

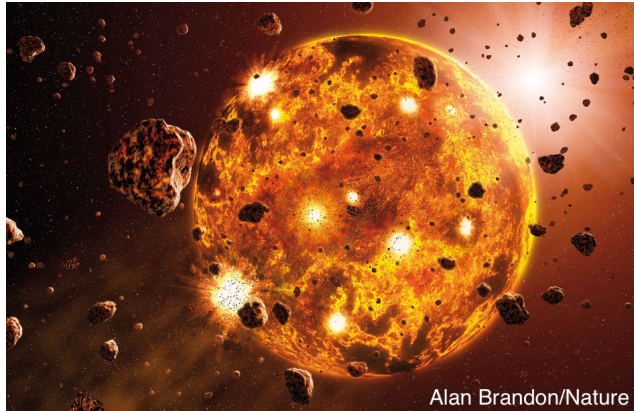
SAND2017-7139C

## Shock states of solid $\text{Mg}_2\text{SiO}_4$

Joshua P. Townsend & Luke Shulenburg

Sandia National Laboratories, Albuquerque, NM 87185, USA





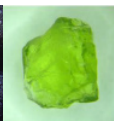
Alan Brandon/Nature

Planets motivate understanding material properties under extreme conditions.

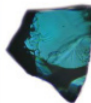
Silicates are the building blocks of terrestrial planets.



Credit: David Monniaux



Olivine



Wadsleyite



Ringwoodite

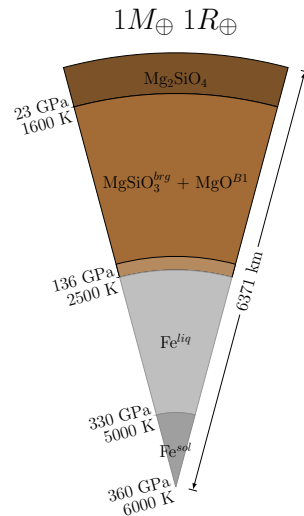


Bridgmanite

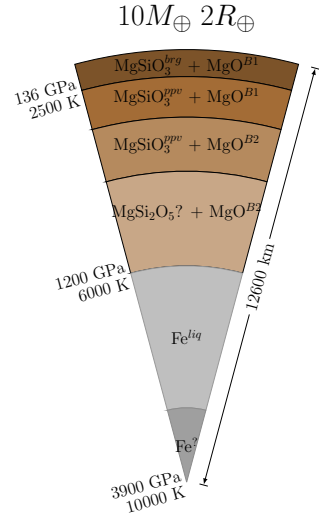
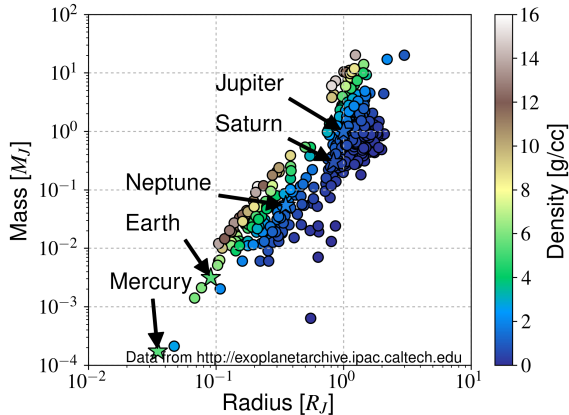


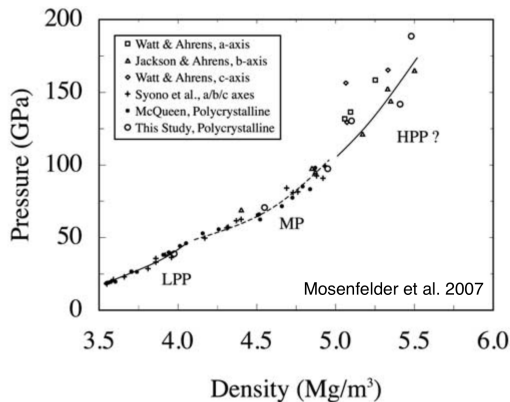
Postperovskite

T.Kawazoe



Properties under super-Earth conditions still uncertain.





