Sandia National Laboratories

The principal Hugoniot of forsterite to 950 GPa

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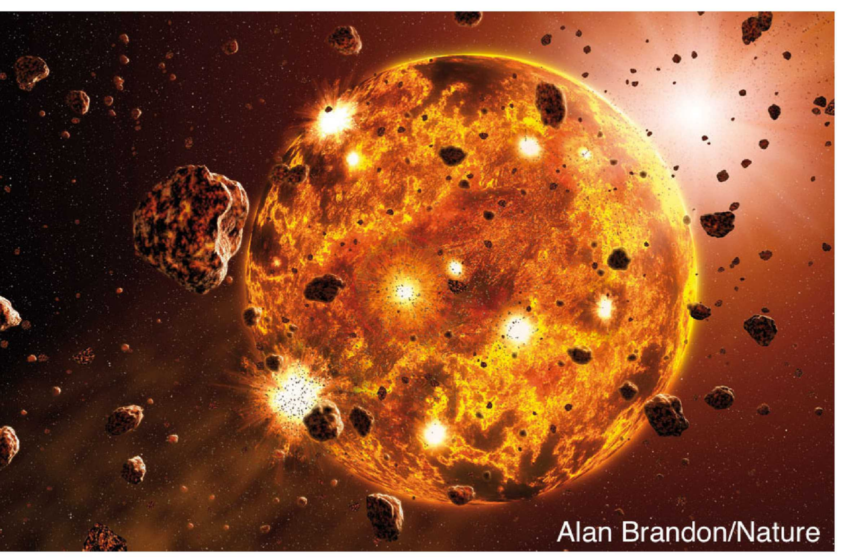
0 - Plain language summary

We performed shock wave compression experiments to investigate the properties of Mg_2SiO_4 olivine above 200 GPa at the Z-Machine at Sandia National Laboratories. In addition to the experiments, we also used quantum mechanical calculations to better understand the experimental results. We find that the measured and calculated shock states are in excellent agreement, but disagree with previous analytic equations of state extrapolated from lower pressure data. In addition, we examine whether liquid Mg2SiO4 de-mixes into solid MgO + liquid $MgSiO_3$ and show that all experimental data to-date cannot distinguish a de-mixed from a single liquid phase from the shock states alone.

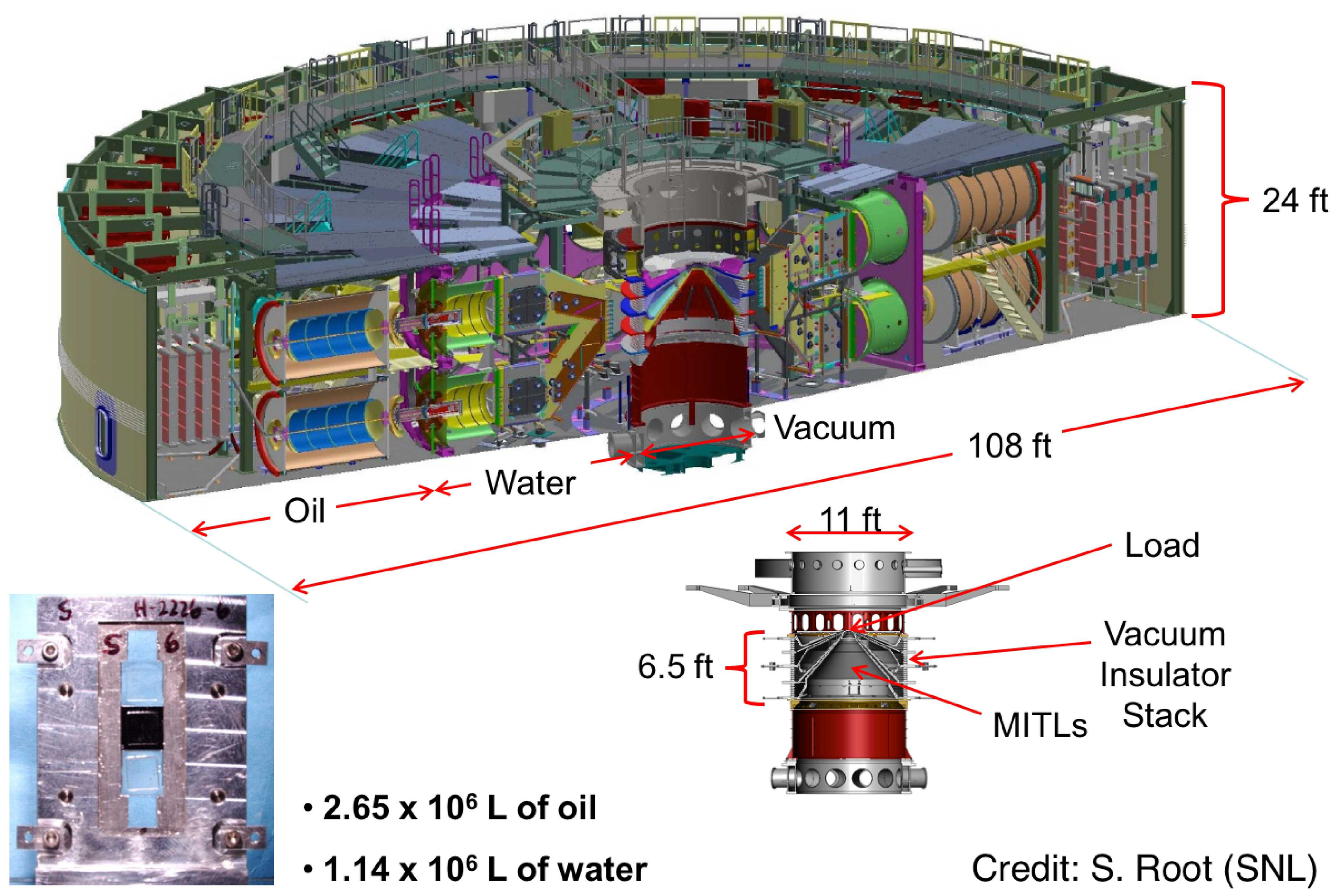
1 - Importance of accurate Hugoniots for planetary materials



