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SAND2013-5370C

Joint 18th APS SCCM / 24th AIRAPT Conference, Seattle, WA, July 7-12, 2013

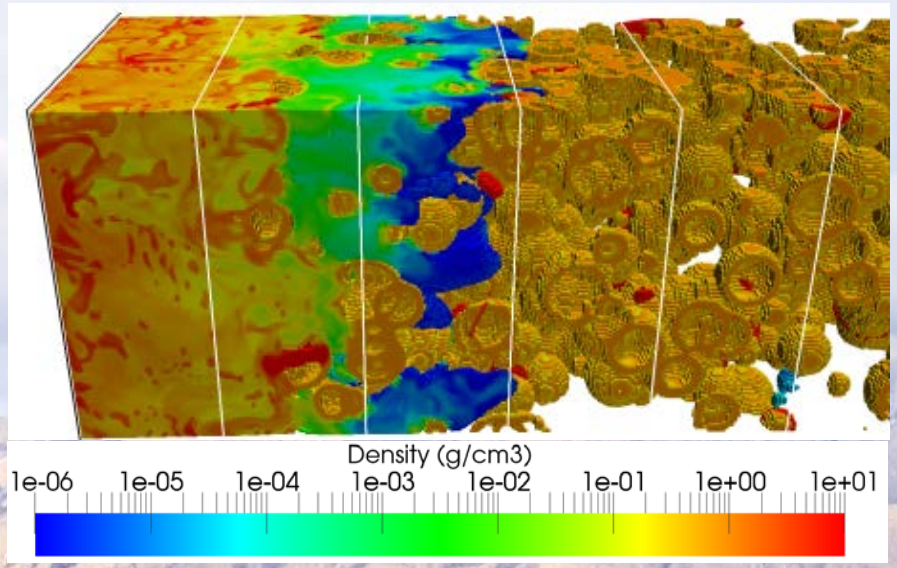
Shock Propagation Modeling in Heterogeneous Foams

Thomas A. Haill

Pulsed Power Sciences Center

Sandia National Laboratories

Albuquerque, NM



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Our motivation for modeling heterogeneous foams is to ultimately verify equation-of-state mixture rules

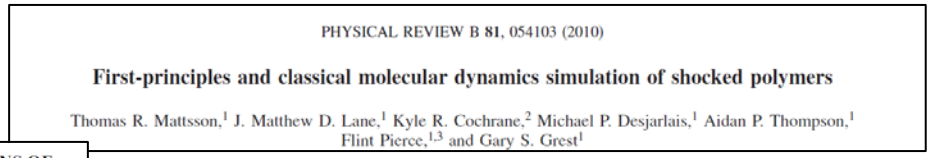
- **Model individual components**
  - Atomistic
  - Nanoscale
  - Mesoscale
  - Continuum
- **Model mixtures**
  - Atomistic
  - Nanoscale
  - Mesoscale
  - Continuum
- **Mixtures currently under study**
  - Uniform (miscible) mixtures
    - *Xenon / ethane*
    - *Xenon / deuterium*
    - *Xenon / argon*
  - Non-uniform (heterogeneous) mixtures
    - *PMP foam / platinum particles*
    - *Porous tantala (Ti_2O_3)*

Magyar: J4.001 (Tues 11:00)

Root: L2.007 (Tues 3:45)

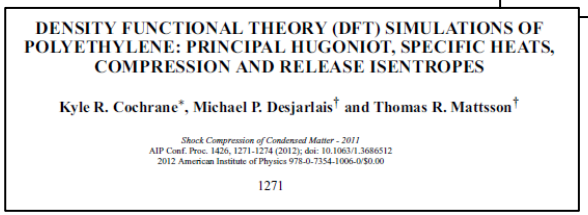
Mattsson: Z5.001 (Fri 11:00)

Cochrane: O2.001 (Wed 9:15)


PHYSICAL REVIEW B 81, 054103 (2010)

First-principles and classical molecular dynamics simulation of shocked polymers

Thomas R. Mattsson,[1] J. Matthew D. Lane,[1] Kyle R. Cochrane,[2] Michael P. Desjarlais,[1] Aidan P. Thompson,[1] Flint Pierce,[1,3] and Gary S. Grest[1]


DENSITY FUNCTIONAL THEORY (DFT) SIMULATIONS OF POLYETHYLENE: PRINCIPAL HUGONIOT, SPECIFIC HEATS, COMPRESSION AND RELEASE ISENTROPES

Kyle R. Cochrane*, Michael P. Desjarlais† and Thomas R. Mattsson†

Shock Compression of Condensed Matter - 2011
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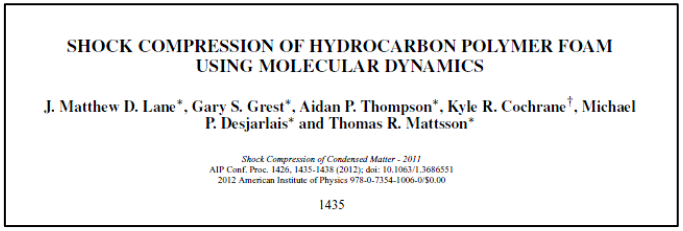
1271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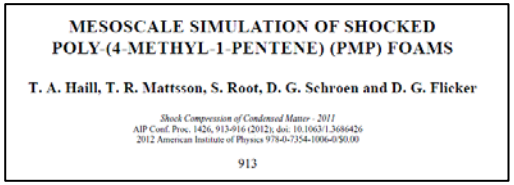
1435


MESOSCALE SIMULATION OF SHOCKED POLY-(4-METHYL-1-PENTENE) (PMP) FOAMS

T. A. Haill, T. R. Mattsson, S. Root, D. G. Schroen and D. G. Flicker

Shock Compression of Condensed Matter - 2011
AIP Conf. Proc. 1426, 913-916 (2012); doi: 10.1063/1.3686426
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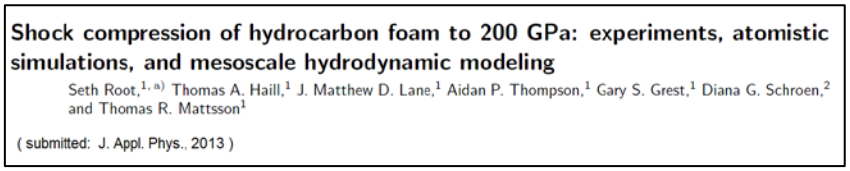
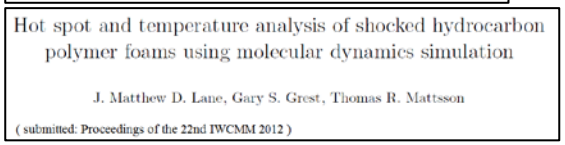

Shock compression of hydrocarbon foam to 200 GPa: experiments, atomistic simulations, and mesoscale hydrodynamic modeling

Seth Root,[1, a)] Thomas A. Haill,[1] J. Matthew D. Lane,[1] Aidan P. Thompson,[1] Gary S. Grest,[1] Diana G. Schroen,[2] and Thomas R. Mattsson[1]

(submitted: J. Appl. Phys., 2013)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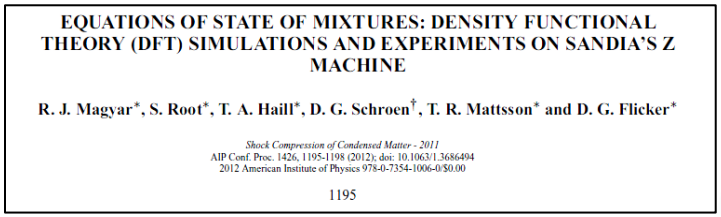
EQUATIONS OF STATE OF MIXTURES: DENSITY FUNCTIONAL THEORY (DFT) SIMULATIONS AND EXPERIMENTS ON SANDIA'S Z MACHINE

R. J. Magyar*, S. Root*, T. A. Haill*, D. G. Schroen†, T. R. Mattsson* and D. G. Flicker*

Shock Compression of Condensed Matter - 2011
AIP Conf. Proc. 1426, 1195-1198 (2012); doi: 10.1063/1.3686494
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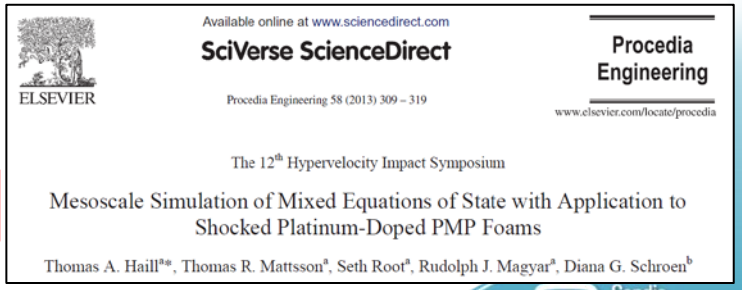
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Procedia Engineering 58 (2013) 309 – 319

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The 12th Hypervelocity Impact Symposium

