

Shock states of solid Mg_2SiO_4

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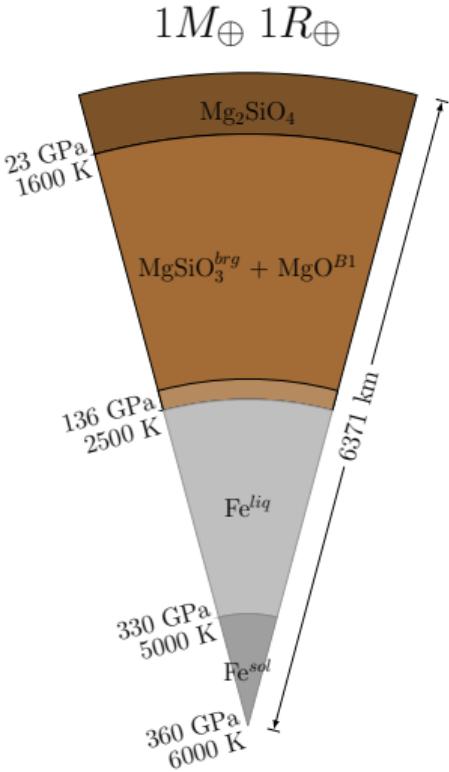
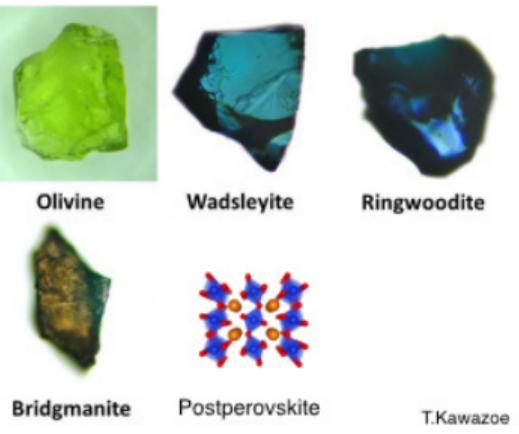


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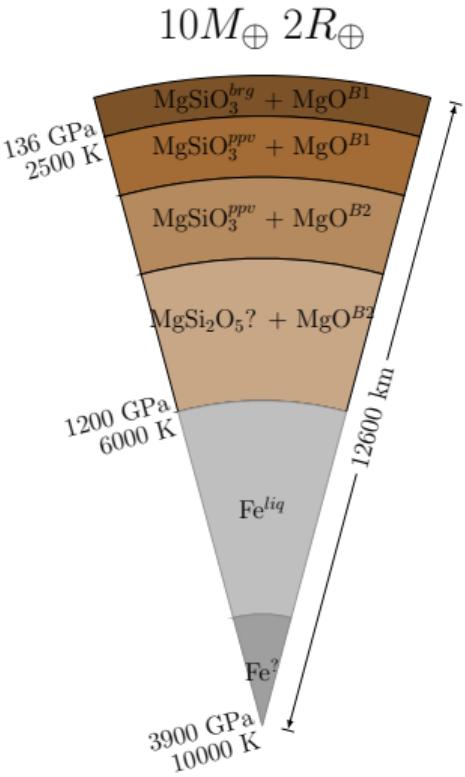
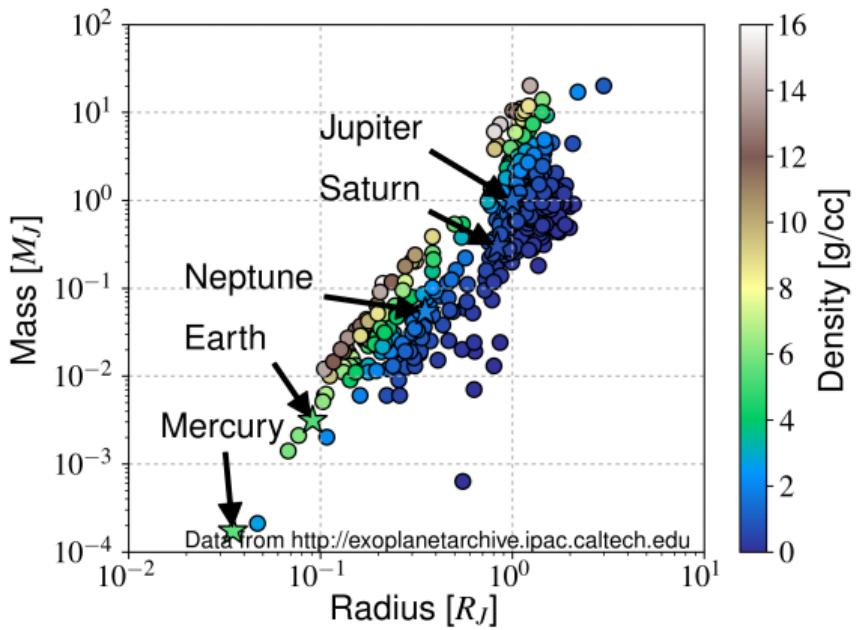