- Hypervelocity impacts generate strong shock waves in thermodynamic regimes far beyond those found in present Earth.
- Accurate Hugoniots and thermodynamic properties required for accurate accretion and differentiation models.

2 - Shock wave compression experiments on the Z-Machine

The Z-Machine is the largest pulsed power facility in the world and is capable of generating 20 MA currents in 100 ns, and is used to accelerate a metal flyer plate to velocities approaching 40 kms/s.



- **2.65 x 10⁶ L of oil**
- **1.14 x 10⁶ L of water**

Credit: S. Root (SNL)

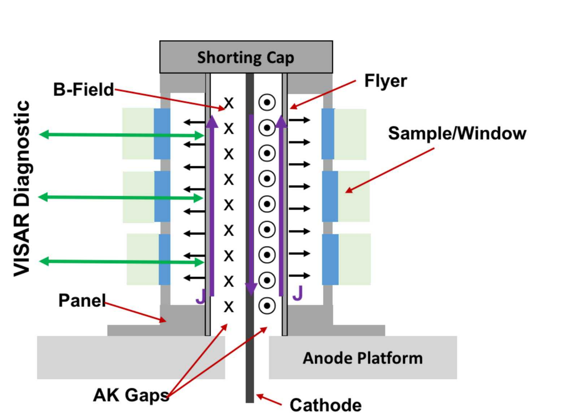


Figure: Sample target schematic.

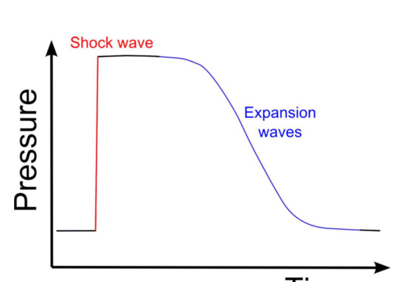


Figure: Schematic illustration of shock wave propagation into the sample due to impact with the flyer.

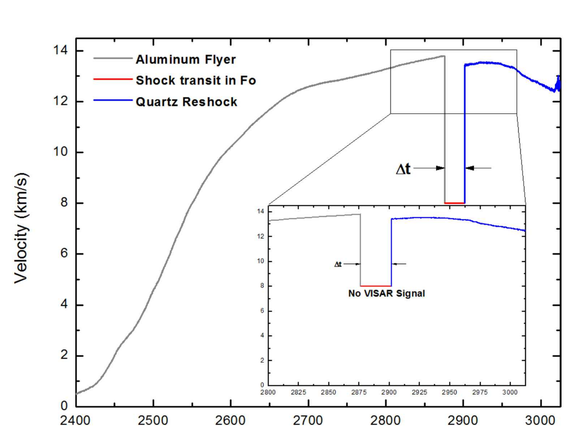


Figure: Velocity history of experiment.