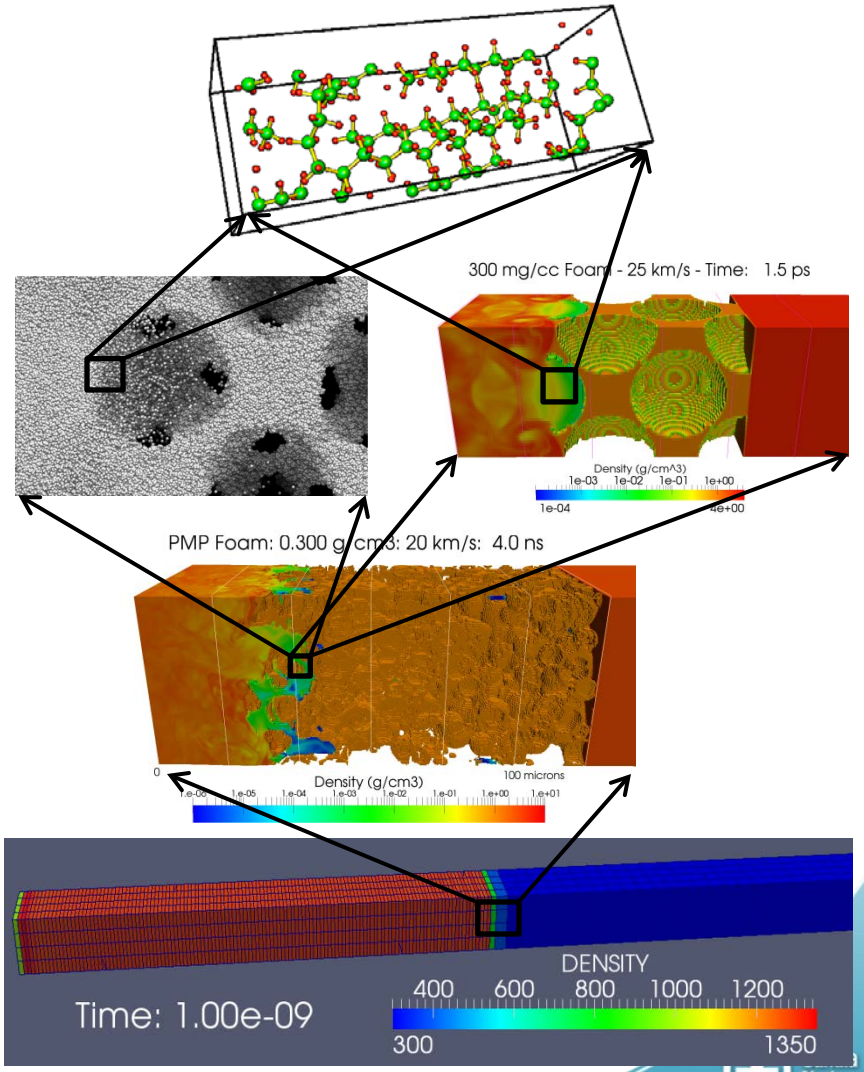
Mesoscale Simulation of Mixed Equations of State with Application to Shocked Platinum-Doped PMP Foams

Thomas A. Haill[a]*, Thomas R. Mattsson[a], Seth Root[a], Rudolph J. Magyar[a], Diana G. Schroen[b]

Sandia National Laboratories

Foam modeling efforts span 9 orders of magnitude from the atomistic scale (Å) to the continuum scale (cm)

- **Polymers under consideration:**
  - **Poly-(4-methyl-1-pentene)**
    i.e., PMP or TPX™
  - **Polyethylene (PE)**
- **Atomistic: O(10^{-10} m)**
  - **DFT (VASP)**
  - **Classical MD (LAMMPS)**
- **Nanoscale: O(10^{-9} m)**
  - **Classical MD (LAMMPS)**
  - **Hydrodynamics code (ALEGRA)**
- **Mesoscale: O(10^{-6} m)**
  - **Hydrodynamics code (ALEGRA)**
- **Continuum: O(10^{-2} m)**
  - **Hydrodynamics code (ALEGRA)**
  - **Hydrodynamics code (KULL)**



Scaling shows why the hydrodynamic equations may be solved over 9 orders of magnitude in spatial scales

Hydrodynamic Equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = 0$$

$$\rho\left(\frac{\partial \vec{V}}{\partial t} + \left(\vec{V} \cdot \nabla\right)\vec{V}\right) = -\nabla \cdot P$$

$$\rho\left(\frac{\partial e}{\partial t} + \left(\vec{V} \cdot \nabla\right)e\right) = -P : \nabla \vec{V}$$

Variable Scaling

$$\tilde{\rho} = \frac{\rho}{\rho_0} \qquad \tilde{t} = \frac{t}{L/U_P}$$

$$\tilde{\vec{V}} = \frac{\vec{V}}{U_P} \qquad \tilde{P} = \frac{P}{\rho_0 U_P^2}$$

$$\tilde{\vec{x}} = \frac{\vec{x}}{L} \qquad \tilde{e} = \frac{e}{\rho_0 U_P^2}$$

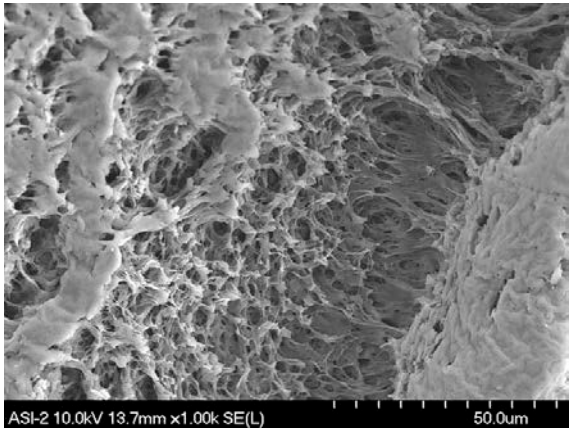
- **Scale by mean initial density ρ_0, particle (piston) velocity U_P, and void size L**
- **Density, velocity, pressure, and specific internal energy are independent of scale length**
- **Gradients inversely dependent on scale length**
- **Shock front thickness defined by scale length**

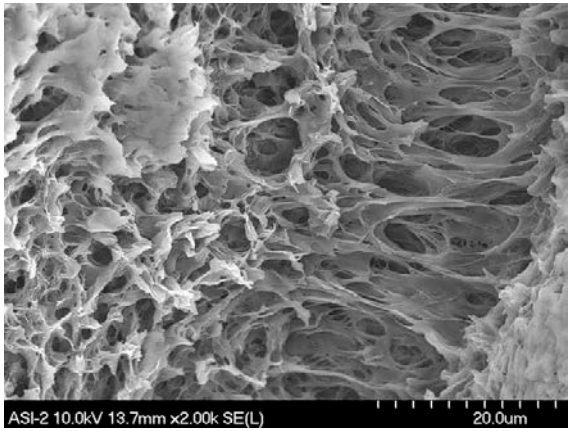
Optical and scanning electron emission images of pure and platinum-doped PMP foam show 1-5 micron voids and 1-3 micron platinum particle sizes