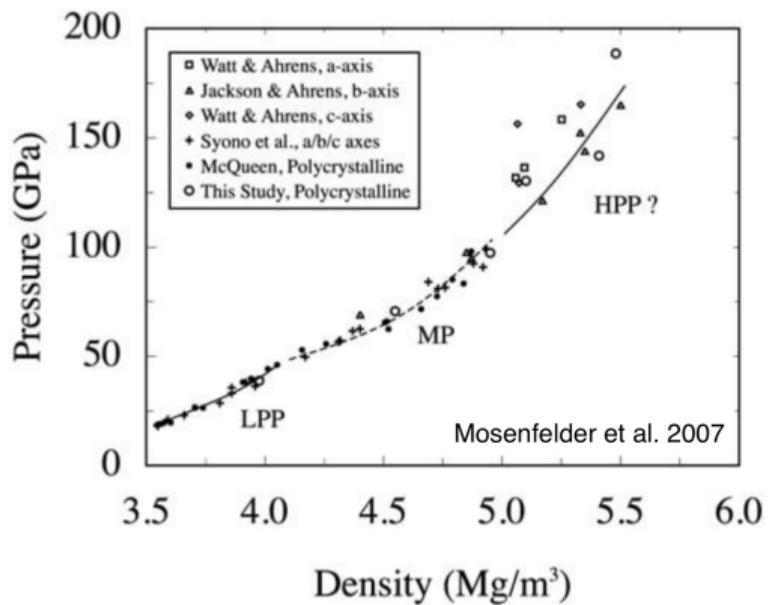
Planets motivate understanding material properties under extreme conditions.

Silicates are the building blocks of terrestrial planets.



Properties under super-Earth conditions still uncertain.





Summary:

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

Hugoniot equation:

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

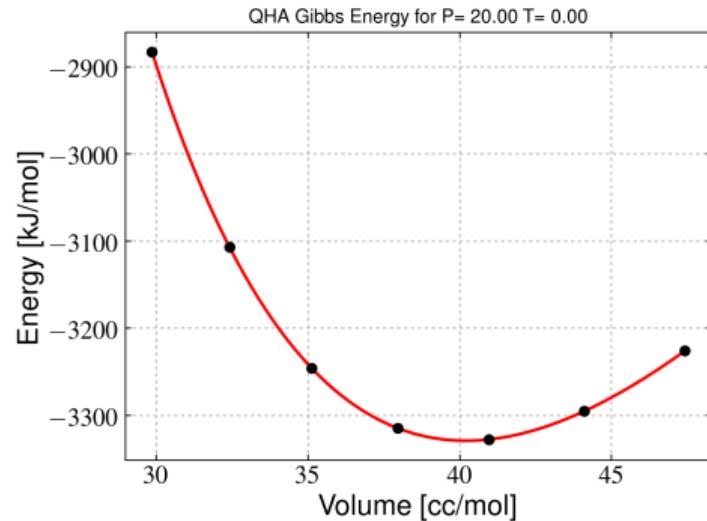
V_0 matches expt. 3.22 g/cc at 300 K.

- ▶ 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:

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

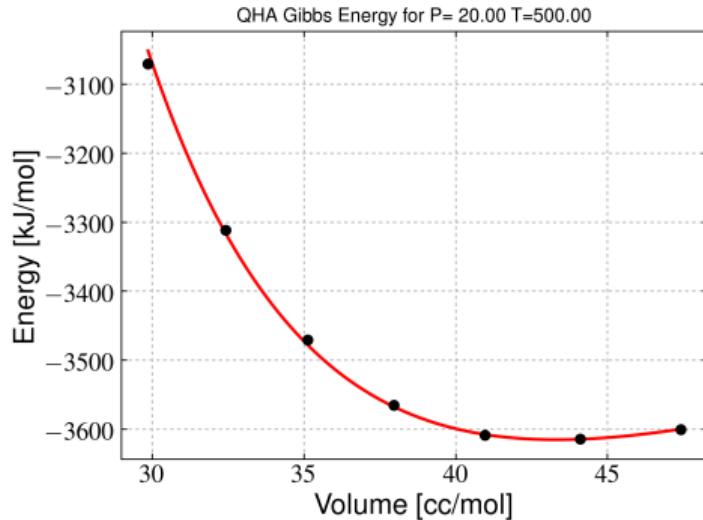
- ▶ Fit to isothermal EOS



Constant P - T properties:

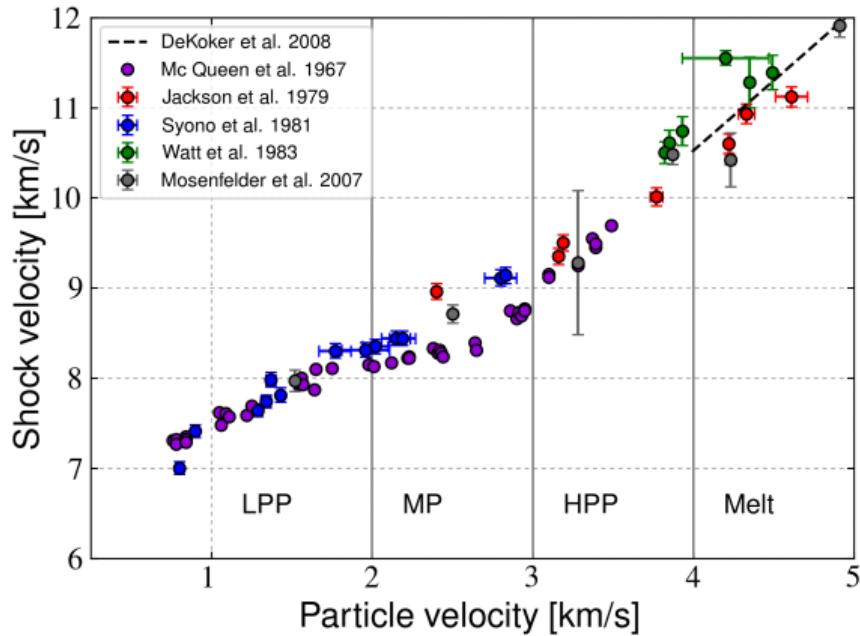
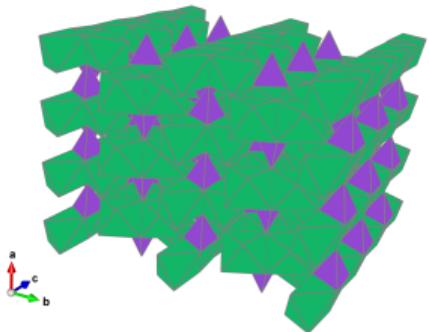
$$G = \min_V \{ U(V, T) - TS(V, T) + P(V, T)V \}$$

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



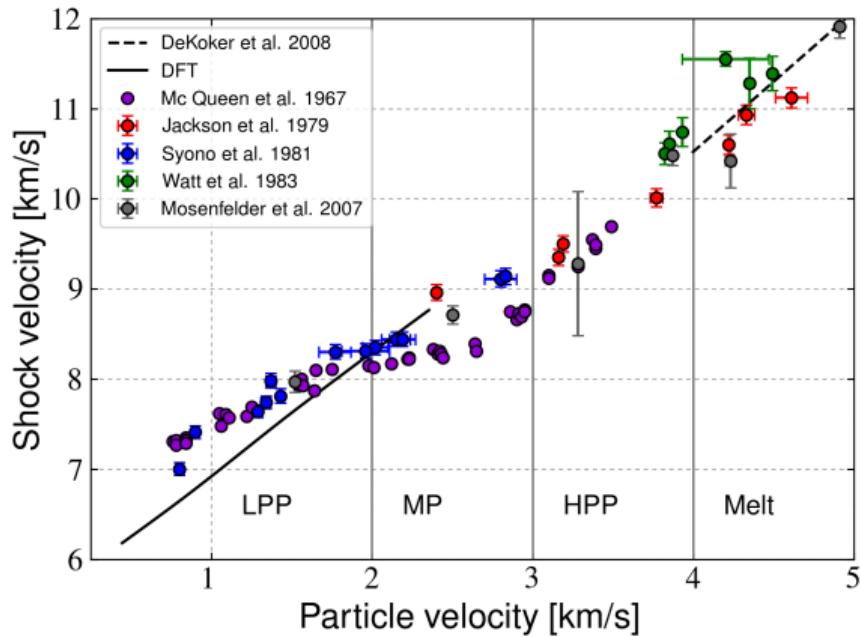
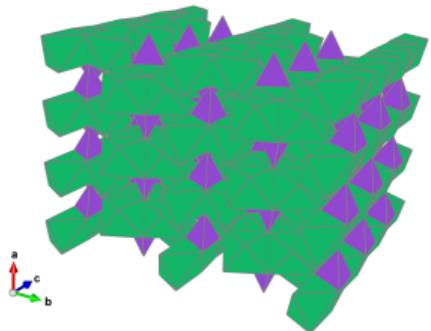
Hugoniot of solid forsterite - LPP