3 - Density functional theory based molecular dynamics

In quantum molecular dynamics the electronic charge density comes from a self-consistent calculation of a set of single particle states via the Kohn-Sham implementation of density functional theory:

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

The exchange correlation functional ($E_{XC}[\rho]$) captures the correlation energy missed in the single particle approximation, and is parametrically given in this work according to the generalized gradient approximation (GGA):

$$E_x^{GGA} = \int d\mathbf{r}\rho(\mathbf{r})F_x^{GGA}(s)\epsilon_x^{hom}(\rho(\mathbf{r})) \quad (2)$$

Where $s = |\nabla\rho|/2k_f\rho$, $k_f = (3\pi^2\rho)^{1/3}$, and ϵ_x^{hom} is the correlation energy of the homogeneous electron gas. The atoms are moved according to the classical equations of motion:

$$\mathbf{r}(t+\Delta t) = 2\mathbf{r}(t) - \mathbf{r}(t-\Delta t) + \frac{\mathbf{f}(t)}{m}\Delta t^2 + \mathcal{O}(\Delta t^4) \quad (3)$$

Where **f** is the force on the atom, computed from the Hellman-Feynman theorem.

This approach makes accessible thermodynamic quantities such as E, P, T, V, directly without making any assumptions about the response of the material.

4 - Hugoniot State Estimation

The Hugoniot states are inferred from the Rankine-Hugoniot relations:

$$P = \rho_0 U_S u_P, \qquad \rho = \rho_0\frac{1}{1-\frac{u_P}{U_S}} \quad (4)$$

And satisfy the Hugoniot equation:

$$E - E_0 = \frac{1}{2}(P + P_0)(V_0 - V) \quad (5)$$

Where the subscript 0 indicates the initial state of the material. In the experiments, the shock U_S, and particle u_P velocities are measured via the impedance matching technique[1]. For the QMD calculations, the Hugoniot states are computed from the interpolation of a number of calculations with the same volume, but different temperature.

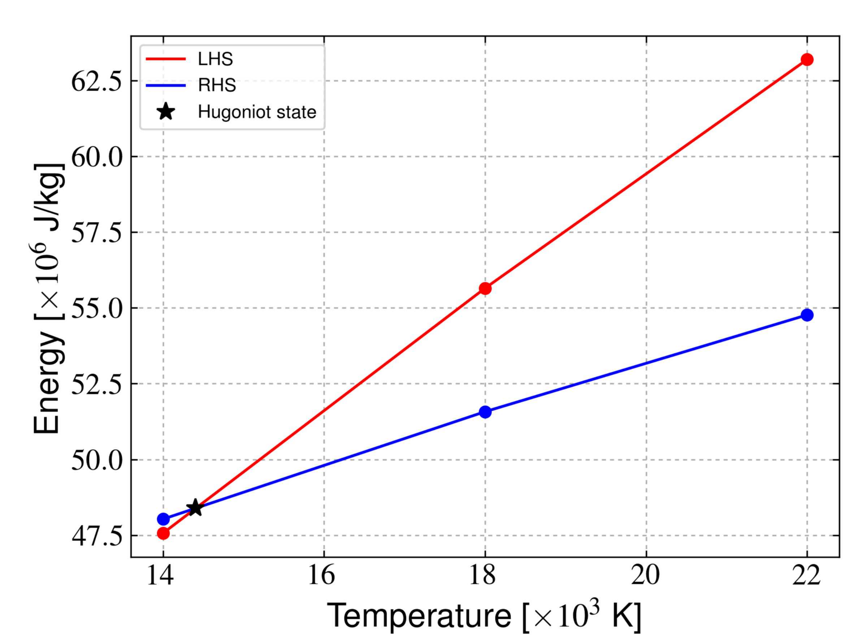


Figure: QMD estimation of the Hugoniot state from a series of isochoric calculations.