50 μm resolution

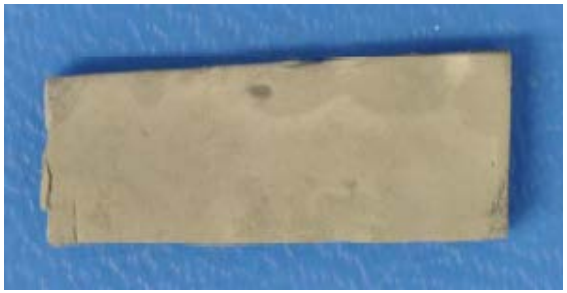
20 μm resolution

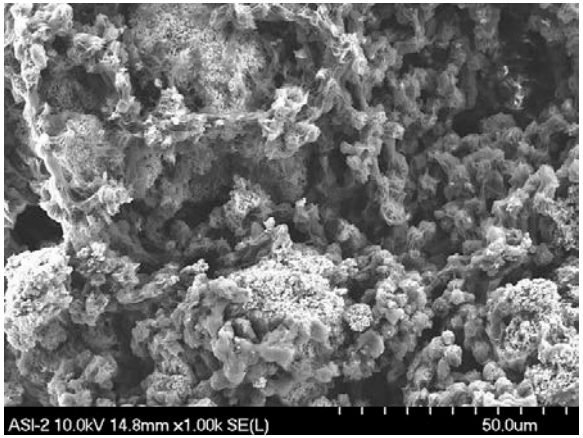
Pure 300 mg/cm^3 foam

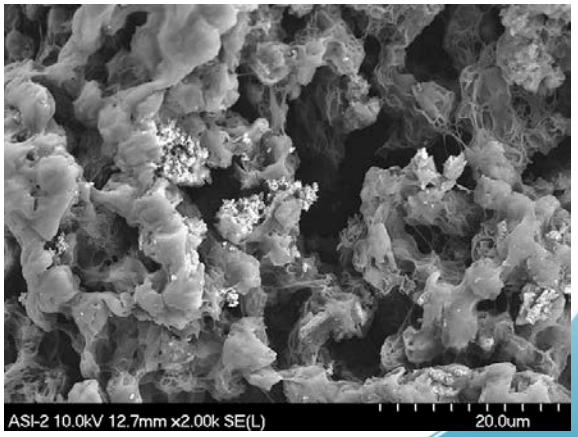




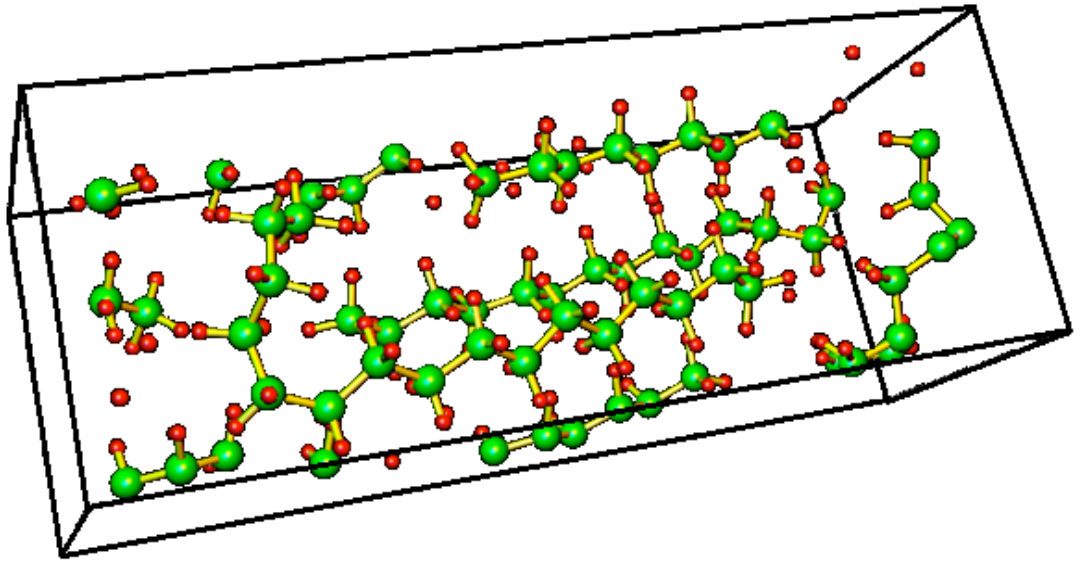
Doped 300 mg/cm^3 foam







Dense Polymers at the Atomistic Scale



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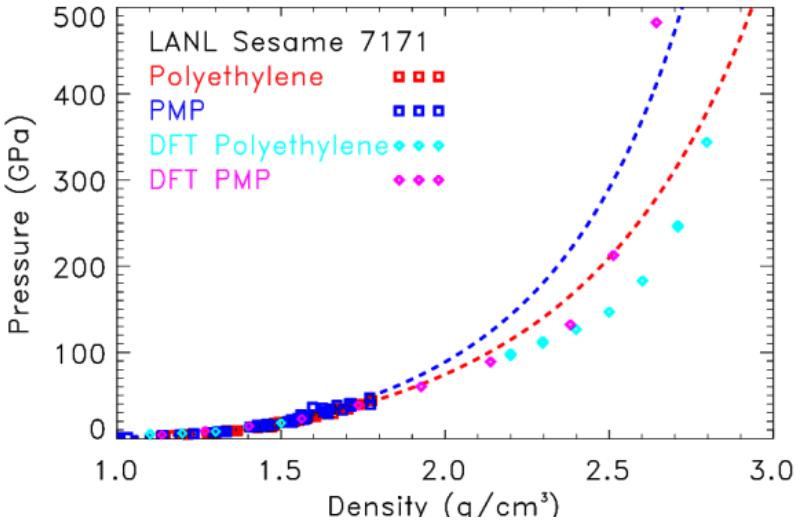
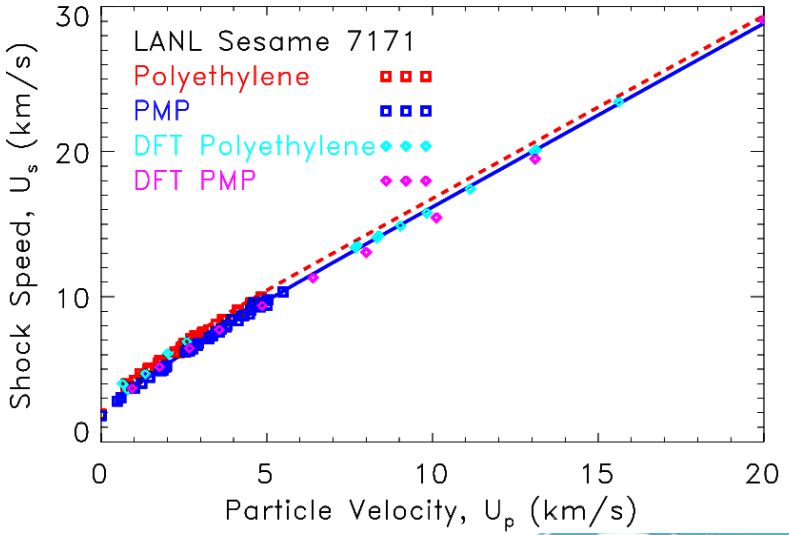
1271

Atomistic scale modeling has been limited to full density PE and PMP polymers

- DFT and classical MD simulations computed Hugoniot states to 350 to 500 GPa
  - DFT: 200 to 440 atoms
  - MD: 22176 atoms
  - $\rho_{PE} = 0.955$ g/cm^3
  - $\rho_{PMP} = 0.83$ g/cm^3
- Comparison to experimental data up to 50 to 70 GPa
- Dissociation of polymer chains between 2000-4000 K and 2 ½ compression
- Sesame 7171 for polyethylene also used to model PMP and polypropylene

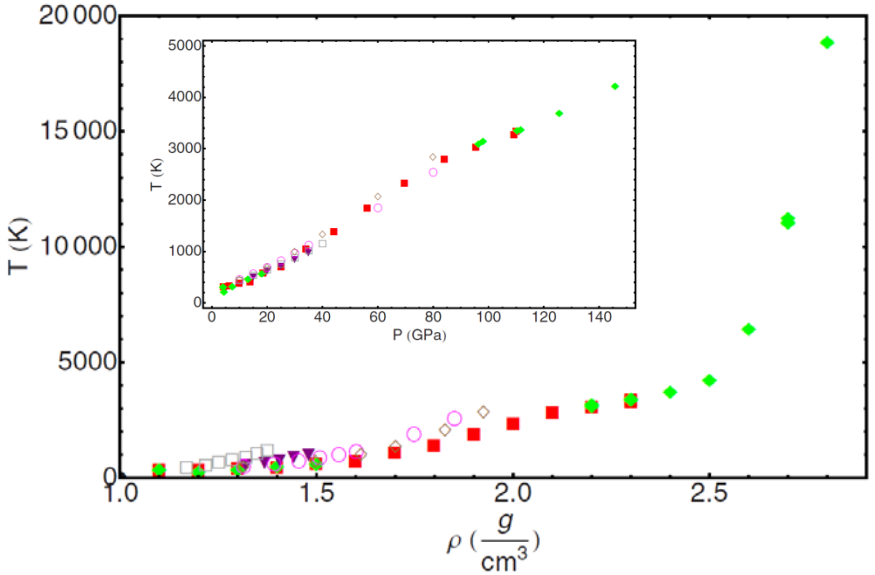


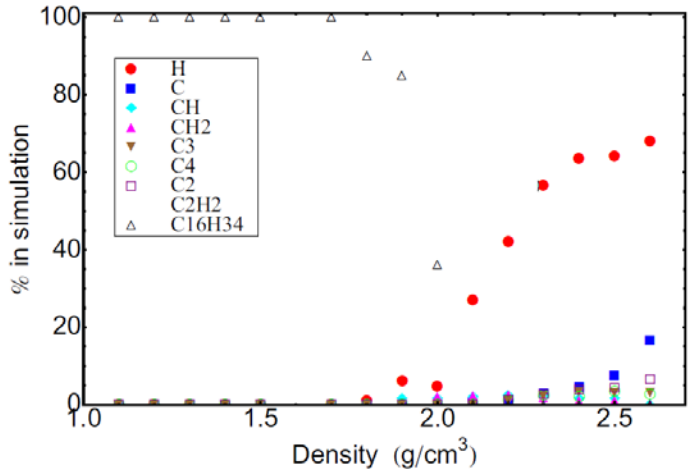


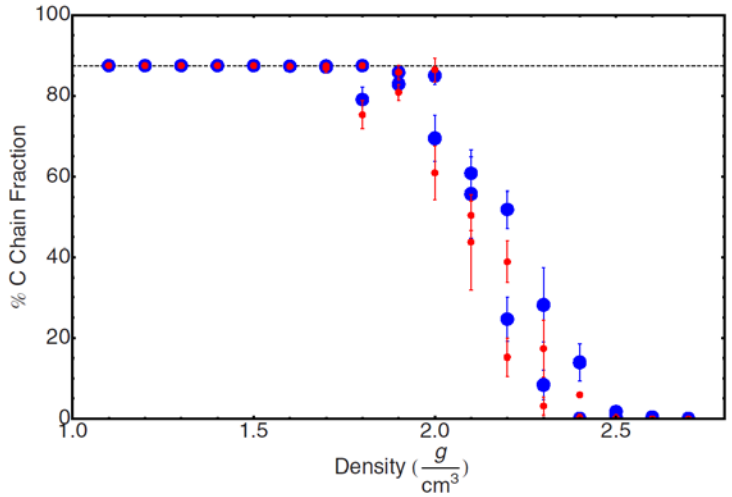
T.R. Mattsson, *et al.*, Phys. Rev. B, 81, 054103 (2010).
M.A. Barrios, *et al.*, Phys. Plasmas, 17, 056307 (2010).

DFT and classical MD simulation illuminate dissociation and chemistry of polymer chains

- DFT and classical MD simulations computed Hugoniot states to 350 to 500 GPa
- Dissociation of polymer chains
  - 3000 - 4000 K
  - 80 – 130 GPa
  - 2 - 2 ½ compression ratio







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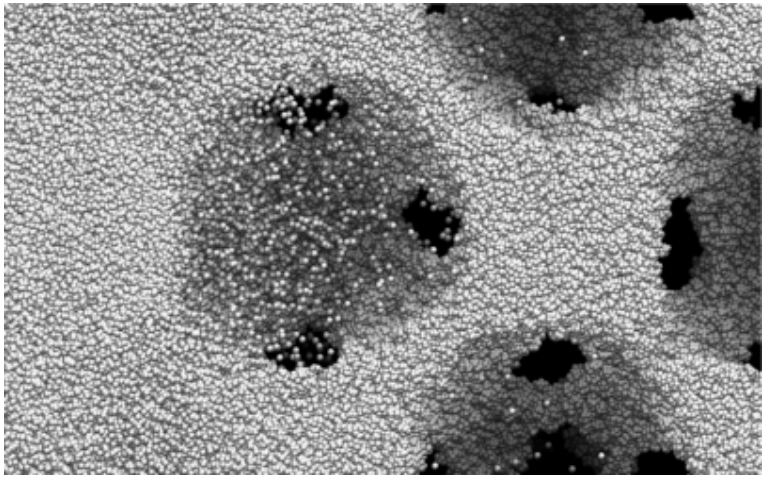
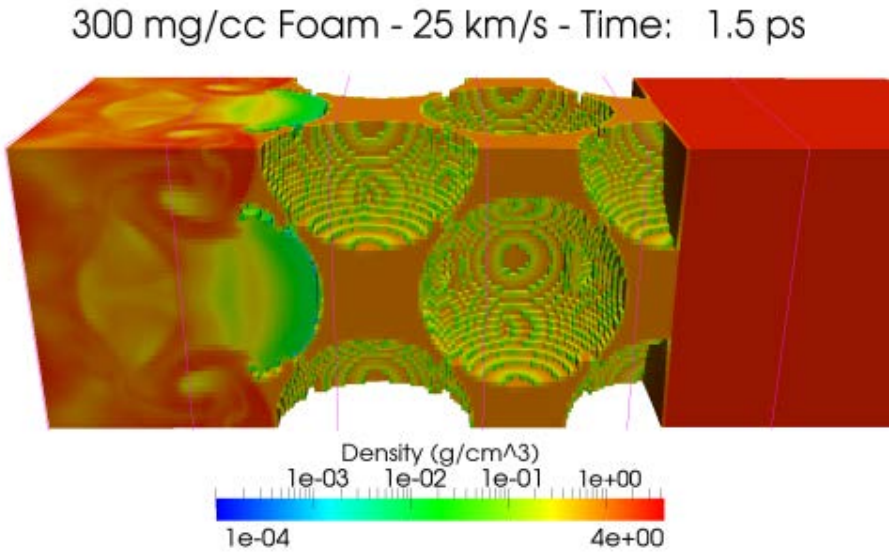
K.R. Cochrane, et al., SCCM, AIP CP 1426, 1271 (2011).