- ▶ LPP data looks good



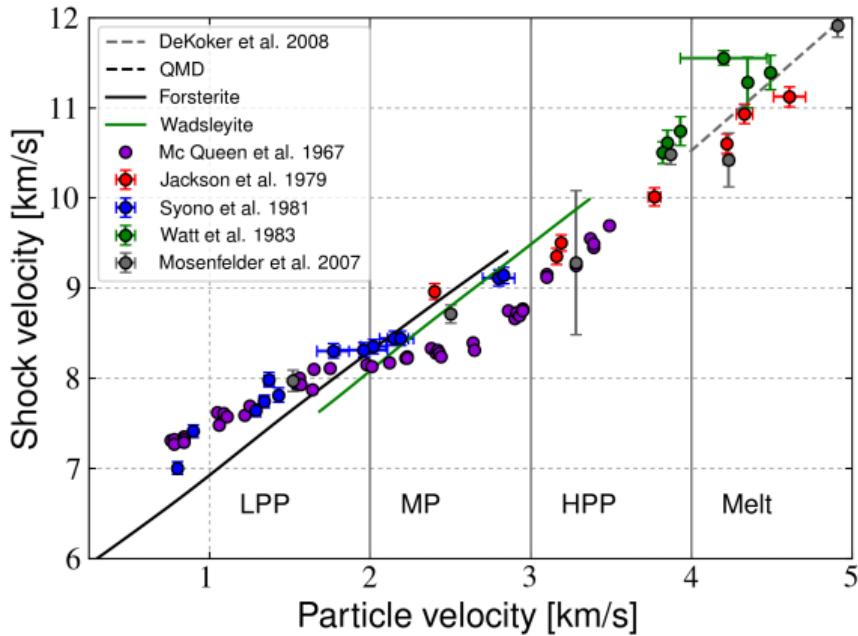
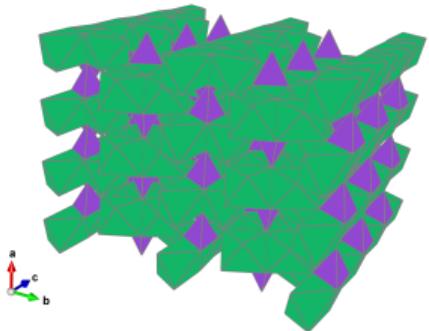
Hugoniot of solid forsterite - LPP

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



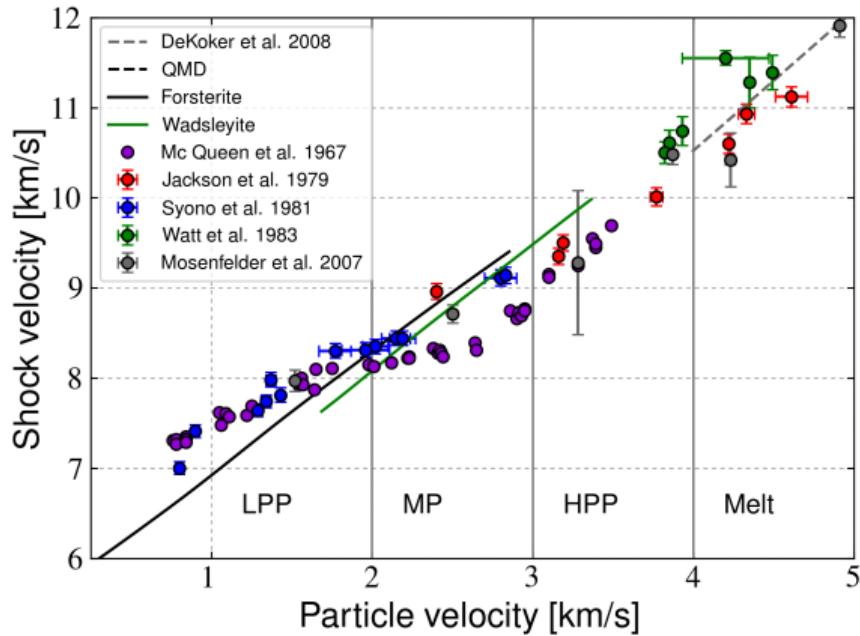
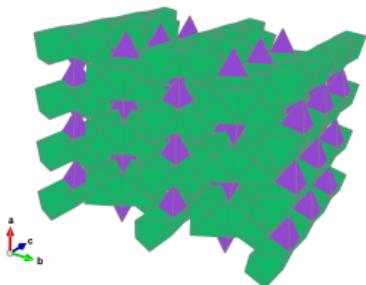
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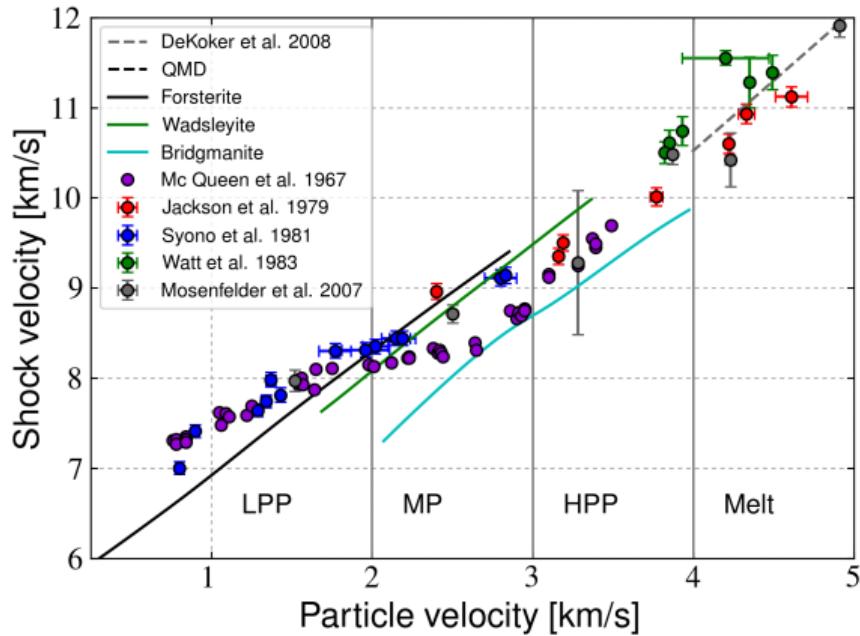
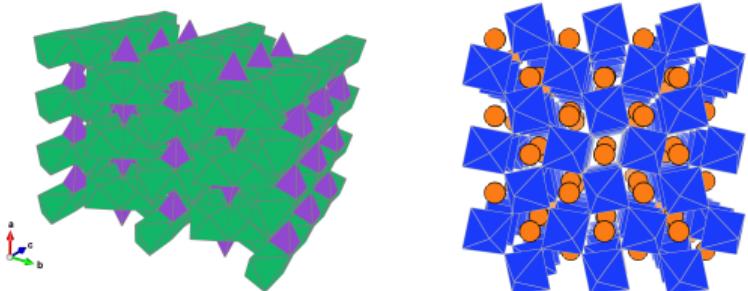
Hugoniot of solid forsterite - MP