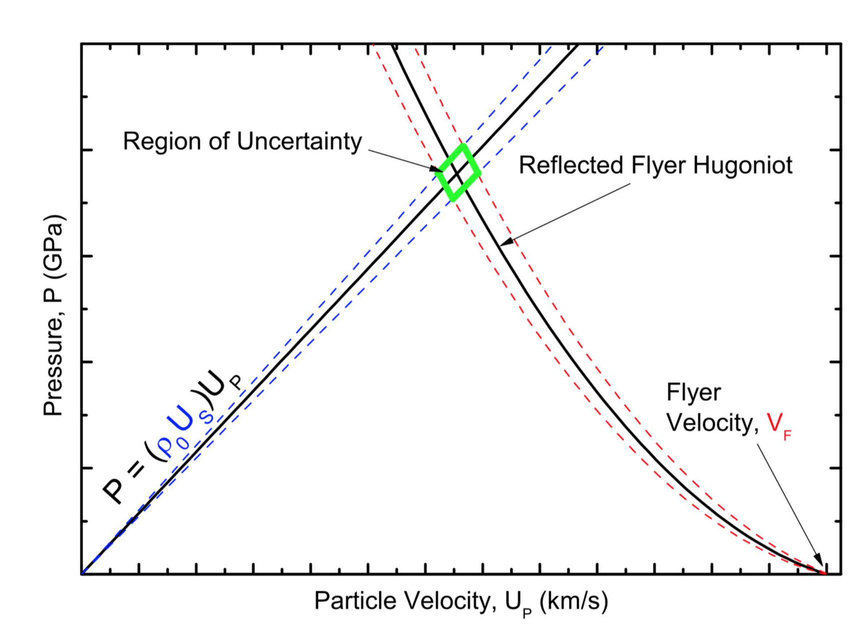
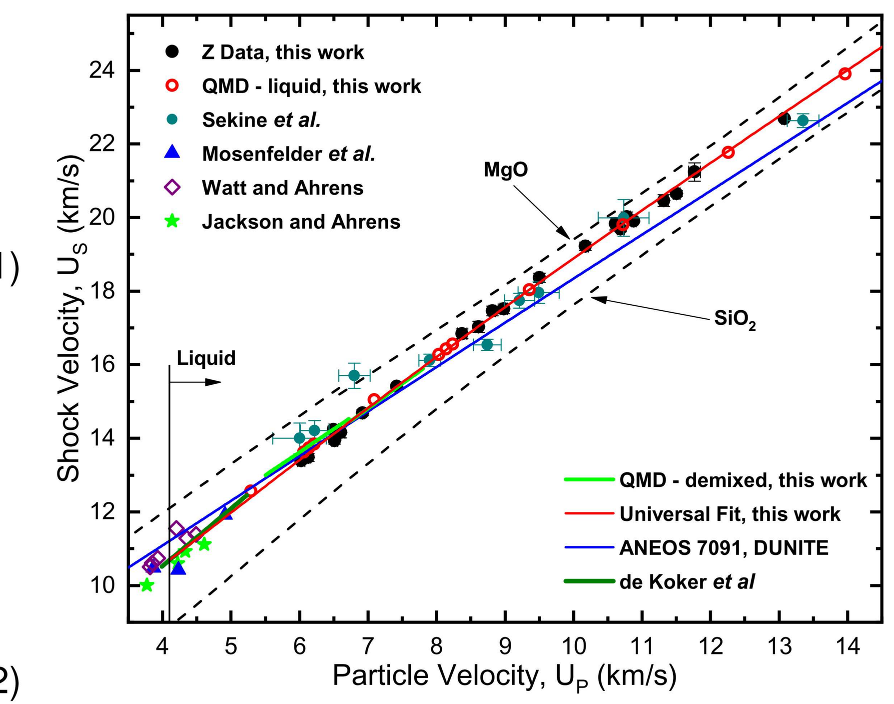