Polymer Foams at the Nanometer Scale





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Hot spot and temperature analysis of shocked hydrocarbon polymer foams using molecular dynamics simulation

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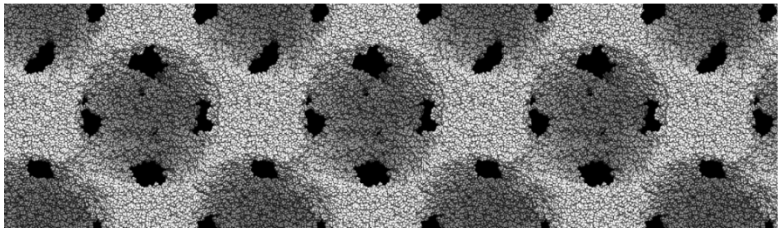
(submitted: Proceedings of the 22nd IWCMM 2012)

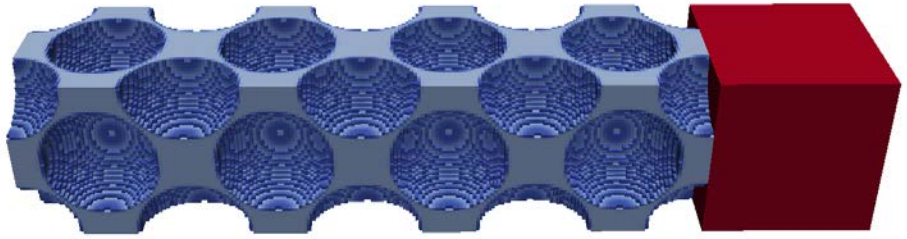
Nanometer Scale: ○●○○

Nanoscale simulations model foams using classical MD (LAMMPS) and hydrodynamics codes (ALEGRA)

LAMMPS



ALEGRA



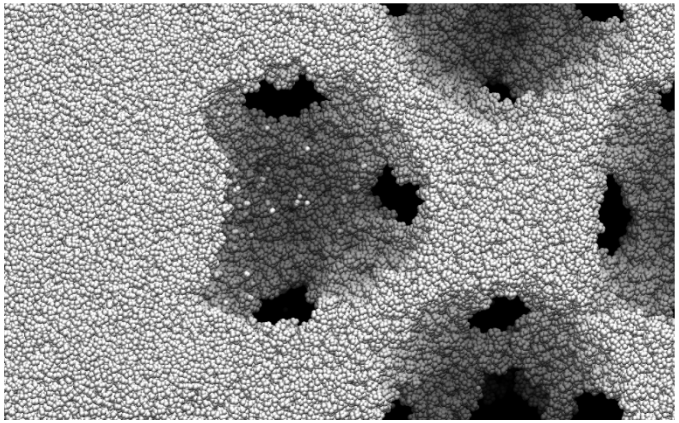
- **Directly compare classical MD and hydrodynamics codes**
  - **Idealized foam: 0.300 g/cm^3**
  - **20 nm × 20 nm × 80 nm foam simulation domains**
  - **Face-centered cubic (FCC) void structure: ~12-nm diameter voids**
  - **5 to 25 km/s impact speeds**
- **LAMMPS**
  - **1.44 million atoms**
- **ALEGRA**
  - **0.57 to 4.33 million elements**
  - **2.5 to 0.33 atoms per element!**

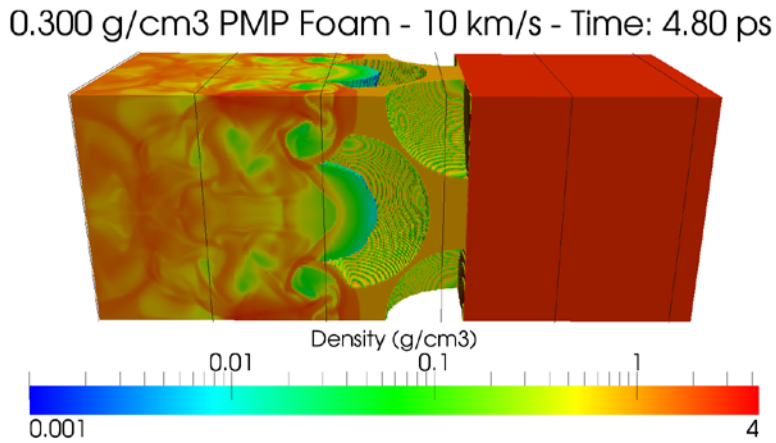
Nanoscale modeling comparing classical MD (LAMMPS) and continuum (ALEGRA) produce comparable results

LAMMPS

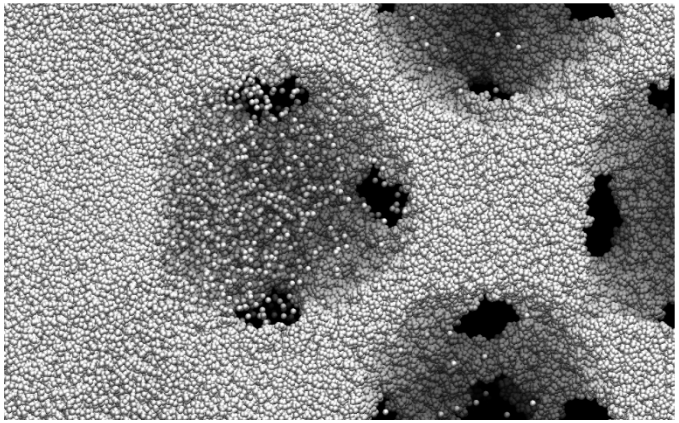
ALEGRA

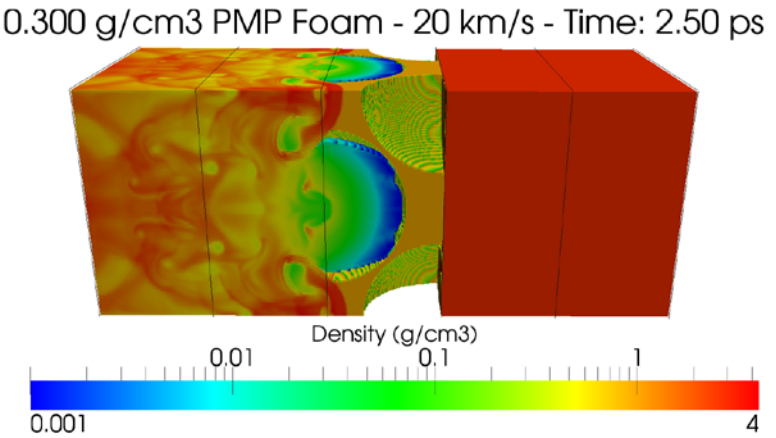
10 km/s





20 km/s





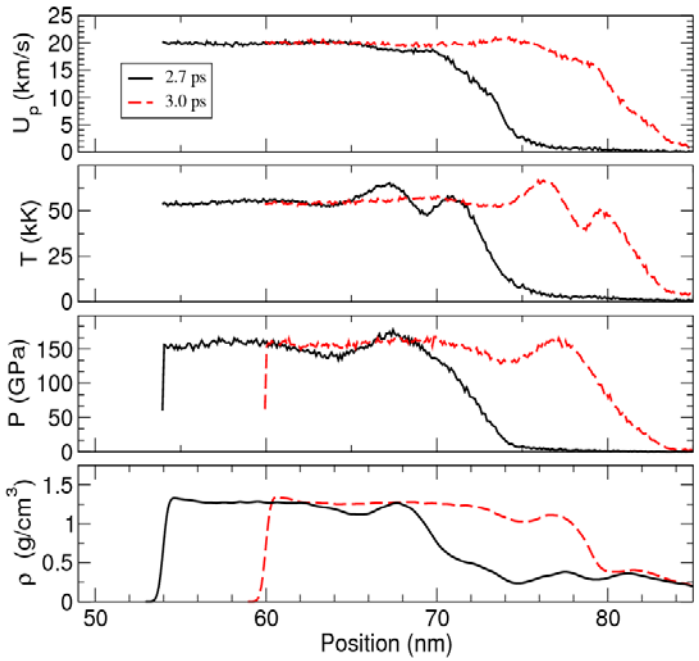
Vaporization and dissociation seen in MD and hydrodynamic simulations.

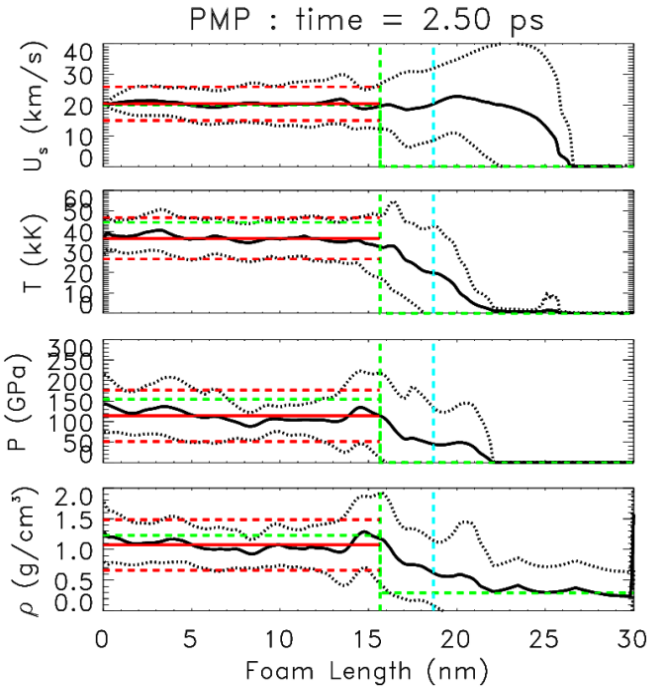
Nanoscale modeling comparing classical MD (LAMMPS) and continuum (ALEGRA) produce comparable results