## Summary:

- ▶ LPP - Fo, wd?, rw?
- ▶ MP - partial transformation to per+brg
- ▶ HPP - per + brg
- ▶ Melting...

Hugoniot equation:

$$U - U_0 = \frac{1}{2}(P + P_0)(V_0 - V)$$

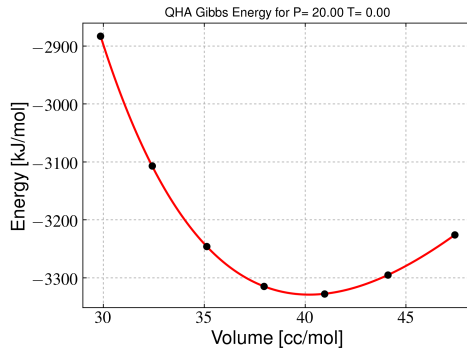
$V_0$  matches expt. 3.22 g/cc at 300 K.

- ▶ DFT calculations using VASP.
- ▶ PAW's with 800 eV cutoff.
- ▶ Frozen phonon calculations on supercells with Phonopy.
- ▶ Thermal properties computed within quasi-harmonic approximation.

Constant  $P$ - $T$  properties:

$$G = \min_V \{U(V, T) - TS(V, T) + P(V, T)V\}$$

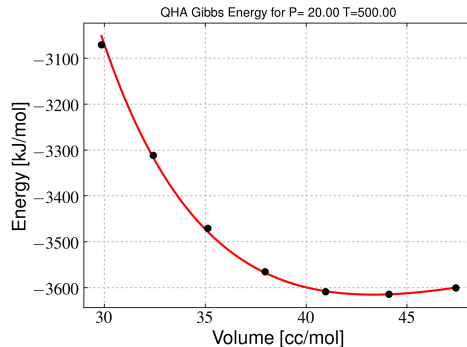
- Fit to isothermal EOS



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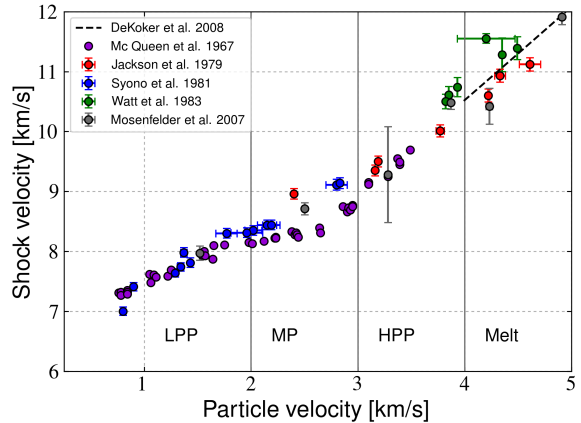
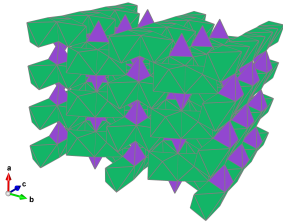
- Fit to isothermal EOS
- Phase diagram, Hugoniot...



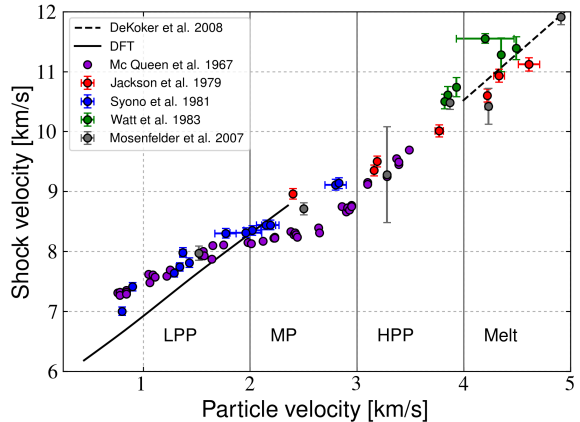
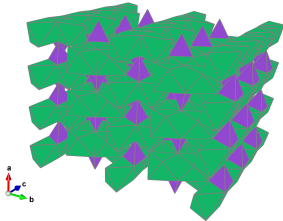


