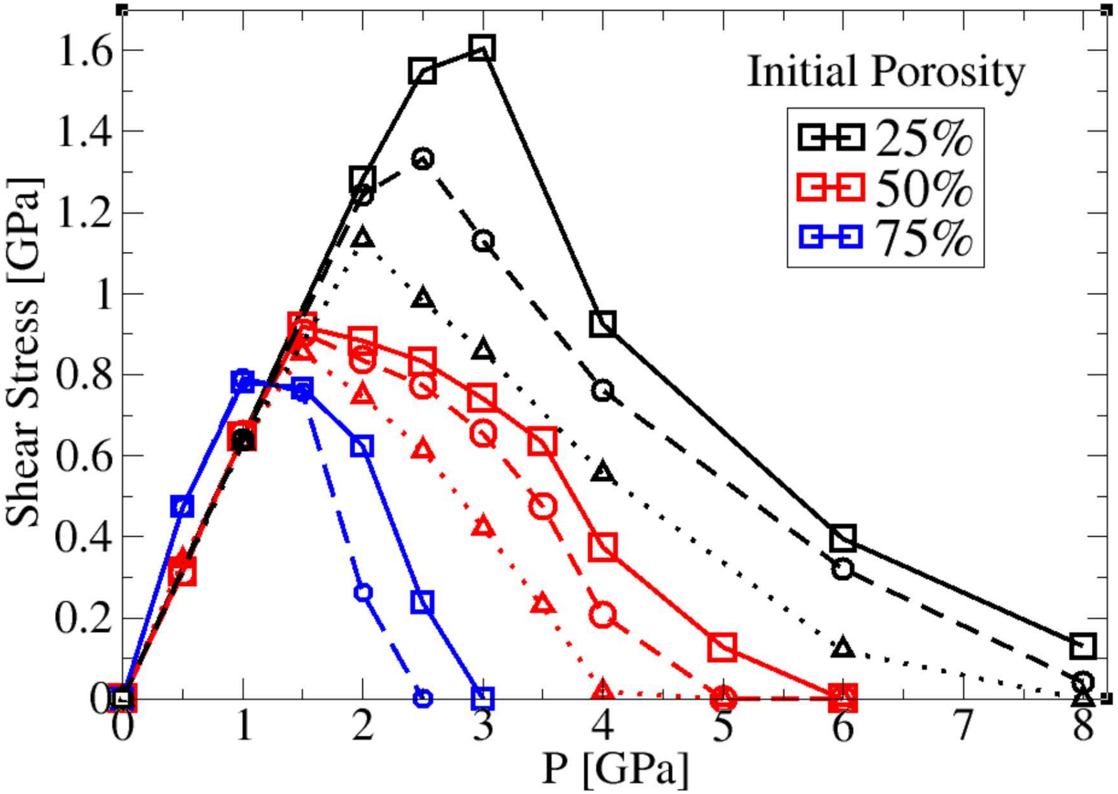


The inclusion of data for an initially fully dense system (0 porosity) indicates a maximum

1. Qualitative conclusions for preheat temperature hold as a function of porosity
2. The relative increase in density with preheat temperature decreases with porosity
3. Indication of maximum where preheat contribution is greatest

Porosity effect on Shear Stress

Squares (Solid): T_0 = 300K
Circles (Dashed): T_0 = 600K
Triangles (Dotted): T_0 = 1000K



1.) Qualitative conclusions for strength hold across different porosity
2.) Elastic to plastic transition (or the Hugoniot Elastic Limit) decreases with porosity and preheat temperature

Conclusions

Preheat Temperature Effect

- When the system is preheated, the Hugoniot curves exhibit the greatest difference in density near the HEL
- In the elastic regime, the strength of the system is not a strong function of preheat temperature while the strength decreases with increasing preheat temperature in the plastic regime

Porosity Effect

- The HEL decreases with increasing porosity and increasing preheat temperature.
- Increasing the porosity decreases the macroscale shear stress at shock pressures greater than the HEL

Future Work/Directions

We want to elucidate mechanistically the energetic contributions to the pore collapse and onset of plasticity

- Demonstrate ***why*** preheat temperature exhibits a max in density increase as a function of porosity and ***why*** both preheat temperature and porosity decrease the HEL
  - Analyze local atomic stress/density/temperature across different compaction regimes, preheat temperatures, and porosities