LAMMPS

ALEGRA

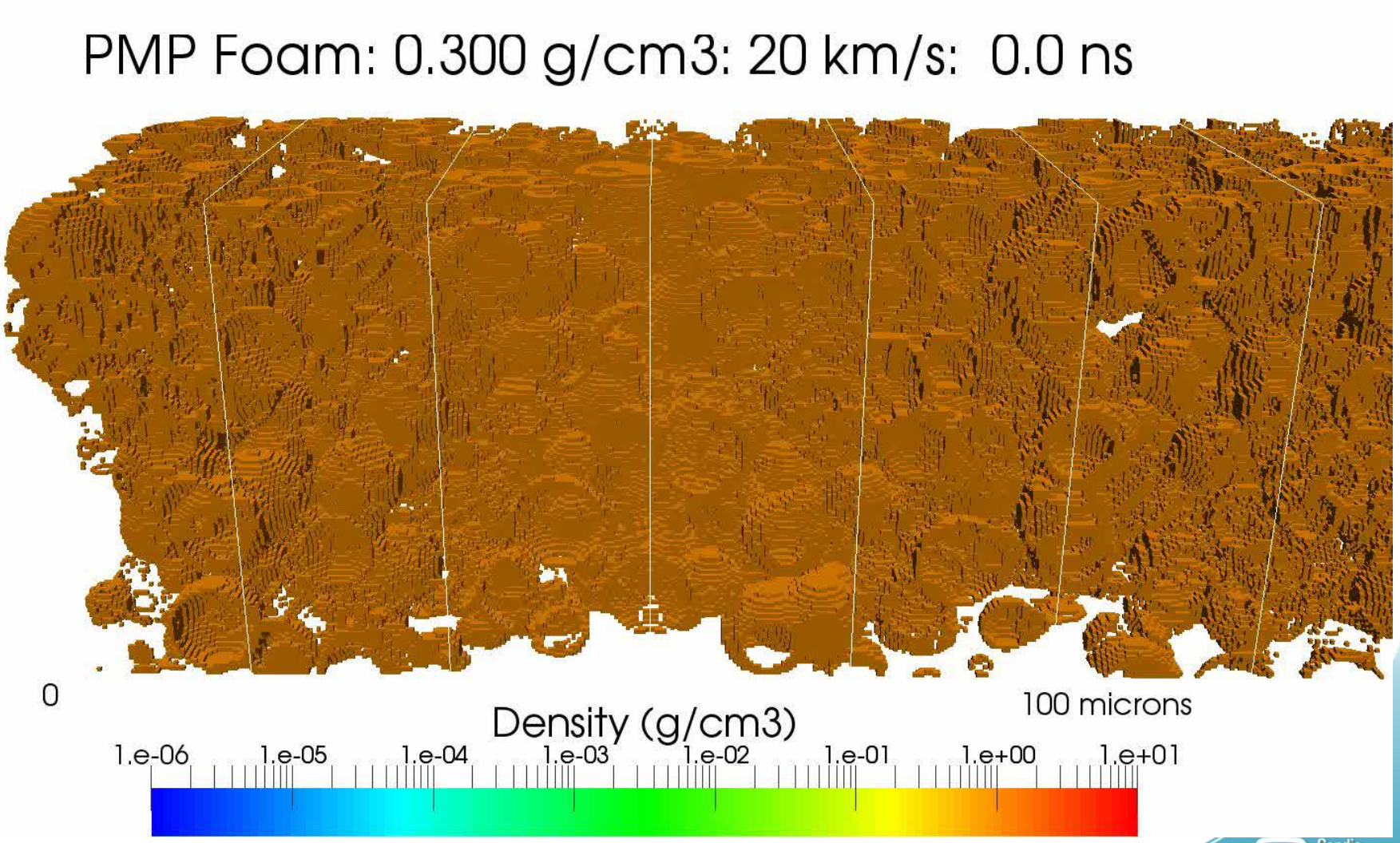
20 km/s





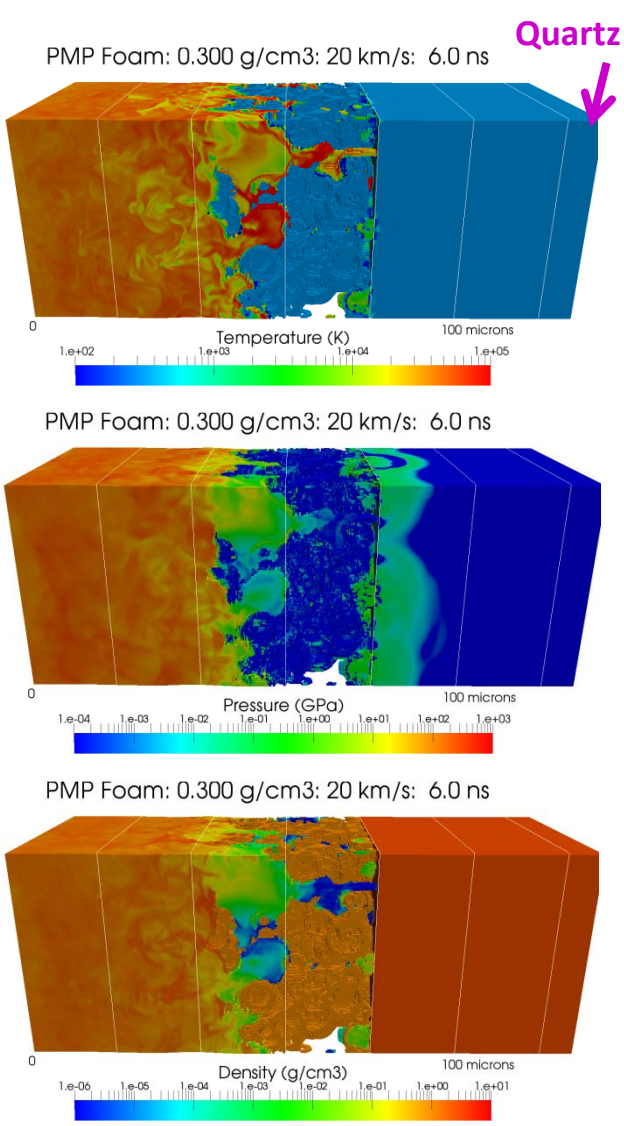
- Mean post-shock values comparable
- Shock location similar when translated by Galilean transformation
- Hydrodynamic simulation have larger RMS deviations due to post-shock turbulence seeded by large initial density perturbation
- Mean density, pressure, Us, Up data are compared to experiments

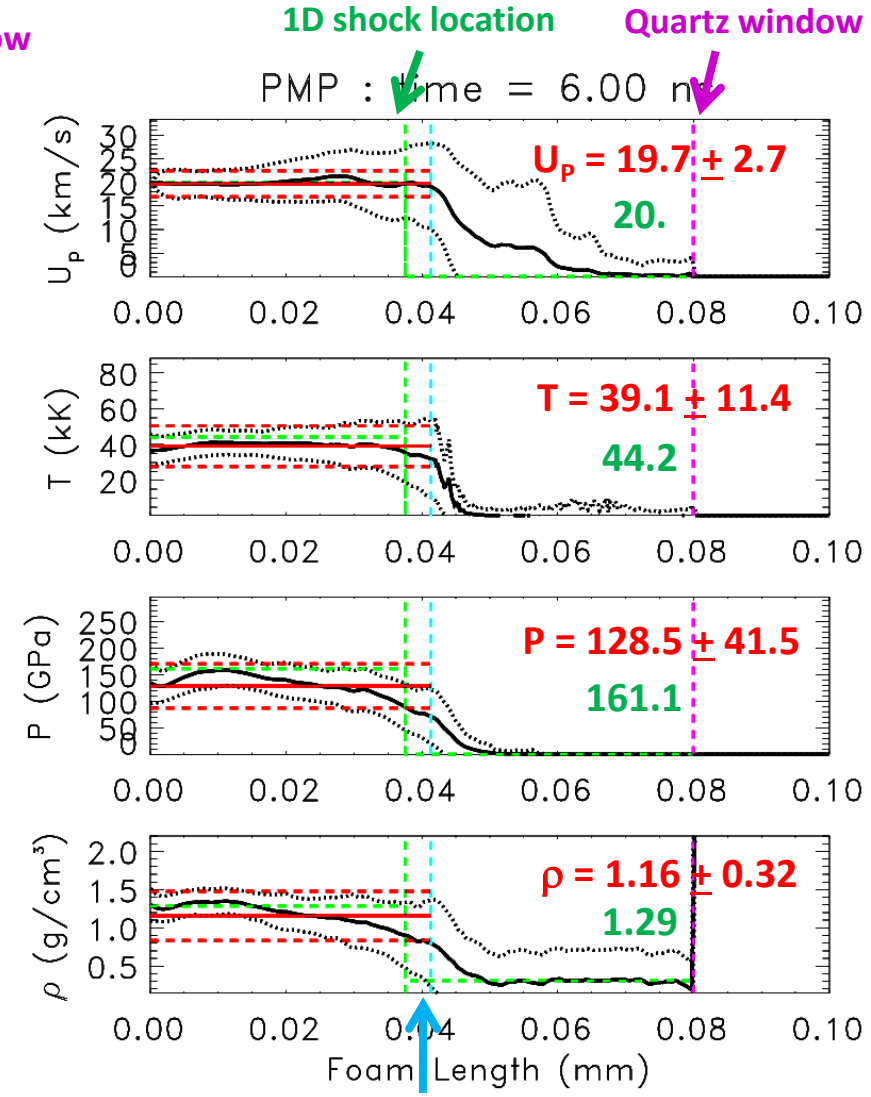
Pure PMP Foams at the Micrometer Scale (Mesoscale)



Micrometer Scale: ○●○○

Noh simulation of 0.300 mg/cm³ foam at 20 km/s – Foam compresses with a diffuse shock front