# Hugoniot of solid forsterite - LPP

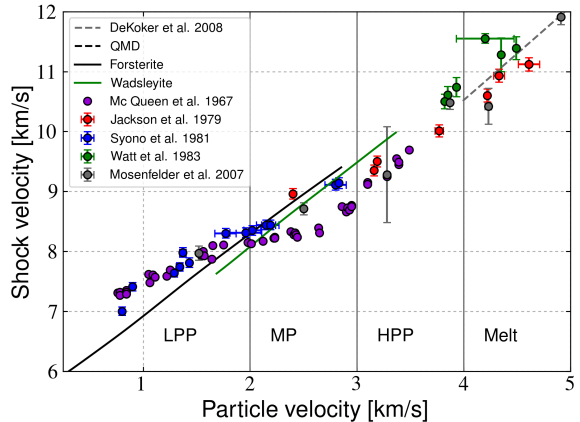
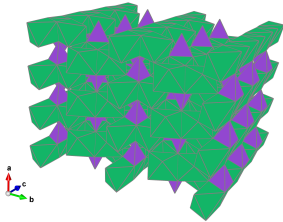
- ▶ LPP data looks good



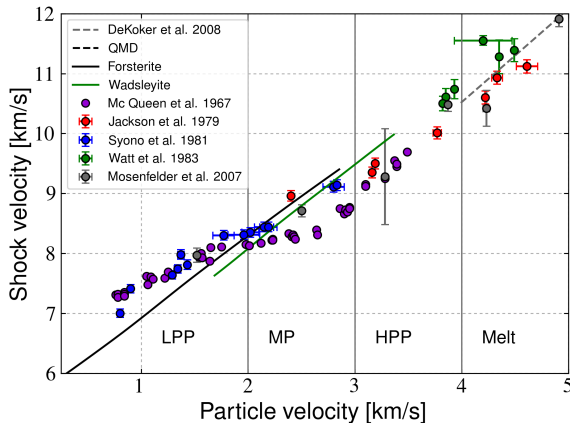
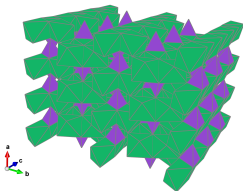
- ▶ LPP data looks good
- ▶ Spread in MP, HPP, and melt
- ▶ Forsterite DFT agrees with LPP



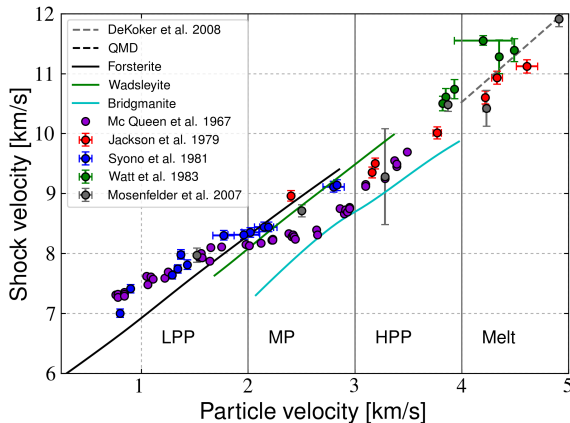
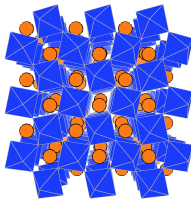
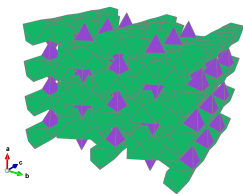
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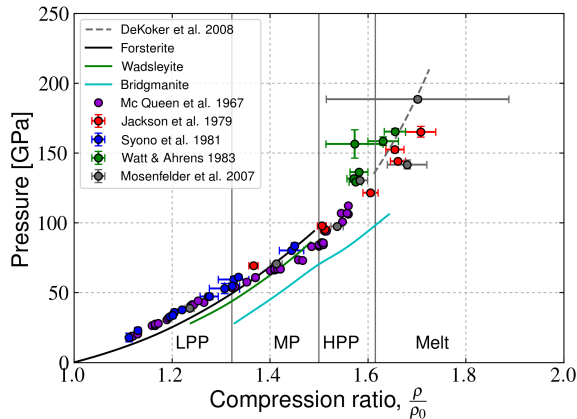
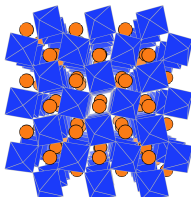
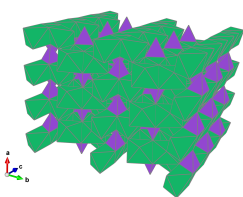
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- ▶ MP data show more scatter
- ▶ Mixture of wd, brg, per?

