Molecular dynamics study of shock compression in porous silica glass

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Motivation for studying porous silica

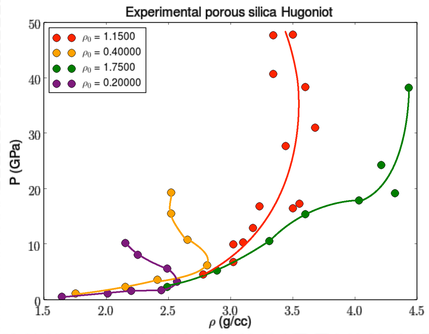
- Low density silica aerogels with a range of initial densities are commonly used in extreme conditions:
  - Space missions [1,2]
  - High P research [3,4,5]
- Gaining a more detailed understanding of the processes occurring under these conditions is important.
- Validate model by comparison with experiment.

1. M. Burchell et al., *Annu. Rev. Earth Planet. Sci.* **34**, 385 (2006).
2. D. Brownlee et al., *Science* **314**, 1711 (2006).
3. M. D. Knudson, J. R. Asay, and C. Deeney, *J. Appl. Phys.* **97**, 073514 (2005).
4. N. Holmes, High-Pressure Science and Technology—1993 (AIP, New York, 1994), p. 153.
5. M. D. Knudson and R. W. Lemke, *J. Appl. Phys.*, **114**, 053510 (2013).

An anomalous density inversion in the Hugoniot is observed experimentally at high shock pressures for highly porous silica [6]. This is due to shock energy being converted into kinetic energy as particles are vaporized into the void space. Thermal expansion occurs with respect to the same system shocked to a lower pressure. Local heating during void collapse has been studied [7].

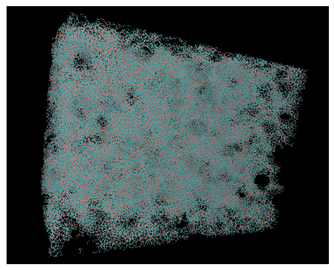
Can we model this density inversion with molecular dynamics?

Can we model with density inversion without using the expensive, propagating, non-equilibrium molecular dynamics (NEMD) model for dynamical shock simulation?



6. R. F. Trunin, *Experimental data on shock compression and adiabatic expansion of condensed matter* (2001).
7. J. Matthew D. Lane et al., *Comp. Mat. Sci.* ***79****, 873-876 (2013).*

Preparation of an initial porous state



ρ_0 (g/cc)	% Porosity
2.212	0
2.09	~5
1.08	~50
0.56	~75
0.23	~90
0.14	~95

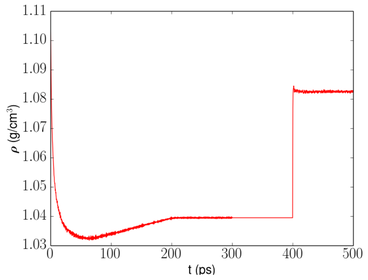
Fully atomistic molecular dynamics.

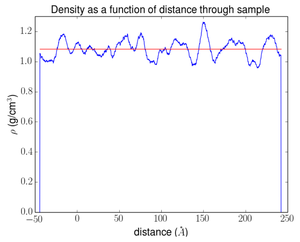
Short/medium range interactions are calculated using the BKS SiO_2 potential. B. W. H. van Beest et al., *Phys. Rev. Lett.* **64**(16), 1955 (1990).

Long range interactions are calculated using an Ewald sum.

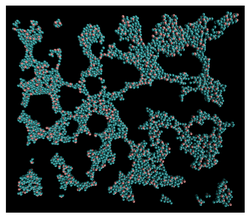
- Expand spherical voids at 2500 K until desired porosity is reached.
- Cool to 300 K.
- Equilibrate.
- Remove voids and re-equilibrate

Periodic boundary conditions
Timestep: 1 fs
Number of atoms: 373248



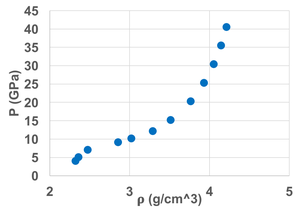


Each data point - 4 Å slice throughout 50 % porous sample
Average density: 1.08 g/cc
Average pore diameter: 20.0 Å
Number of atoms: 373248
Box dimensions: 182 x 217 x 290 Å^3



Reproducing the Hugoniot in MD

Hugoniot: the locus of points representing a series of final states originating from a single reference state, when the final and reference states are separated by a discontinuity (a shock), satisfying the jump conditions (energy, mass, and momentum conservations) which relate the initial state to the final state.



Reproducing the final state in MD

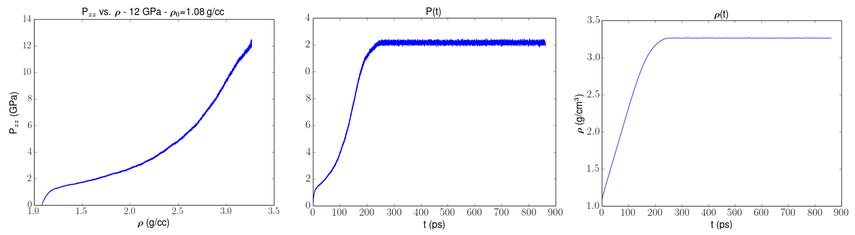
1. Non-equilibrium molecular dynamics. Propagate a shock through the material via a momentum mirror [7,8], calculate state variables to verify jump conditions.
   - Expensive and requires large system sizes.
   - Effectively reproduces experimental Hugoniot data for porous systems [7].

