SAND2018-10204C

Shock states and thermodynamic properties of liquid silicates

Joshua P. Townsend[1], Seth Root[1], Erik Davies[2], Raymond W Lemke[1], David E Bliss[1], Dayne E Fratanduono[3], Richard G Kraus[3], Marius Millot[3], Dylan K Spaulding[2], Sarah T. Stewart[2], Stein B Jacobsen[4], Luke Shulenburger[1]

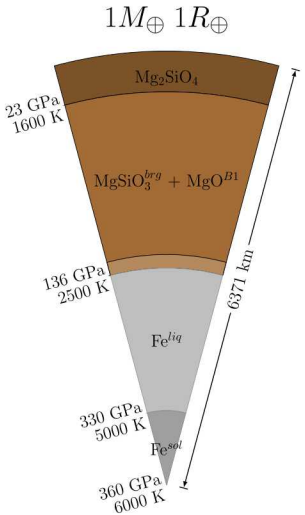
[1]High Energy Density Physics Theory, Sandia National Laboratories, Albuquerque, NM, USA
[2]Department of Earth and Planetary Sciences, University of California Davis, Davis, CA, USA
[3]Lawrence Livermore National Laboratory, Livermore, CA, USA
[4]Department of Earth and Planetary Sciences, Harvard University, Cambridge, MA, USA

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy?s National Nuclear Security Administration under contract DE-NA0003525.

Why dynamic compression?

Sandia National Laboratories

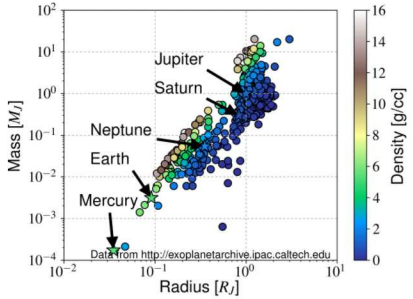
Giant impacts explore exotic P, T states

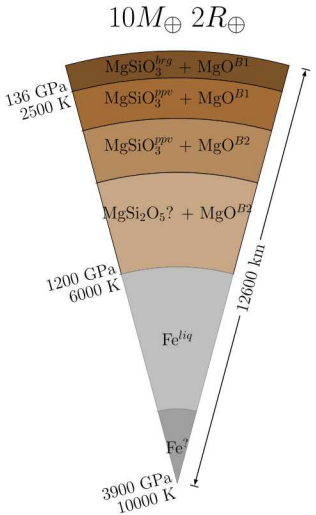


Why dynamic compression?