- ▶ MP data show more scatter



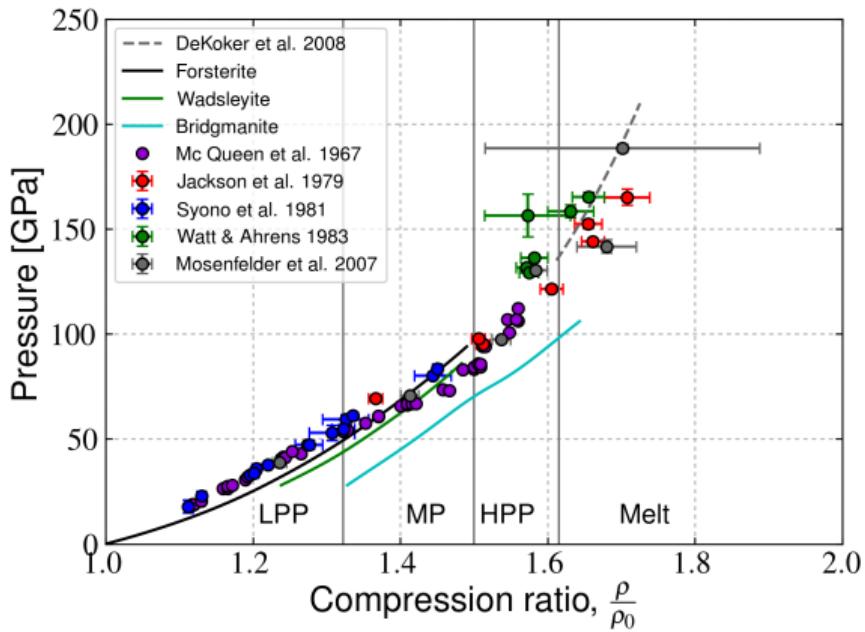
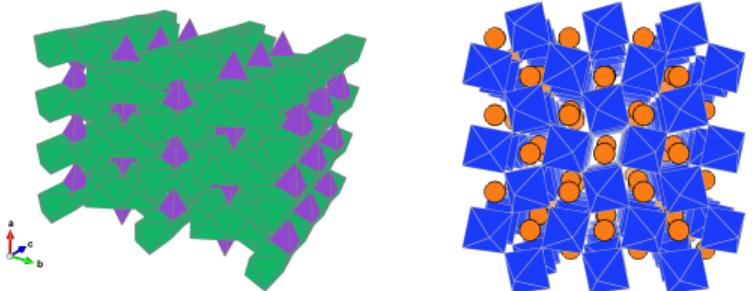
Hugoniot of solid forsterite - MP