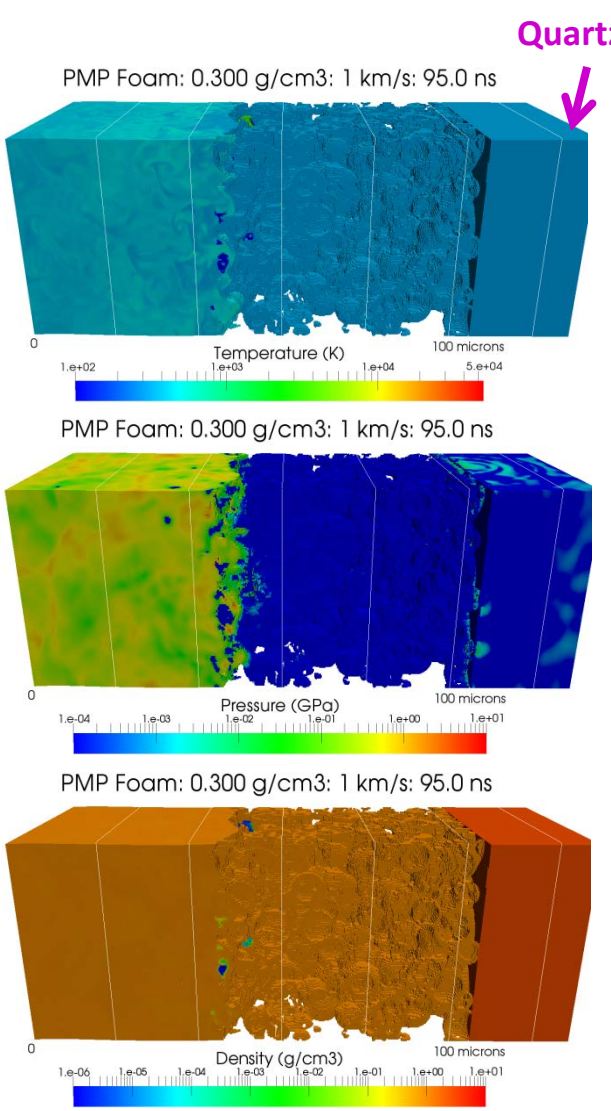


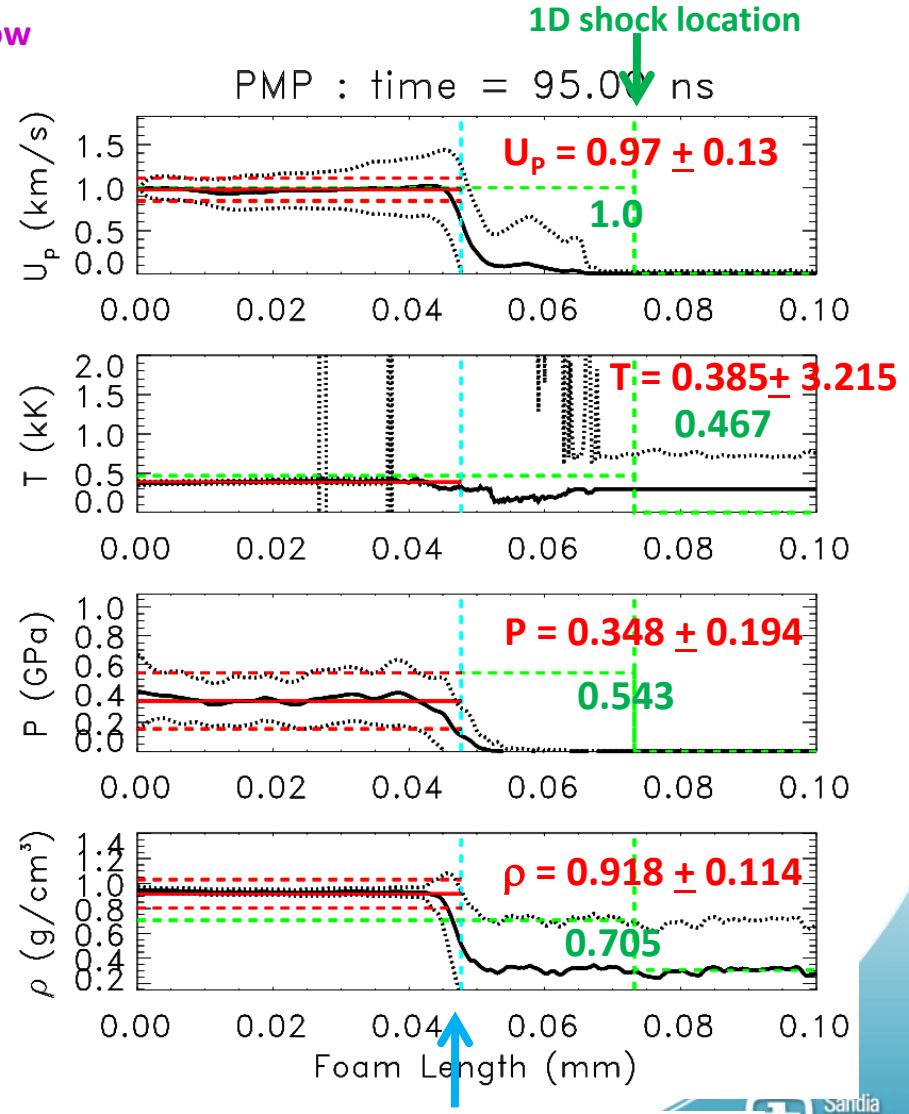


Average of pre- and post-shock 1D density

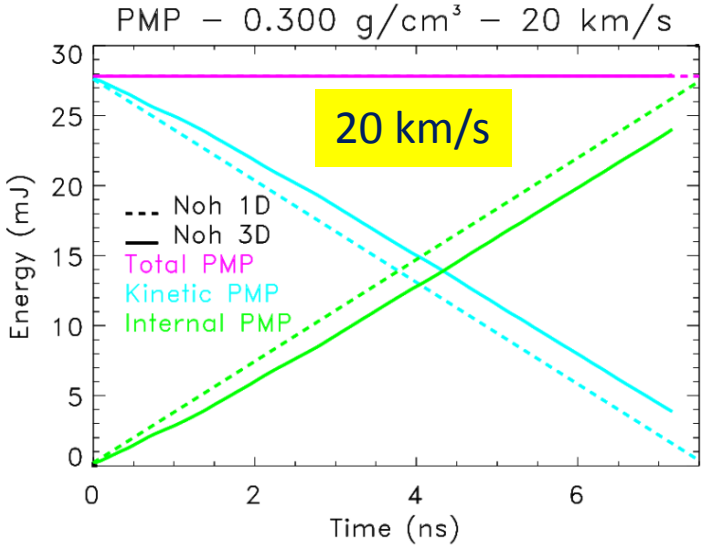
Micrometer Scale: ○○○●

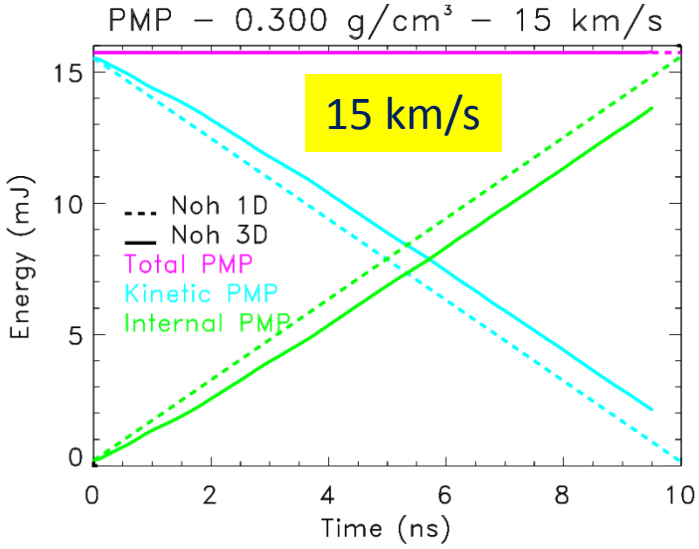
Noh simulation of 300 mg/cm³ foam at 1 km/s – Foam compacts to dense polymer

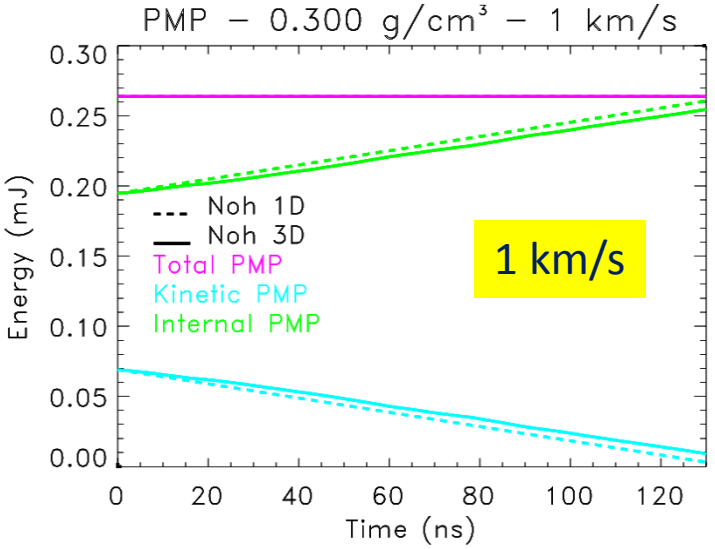




Comparison of 3D and 1D energy tallies show 3D retains more kinetic energy consistent with post-shock vorticity





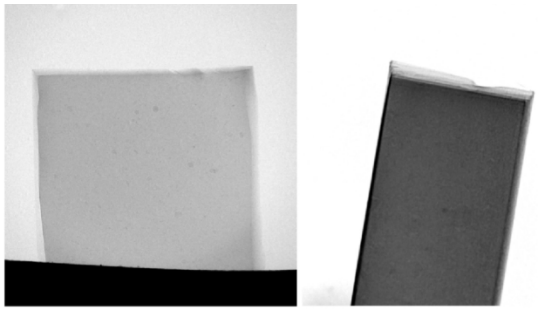


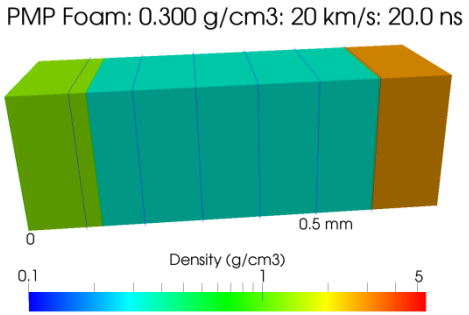
- **Kinetic energy converts to internal energy**
- **3D kinetic energy loss ~8% less than 1D**
  - **KE stored in post-shock vorticity as represented by RMS deviation and fluctuations**
- **3D internal energy increase ~8% less than 1D**
- **Contributes to lower pressure in 3D**

Polymers and Foams at the Continuum Scale

Optical image of 0.300 g/cm^3 PMP foam

Radiographs of 0.300 g/cm^3 PMP foam





Shock compression of hydrocarbon foam to 200 GPa: experiments, atomistic simulations, and mesoscale hydrodynamic modeling

Seth Root,[1, a)] Thomas A. Haill,[1] J. Matthew D. Lane,[1] Aidan P. Thompson,[1] Gary S. Grest,[1] Diana G. Schroen,[2] and Thomas R. Mattsson[1]