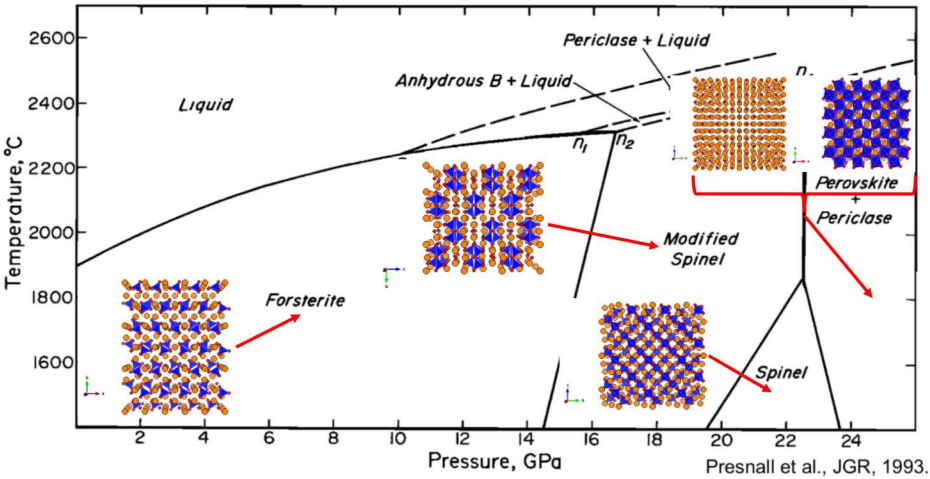
Sandia National Laboratories

Planetary interior models unconstrained





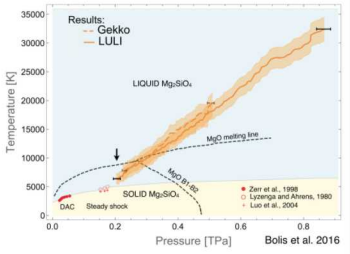
Low pressure phase diagram

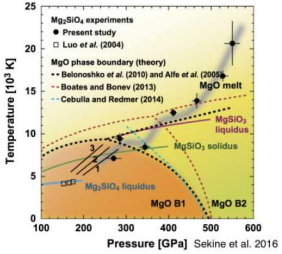


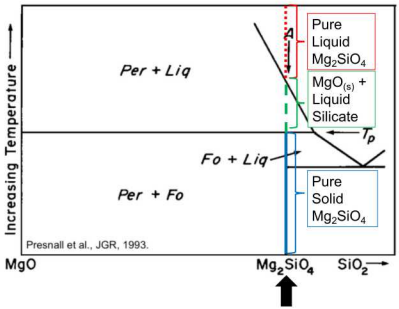
Presnall et al., JGR, 1993.

Hugoniot state interpretation

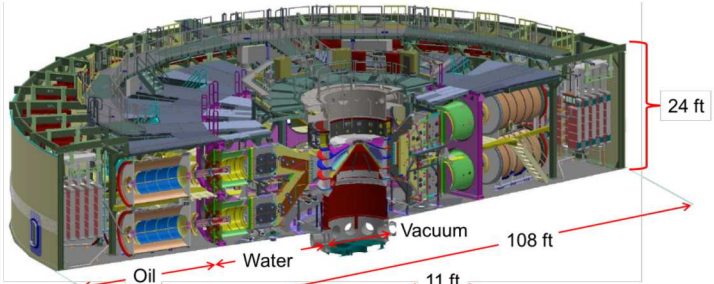
- Multi-component system
- Incommensurate melting
- Melting $\sim$ 120-160 GPa
- No XRD, indirect phase ID





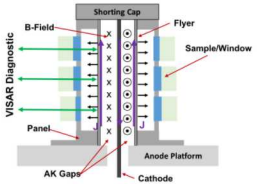


Planetary science on the Z Machine



- **2.65 x 10^6 L of oil**
- **1.14 x 10^6 L of water**

Credit: S. Root (SNL)



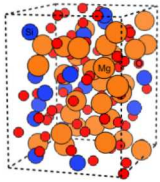
$$E = 35 \text{ MJ}$$
$$I = 20 \text{ MA}$$
$$\Delta t = 20 \text{ ns}$$

DFT-based molecular dynamics

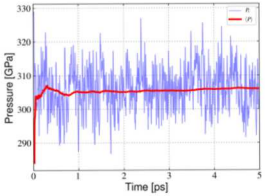
Sandia National Laboratories

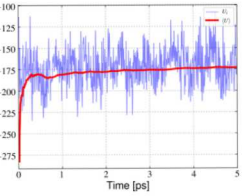
Basic idea: Solve $\mathbf{F} = m\mathbf{a}$ for the ions, with the force due to electrons computed self-consistently from solution of the Kohn-Sham hamiltonian:

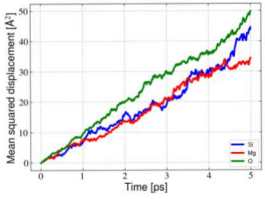
$$\left(-\frac{1}{2}\nabla^2 + V_{ext}(\mathbf{r}) + \int d\mathbf{r}' \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} + \frac{\delta E_{xc}[\rho]}{\delta\rho(\mathbf{r})}\right)\phi_i(\mathbf{r}) = \epsilon_i\phi_i(\mathbf{r})$$

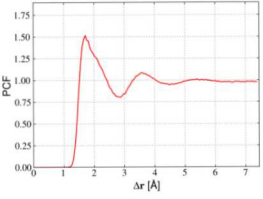


Thermodynamic quantities such as E, P, T, V, directly accessible without making any assumptions about the response or properties of the material *a priori*.