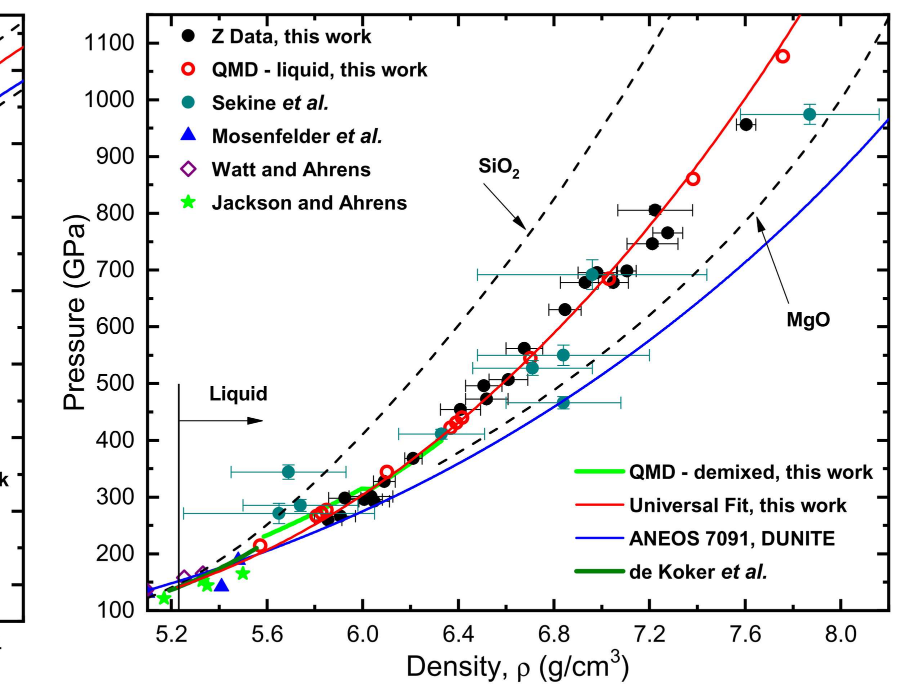
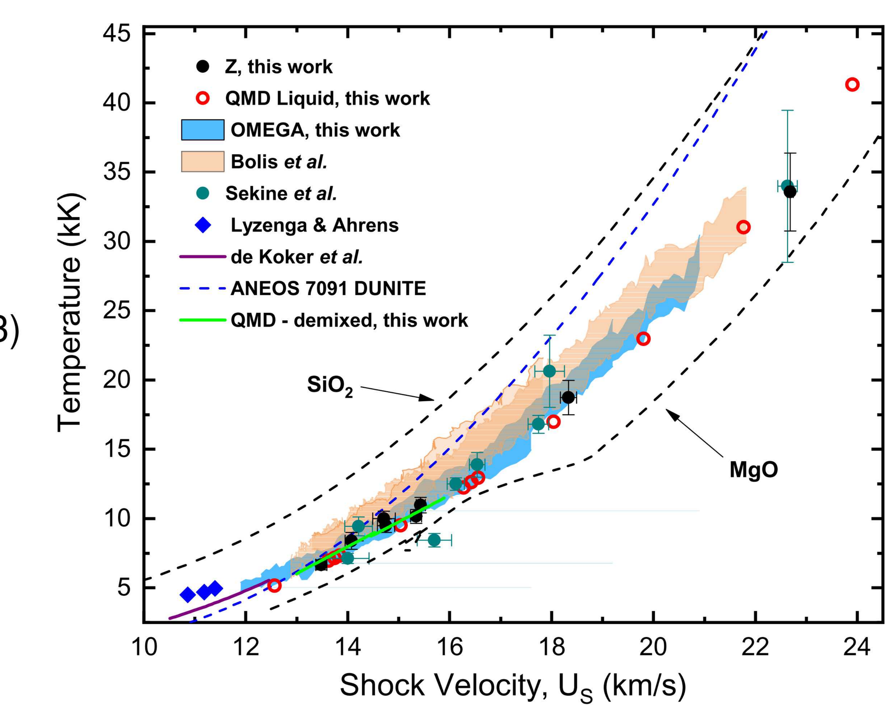