(submitted: J. Appl. Phys., 2013)

MESOSCALE SIMULATION OF SHOCKED POLY-(4-METHYL-1-PENTENE) (PMP) FOAMS

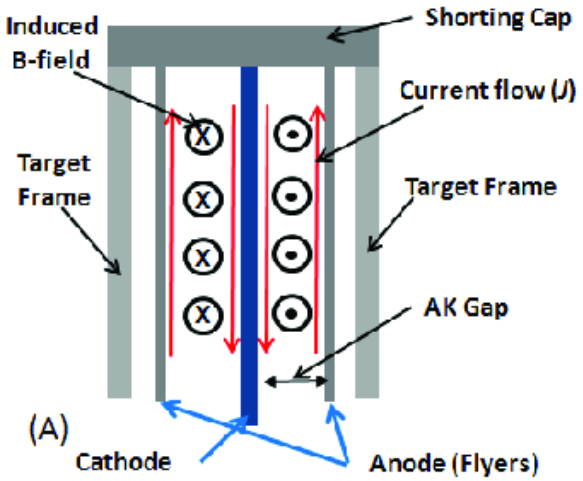
T. A. Haill, T. R. Mattsson, S. Root, D. G. Schroen and D. G. Flicker

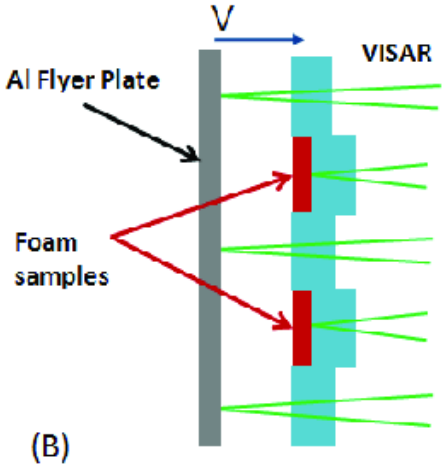
Shock Compression of Condensed Matter - 2011
AIP Conf. Proc. 1426, 913-916 (2012); doi: 10.1063/1.3686426
2012 American Institute of Physics 978-0-7354-1006-0/$0.00

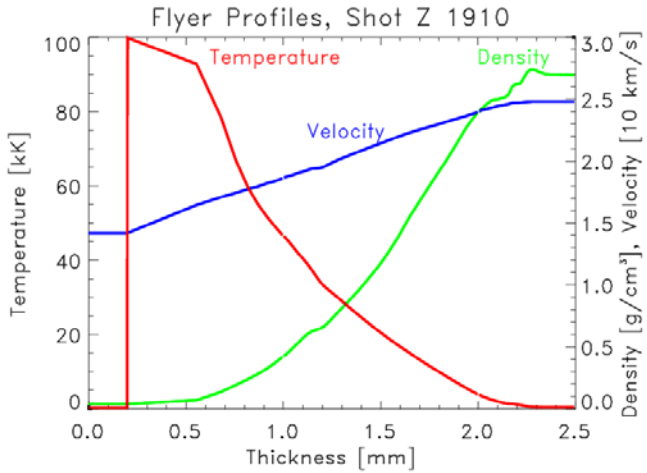
913

Custom 1D simulations of homogenized, P-α foams are driven by realistic graded Al flyer profiles

- Customized foam simulations are based upon Z shot 1910
- P-α model accounts for porosity before compaction
- Average foam densities are tailored to match average experimental densities
- Use Al flyer density, temperature and velocity profiles to impact foam
- Flyer velocity profile peaks are scaled to match unfolded experimental flyer velocities





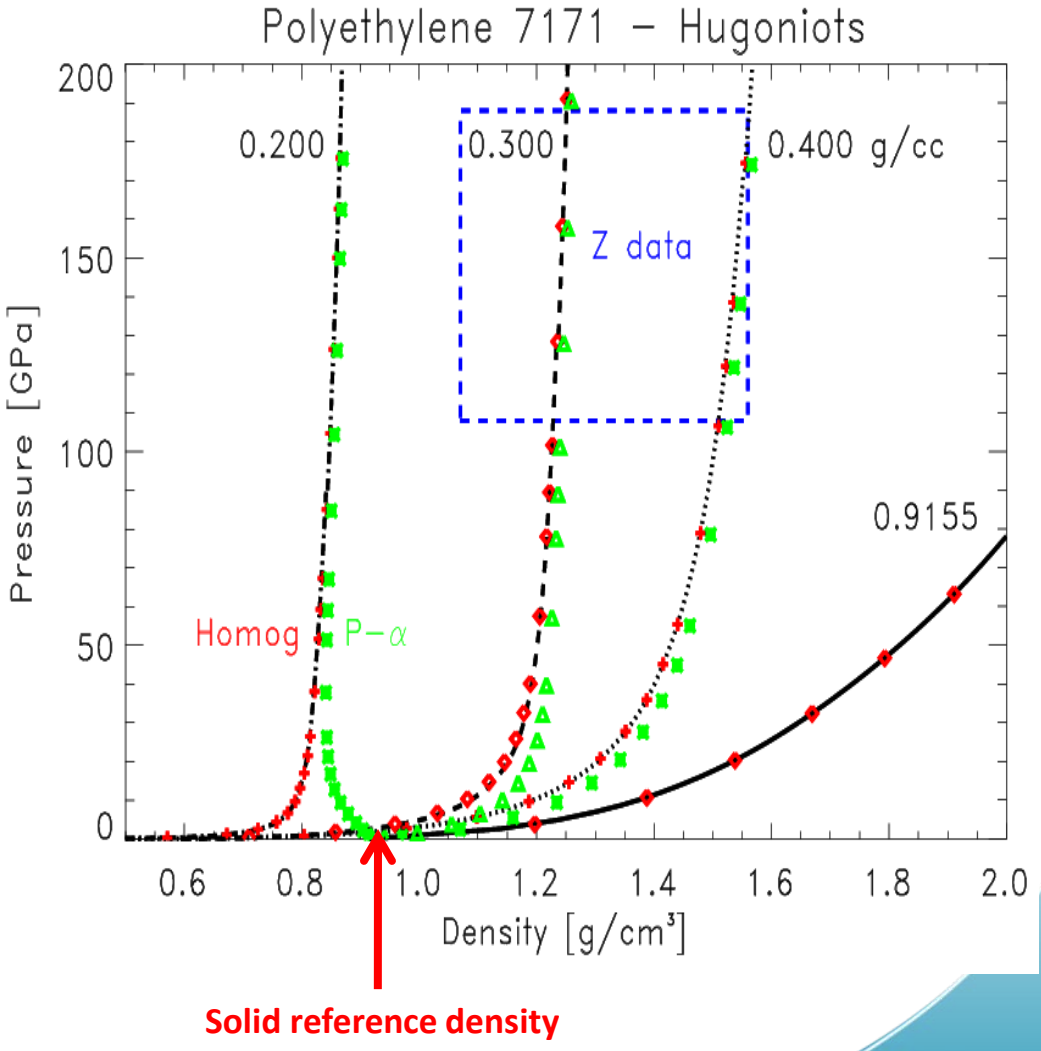


Foam target

Aluminum flyer profiles courtesy of R. Lemke, SNL.

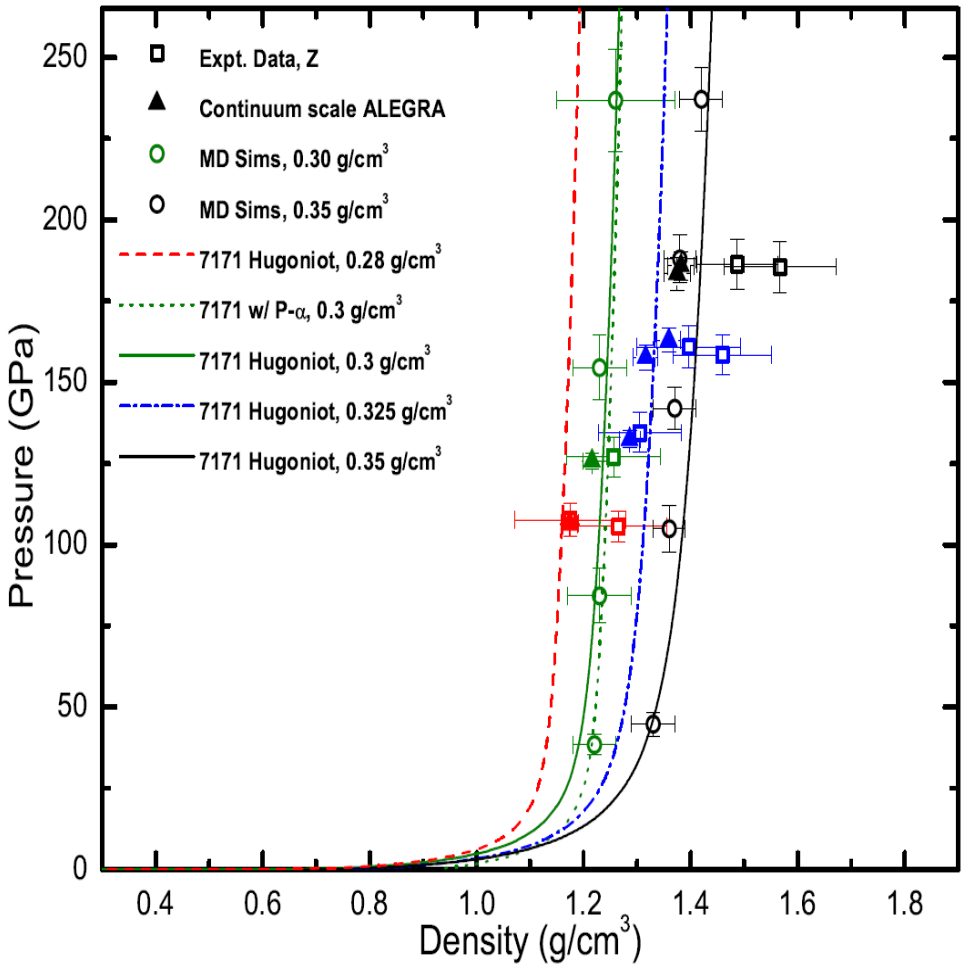
Summary of 1D homogenous foam results: Effect of P-α model on foam Hugoniots