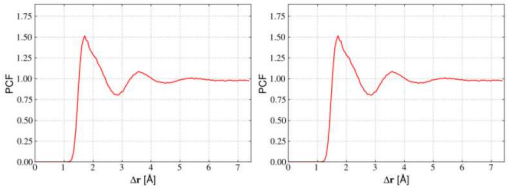


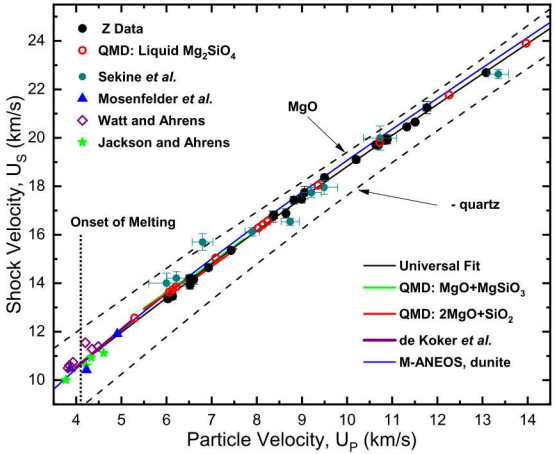




Results

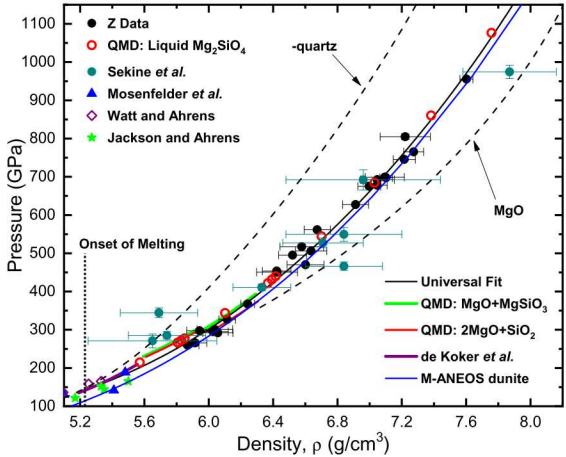
- Data span 13< U_S <24 km/s
- Resolve curvature in Hugoniot
- No discontinuities
- Agree with extrapolated MANEOS





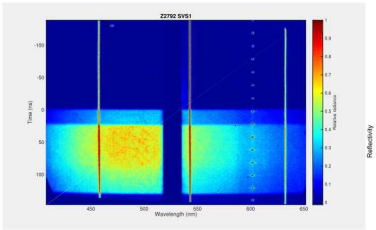
Results

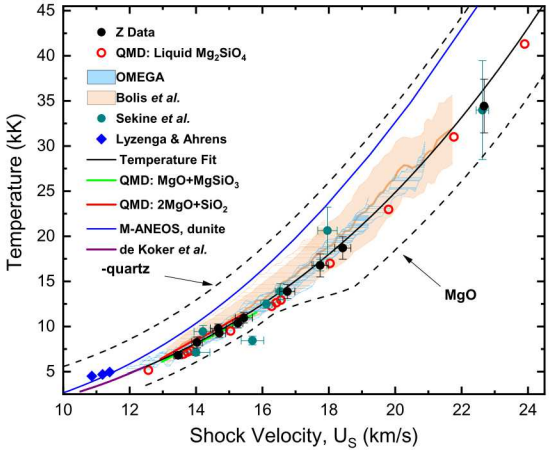
- Data span 13< U_S <24 km/s
- Resolve curvature in Hugoniot
- No discontinuities
- Agree with extrapolated MANEOS