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



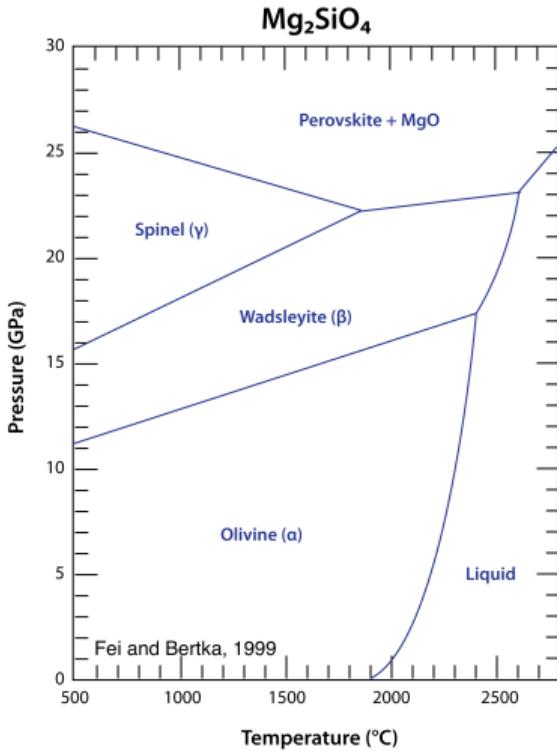
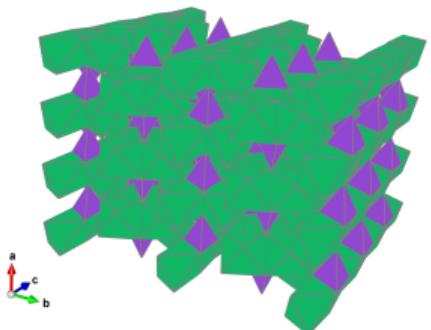
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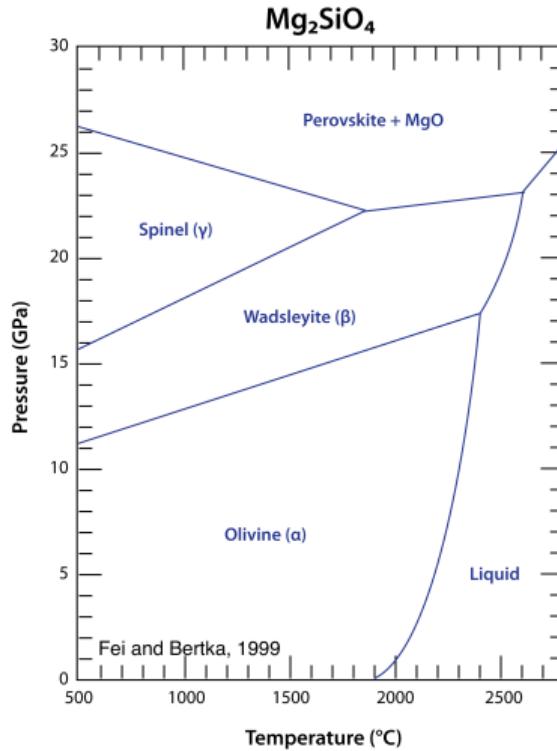
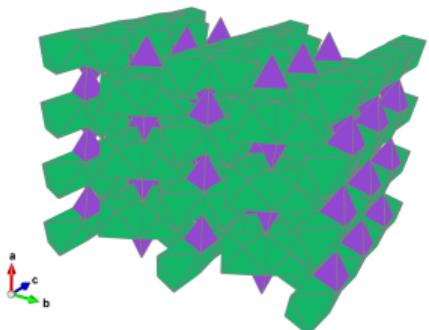
Phase transformations in the Mixed Phase region