- P-α model is relevant below 12 km/s and 40 GPa
- Homogenous and P-α models agree above 12 km/s and 40 GPa
- P-α model is of limited use in modeling Z experiments
  - The approximate range of Z data is outlined



Custom 1D homogenized P-α foam simulation results are consistent with Z experiments

- Incidental slope in data
  - Lower density foams shot at lower flyer velocities
  - Higher density foams shot at higher flyer velocities
- Pressures are consistent between experiment and simulation
- Experimental density range is broader than simulation and analytic density ranges
  - Due to foam non-uniformities not captured by the homogenized simulations?
- Z data lies well above the pressures where P-α model effects would been seen

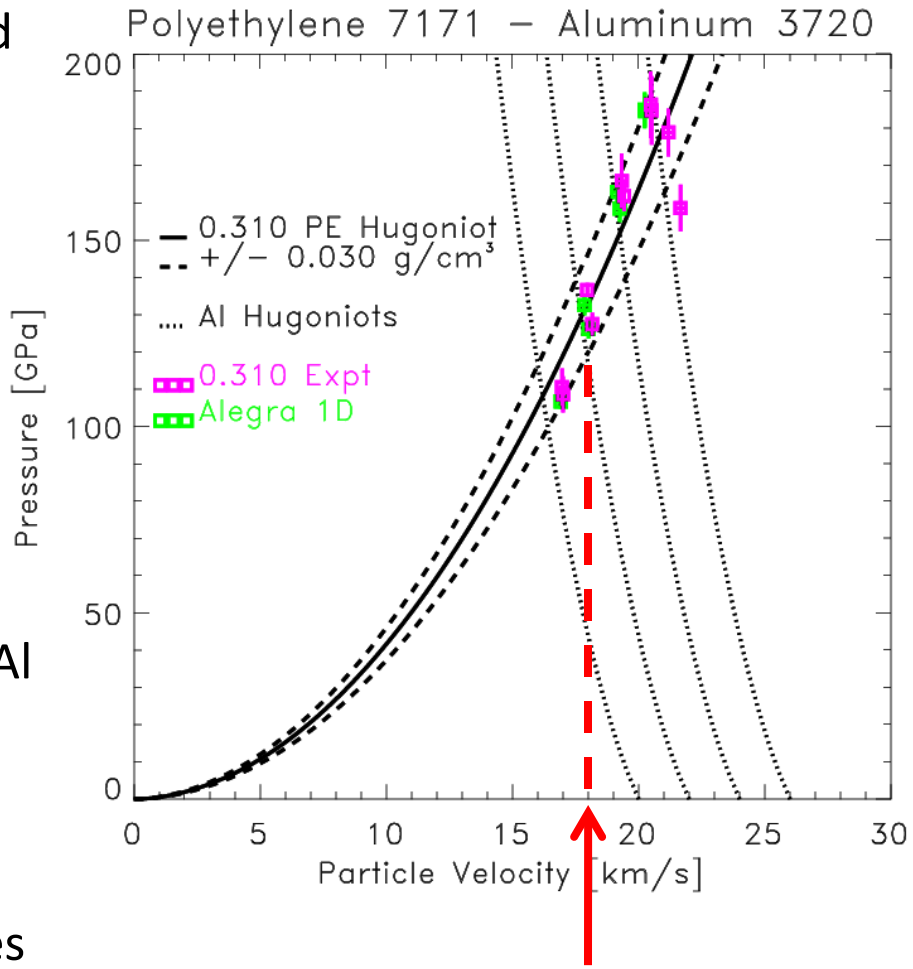


Continuum Scale: ○○○○●○

Summary of Experiments: Hugoniots and Impedance Matching

- Shock Hugoniots are determined from homogenous material EOS
- Impedance curve:

  $P = (\rho_0 * U_s) * u_p$
- Experiments:
  - TPX foam ~ 0.310 g/cm^3
  - Flyer velocity ~ 20 – 26 km/s
- Data roughly lies in region bounded by lower and upper impedance curves for PMP and Al
- Standard shock impedance methods apply!
- Equivalent Noh-type velocity at intersection of impedance curves



Equivalent Noh velocity

Sandia National Laboratories

Continuum Scale: ○○○○●

Summary of Experiments: Hugoniots and Impedance Matching

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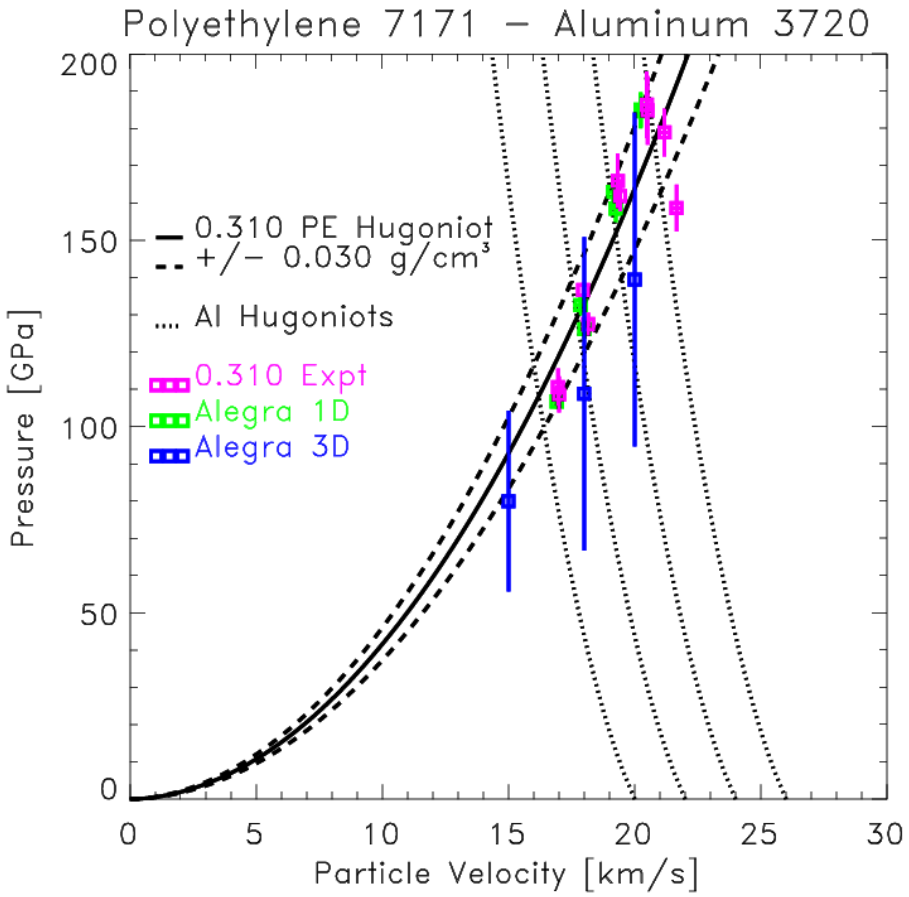
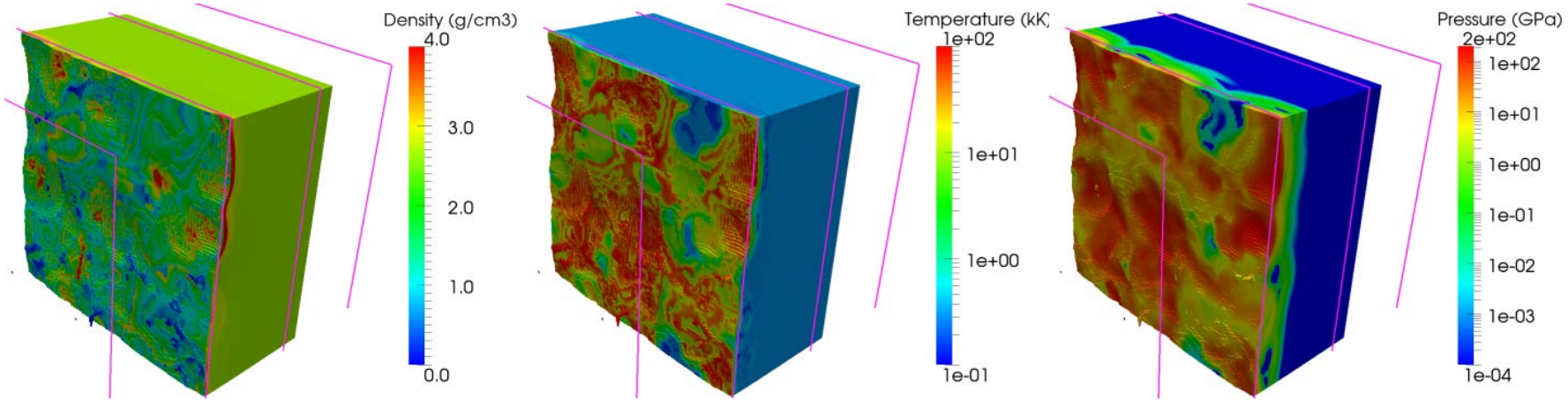


- Equivalent Noh-type velocity at intersection of impedance curves

Buckling of the quartz window face and the non-uniformity of the shock entering the quartz at 7.0 ns is a consequence of the randomness of the foam



- May explain temporary disruption of VISAR signal when shock breaks out of the foam
  - VISAR signal eventually restored after secondary release or perhaps shock enters quartz
- Simulation shock speed = 28.57 km/s
- Experimental shock speed = 27.8 ± 1.0 km/s

Conclusions

- **Atomistic scale**
  - **DFT and classical MD can be used to compute Hugoniot and EOS data for dense polymers at high densities, pressure, temperatures, and shock velocity**
- **Nanometer scale**
  - **Classical MD can be used to model and compute Hugoniot data of polymer foams**
  - **Hydrodynamics simulations at the nanoscale, while not technically valid in terms of large numbers of particles per cell, show good qualitative agreement with classical MD**
- **Micron scale (Mesoscale)**
  - **Shock width correlates with pore size**
  - **RMS deviations independent of scale**
  - **Comparison to experiment**
    - ***Explains loss of VISAR signal***
    - ***Shock speed at high impacts close – lends credibility***
- **Continuum scale**
  - **Experiment and continuum hydro analysis agree – both 1D**
  - **Particle speed and shock arrival times (shock speed) directly measured**
  - **Density and pressure inferred from impedance matching**
    - ***Provides upper bound on density / pressure***