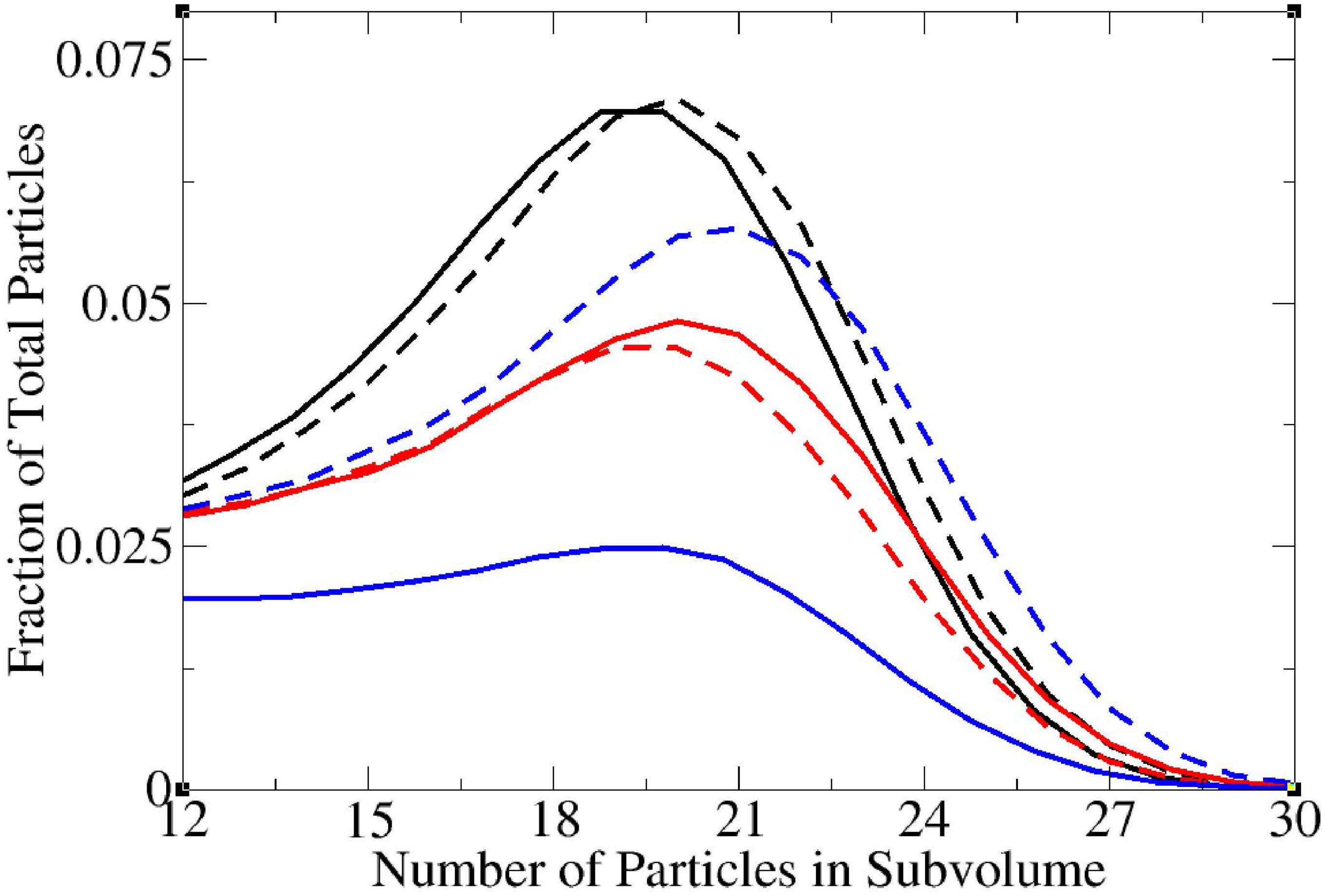
Map to continuum models

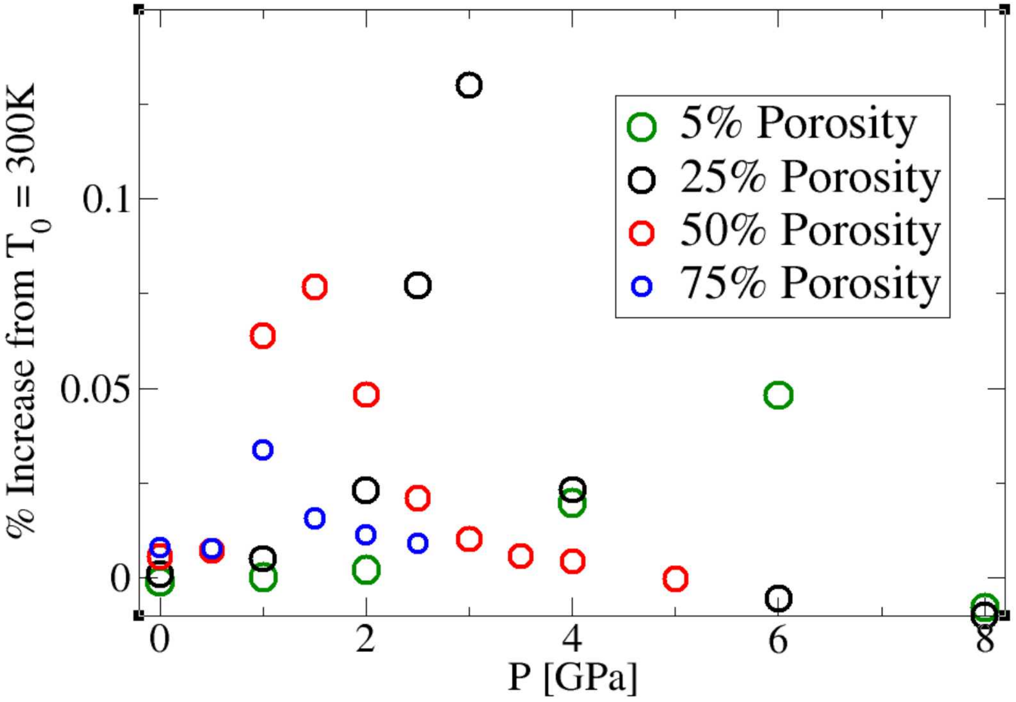
Extra Slides

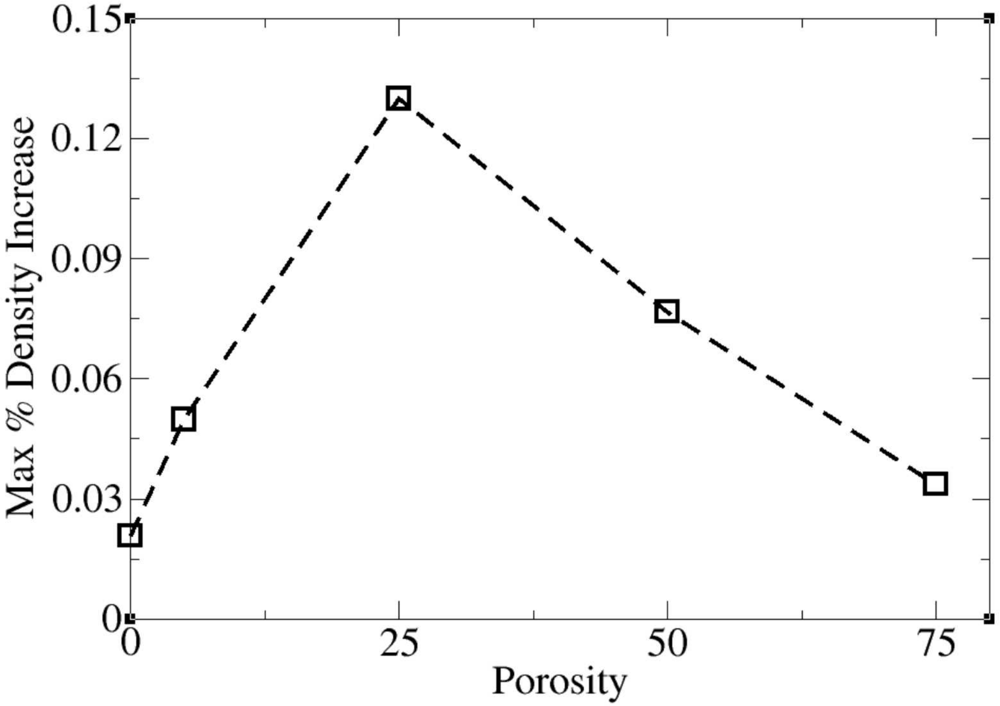
P = 1GPa

Porosity:
Black: 25%
Red: 50%
Blue: 75%

Solid: t = 0ns
Dashed: t = 1ns




% Increase from T_0 = 300K
0.1
0.05
0
0
2
4
6
8
P [GPa]
5% Porosity
25% Porosity
50% Porosity
75% Porosity


Max % Density Increase
0.15
0.12
0.09
0.06
0.03
0
0
25
50
75
Porosity