Results

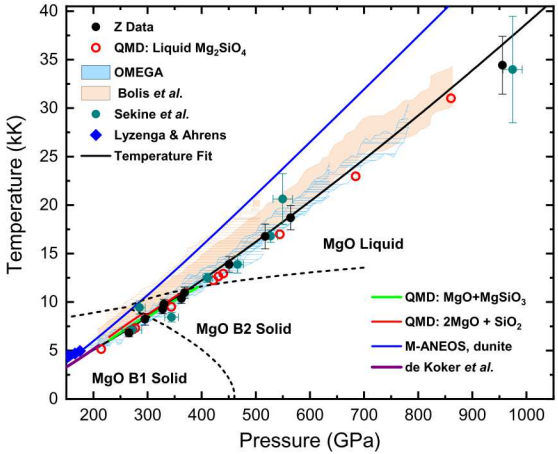
- MANEOS thermal prop's off
- Z, OMEGA, and DFT-MD in agreement





- Data span 13< U_S <24 km/s
- Resolve curvature in Hugoniot
- No discontinuities
- MANEOS thermal prop's off

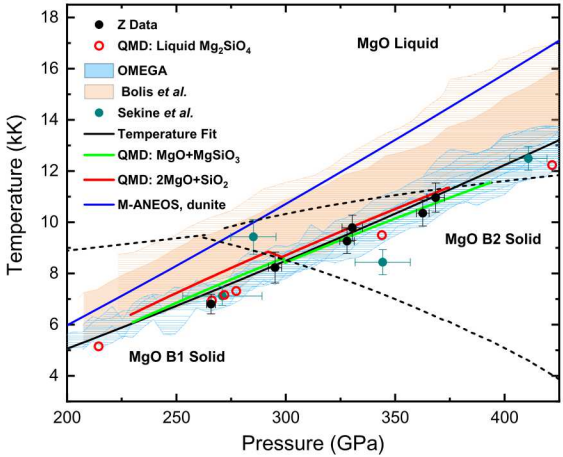
Well... Is it de-mixed, or not?



Results

- Data span 13< U_S <24 km/s
- Resolve curvature in Hugoniot
- No discontinuities
- MANEOS thermal prop's off
- Smaller than expected signal due to de-mixing

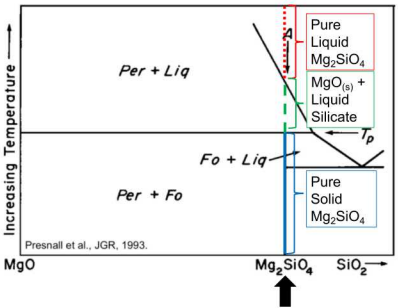
Well... Is it de-mixed, or not?

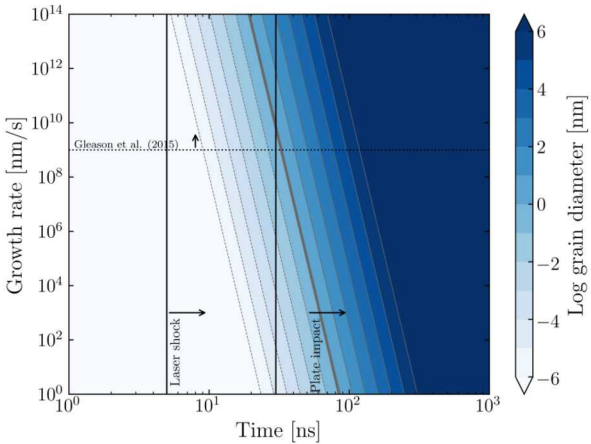


Potential for phase separation

Two things to consider:

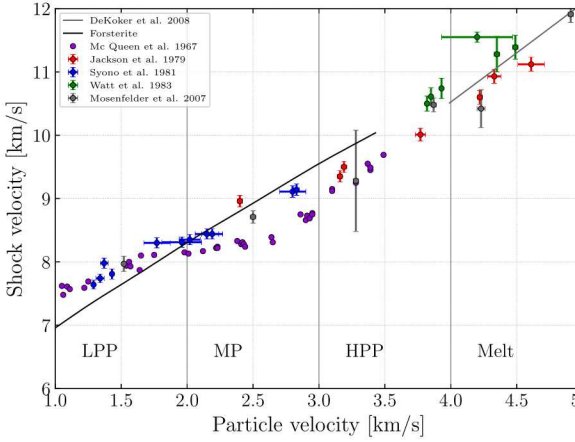
- Incommensurate melting at high pressure?
- Experiments probing equil. states?