- ▶ LPP data looks good



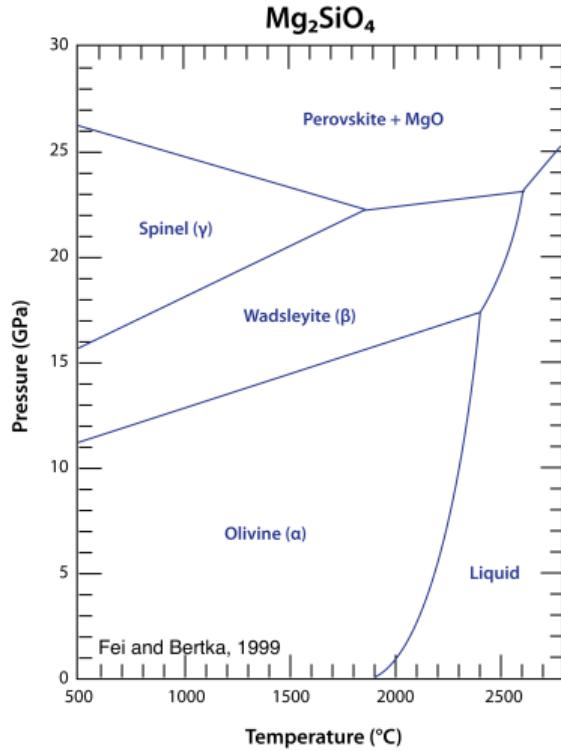
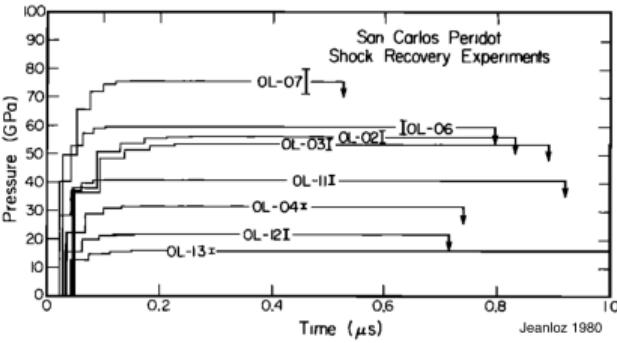
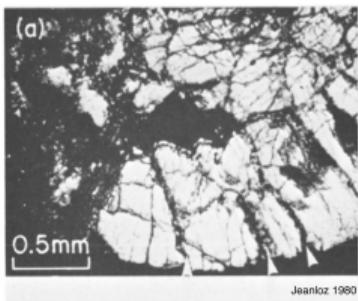
Phase transformations in the Mixed Phase region

- ▶ LPP data looks good
- ▶ Spread in MP, HPP, and melt
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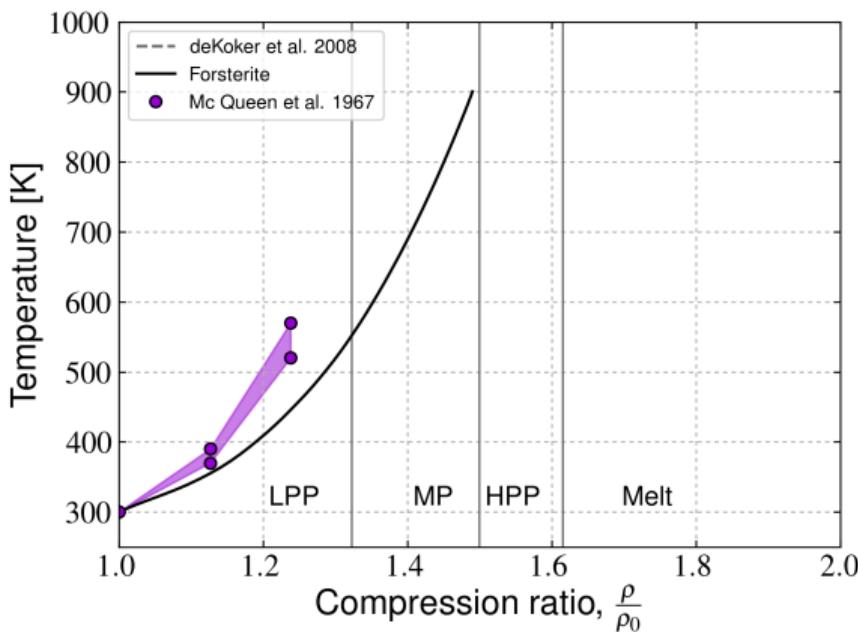
Phase transformations in the Mixed Phase region

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



Temperature on the Hugoniot of solid forsterite

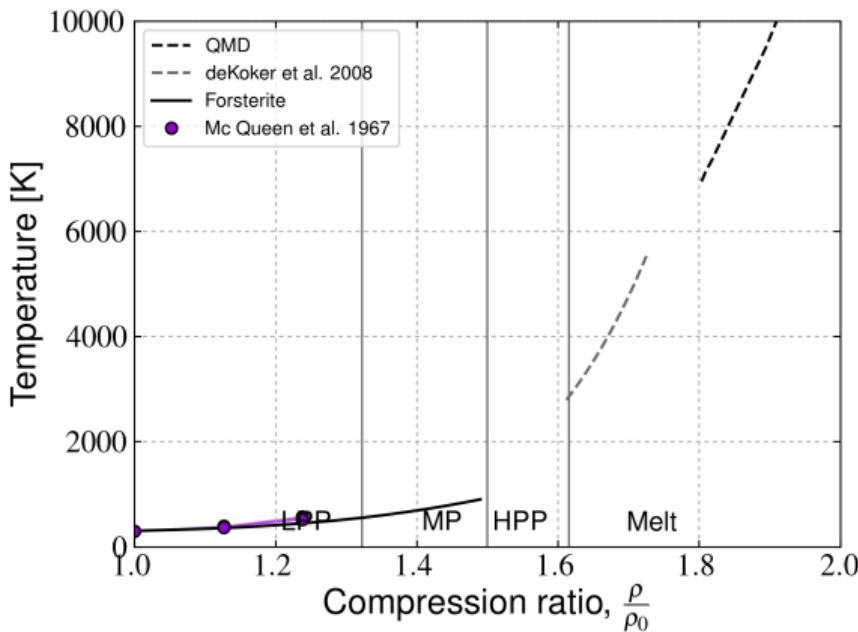
- ▶ Very few experimental data
- ▶ DFT colder than experiments of McQueen et al. 1967
- ▶ Kinetic effects?