Figure: Experimental estimation of the Hugoniot state from the impedance matching technique.

5 - Hugoniot states

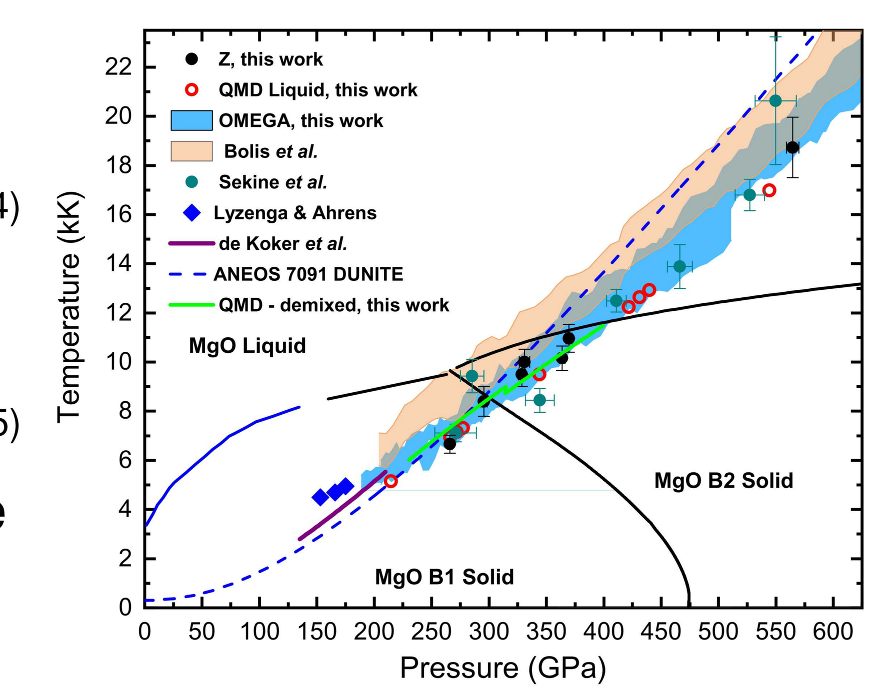


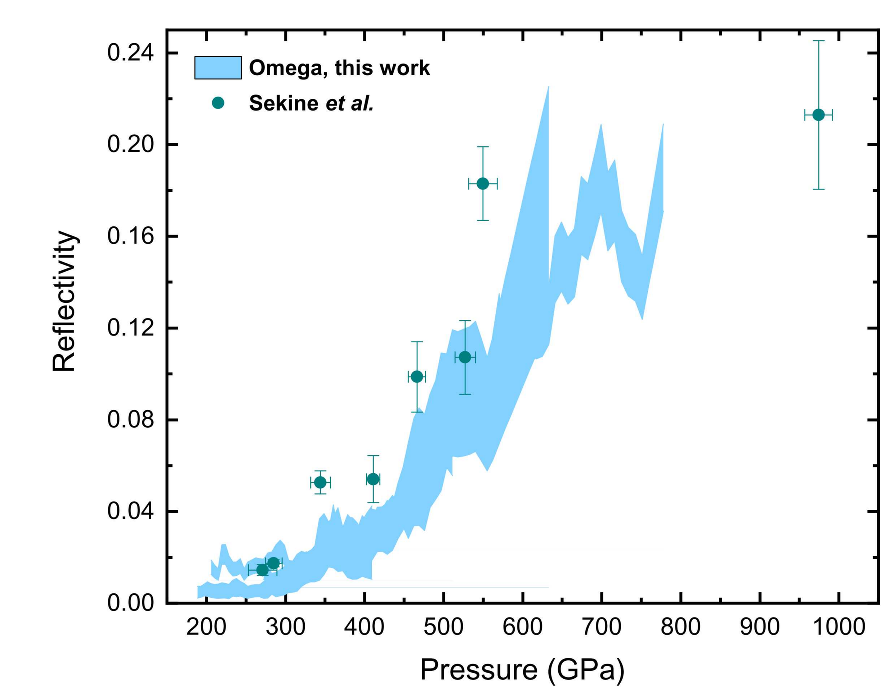




- Hugoniot states of Mg_2SiO_4 fall between those of MgO and SiO_2
- Z & Omega expts. and QMD show remarkable agreement in Hugoniot states
- QMD temperatures tend to be lower than expts
- Dunite ANEOS liquid Hugoniot is softer and hotter than data

6 - Implications for planetary impact models





- Resolved apparent disagreement in interpretation of Hugoniot[2,3]
- Show that previous and current work is insufficient to conclude whether de-mixing occurs
- Current EOS are inaccurate and should incorporate newest data
- Finite reflectivity upon melting suggests poorly conducting liquid

Acknowledgements & References

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References

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