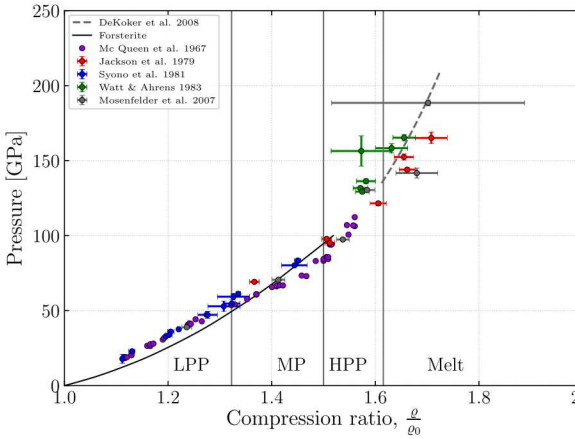
New results on low pressure Hugoniot

- Persistence of Fo to 10's GPa?
- MP and HPP difficult to reproduce
- New XRD experiments suggest metastable Ol to 75 GPa(!)



New results on low pressure Hugoniot

- Persistence of Fo to 10's GPa?
- MP and HPP difficult to reproduce
- New XRD experiments suggest metastable Ol to 75 GPa(!)



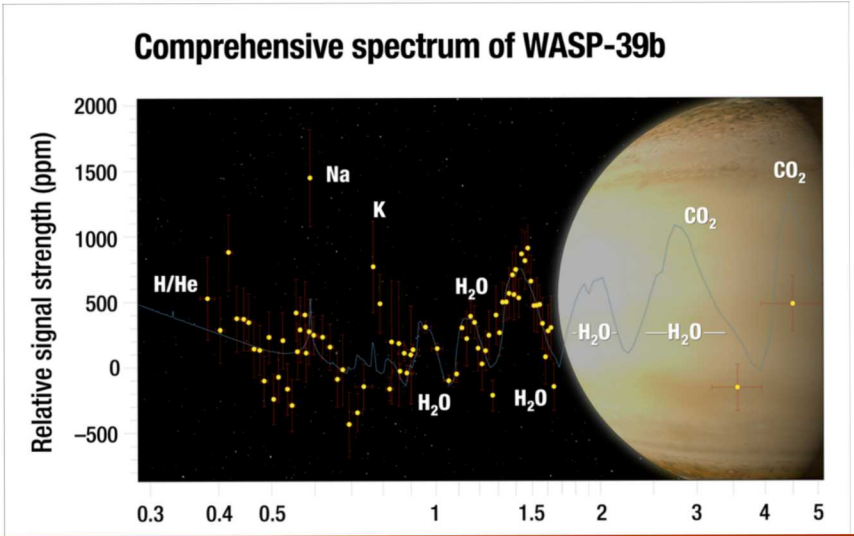
Summary and future work

- Hugoniot states in liquid well constrained
- Possible kinetic effects persist at least up to melting
- Entropy, melting, and release states in progress

Questions?