2. Non-propagating, constant stress Hugoniostat method [9]. Uniaxially compress system until final pressure is reached and jump conditions are met.
   - Less expensive.
   - Well tested in traditional Hugoniot space.
   - Not guaranteed to evolve along Rayleigh line or any other path through ρ, P space.
   - Path and efficiency of path depend on damping coefficients.
   - Previously untested on porous systems.

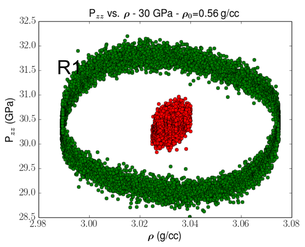
8. B. L. Holian and P. S. Lomdahl, *Science* **280**, 2085 (1998).
9. R. Ravelo et al., *Phys. Rev. B* **70**, 014103 (2004).

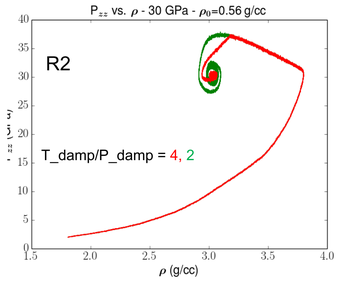
Hugoniostat trajectories

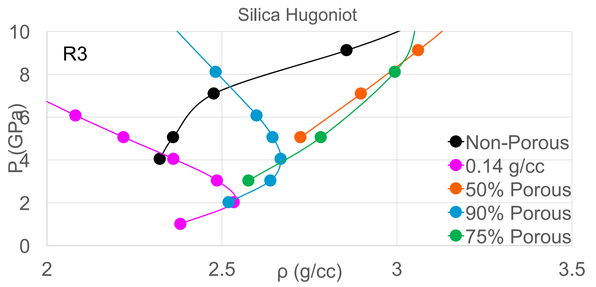
Constant stress Hugoniostat method in action.
50 % porous (1.08 g/cc) silica.
Final pressure: 12 Gpa.
Time step: 0.2 fs.
Temperature damping coeff: 20 ps
Pressure damping coeff: 20 ps

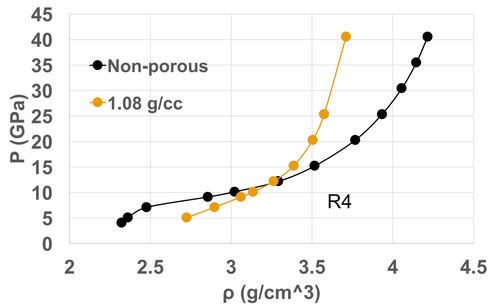


Results

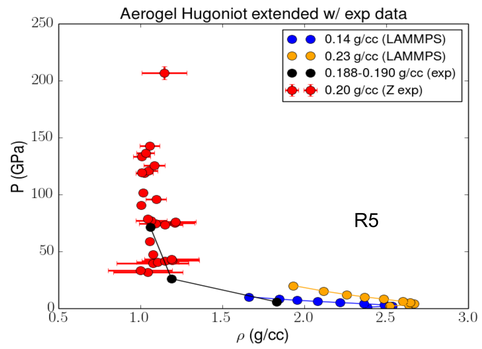


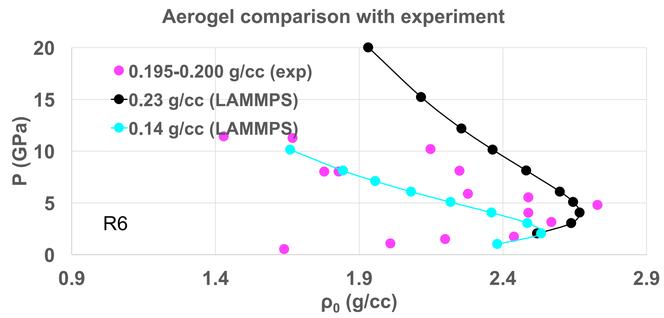






R1, R2 - Final state is not very sensitive to damping coefficient ratios.
R3 - Enhanced densification observed at lower pressures. This has been observed in silicon as well - J. Matthew D. Lane et al. *Phys. Rev. B* **90**, 134311 (2014).
R4 - Enhanced densification is observed at lower pressures.
Normal behavior of shocked porous material relative to shocked non-porous material returns above 10 Gpa.
R5 - Very high pressure experimental data for highly porous silica, collected using the Z-machine [5], plotted against LAMMPS and other experimental data shows a cusp in the Hugoniot. Z machine data is not reproducible with molecular dynamics. Simulation at the level of density functional theory is needed.
R6 - Demonstrated density inversion is in qualitative agreement with experiments





Conclusions

- BKS, a very simple SiO_2 potential, coupled with the constrant stress Hugoniostat reliably reproduces the Hugoniot for porous SiO_2.
- Enhanced densification is observed at lower pressures.
- Negative dP/dρ in the Hugoniot for highly porous SiO_2 is qualitatively captured in this very simple model.

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