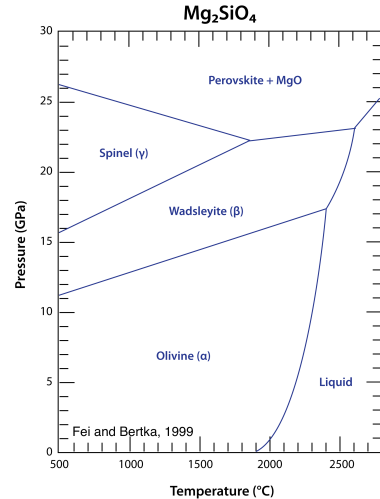
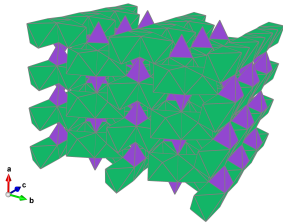


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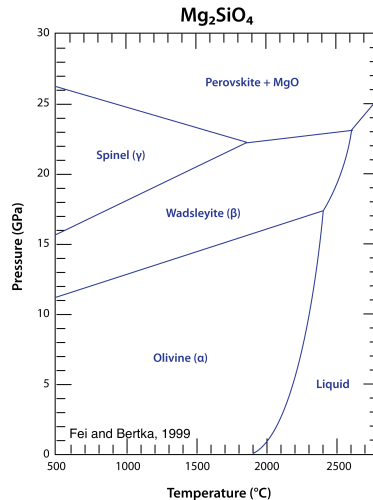
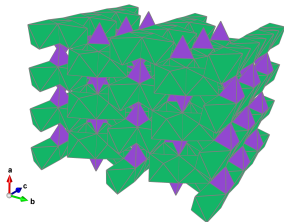


# Phase transformations in the Mixed Phase region

- LPP data looks good

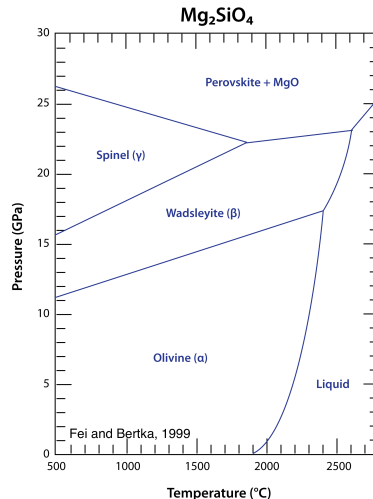
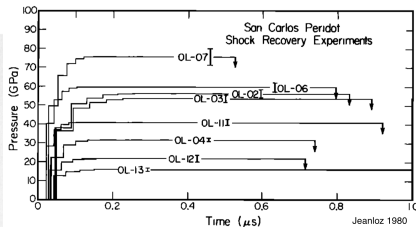
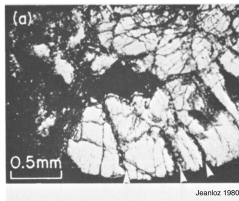


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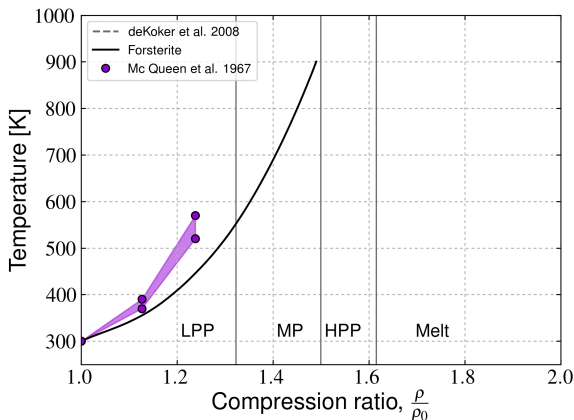




- ▶ LPP data looks good
- ▶ Spread in MP, HPP, and melt
- ▶ Forsterite DFT agrees with LPP
- ▶ Forsterite stable to  $>60$  GPa?