EXTRAS

Sandia National Laboratories



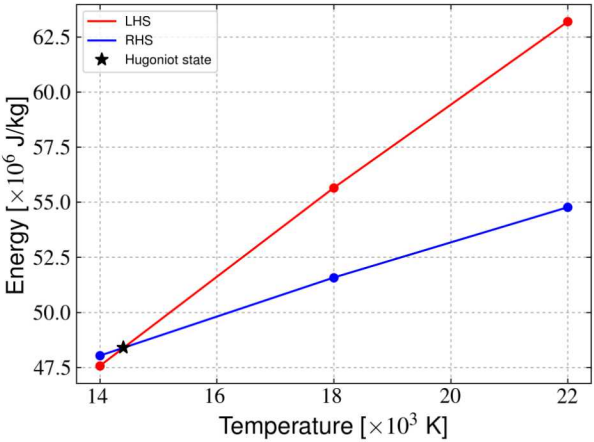
$$P = \rho_0 U_S u_P, \qquad \frac{\rho}{\rho_0} = \frac{U_S}{U_S - u_P}$$

$$\Downarrow$$

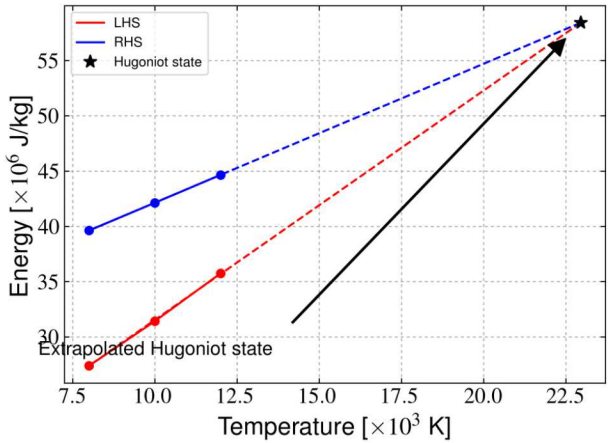
$$E - E_0 = \frac{1}{2}(P + P_0)\left(\frac{1}{\rho_0} - \frac{1}{\rho}\right)$$

- 1d curve, set by choice of reference

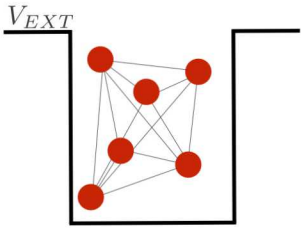
How to estimate the Hugoniot



How to estimate the Hugoniot



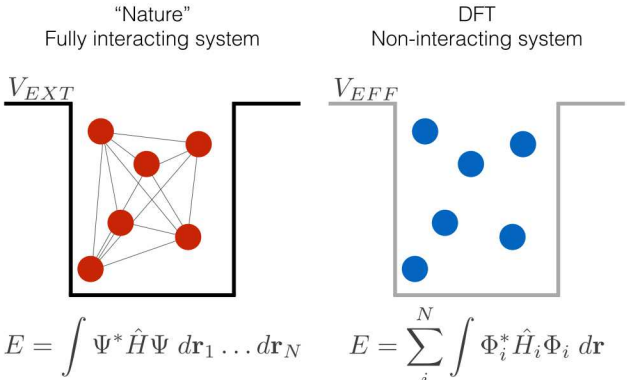
"Nature"
Fully interacting system



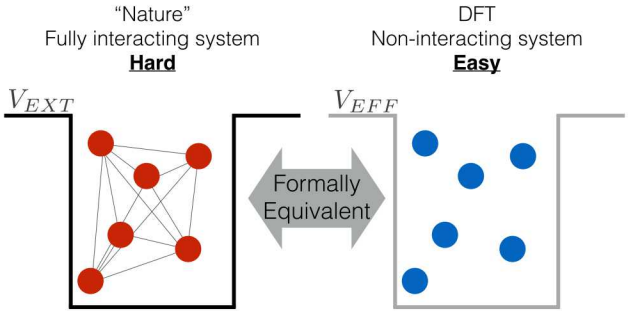
$$E = \int \Psi^* \hat{H} \Psi \; d\mathbf{r}_1 \ldots d\mathbf{r}_N$$

Adapted from Mattsson et al. 2005

Density Functional Theory in 2 minutes



Adapted from Mattsson et al. 2005



Adapted from Mattsson et al. 2005

Planetary science on the Z Machine

Sandia National Laboratories