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.

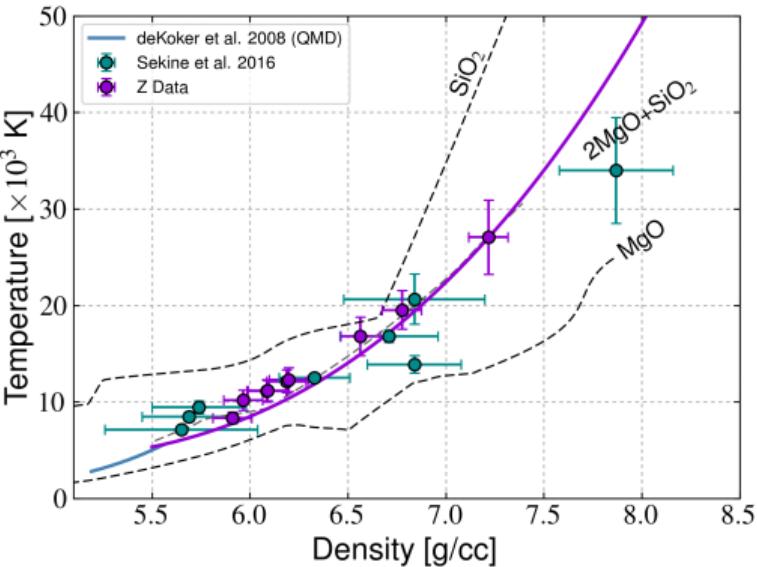
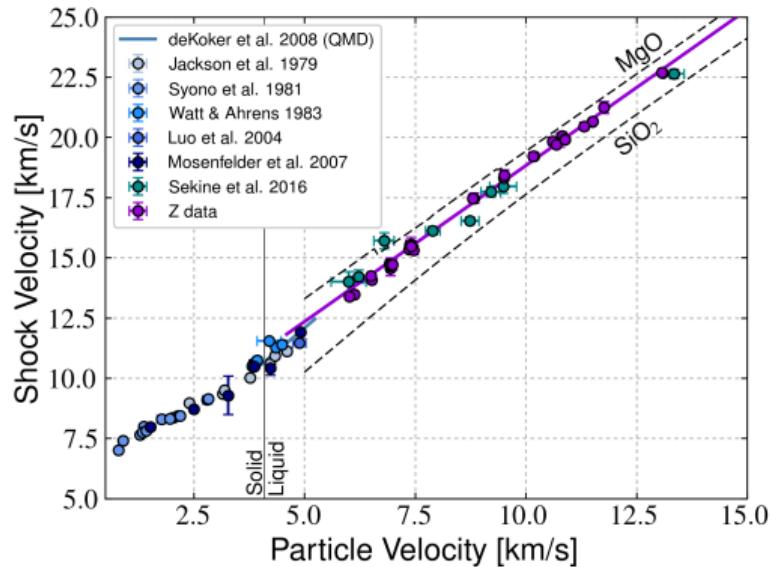
Temperature on the Hugoniot of solid forsterite

- ▶ 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.

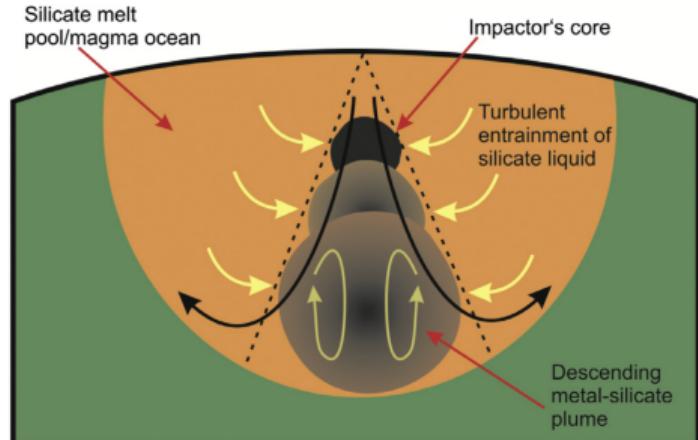


see

Presentation by Seth Root on [FILL IN LATER]

- ▶ We calculated Hugoniot states of forsterite Mg_2SiO_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