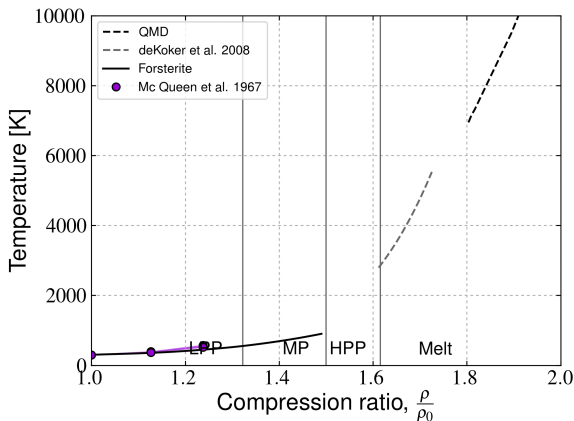


- ▶ Very few experimental data
- ▶ DFT colder than experiments of McQueen et al. 1967
- ▶ Kinetic effects?



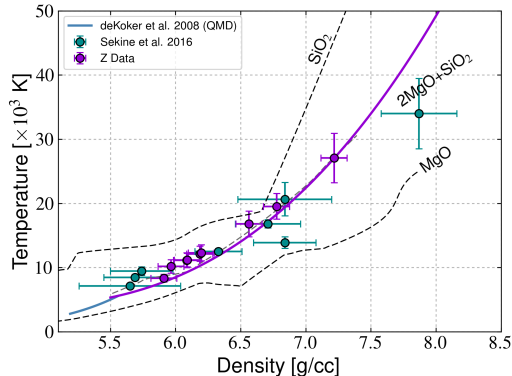
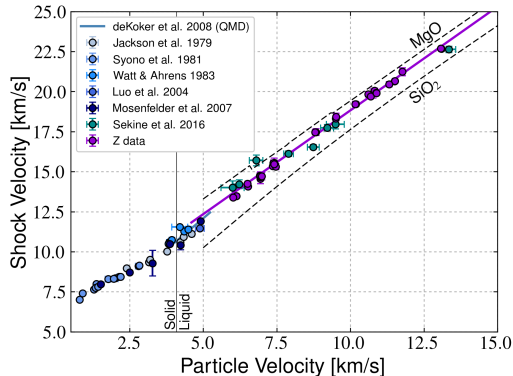
Are low Hugoniot temperatures to blame for persistence of Forsterite to such high pressure? Jeanloz 1980 points out  $\Delta G/k_B \approx 2500$  K at 60 GPa.

- ▶ Very few experimental data
- ▶ DFT colder than experiments of McQueen et al. 1967
- ▶ Kinetic effects?
- ▶ Liquid is much hotter than xtl.



Are low Hugoniot temperatures to blame for persistence of Forsterite to such high pressure? Jeanloz 1980 points out  $\Delta G/k_B \approx 2500$  K at 60 GPa.

Goal is to construct Hugoniot from 0-1000 GPa.



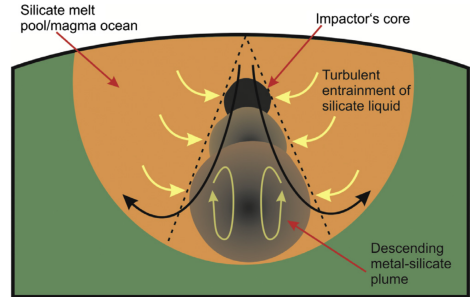
see

Presentation by Seth Root on [FILL IN LATER]

- ▶ We calculated Hugoniot states of forsterite  $\text{Mg}_2\text{SiO}_4$  in LPP and MP regions.
- ▶ At low pressure, DFT and gas gun data differ - *for good reason!*.
- ▶ Forsterite preserved up to 60 GPa - far beyond stability field.
- ▶ Mixed Phase likely composed of a mixture of Fo, possibly Wd, Brg + Per.
- ▶ DFT + QHA calculations fail at higher temperature - *for good reason!*
- ▶ Bridgmanite + Periclase calculations in progress.
- ▶ Next steps: Connect to in-progress work on liquid.



# Supplementary slides



Rubie et al. 2015

New hugoniot data suggests harder to melt planet in impact scenarios