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Shock-ramp compression of iron-rich (Mg,Fe)O: preliminary theory and application to Earth's ultra-low velocity zones

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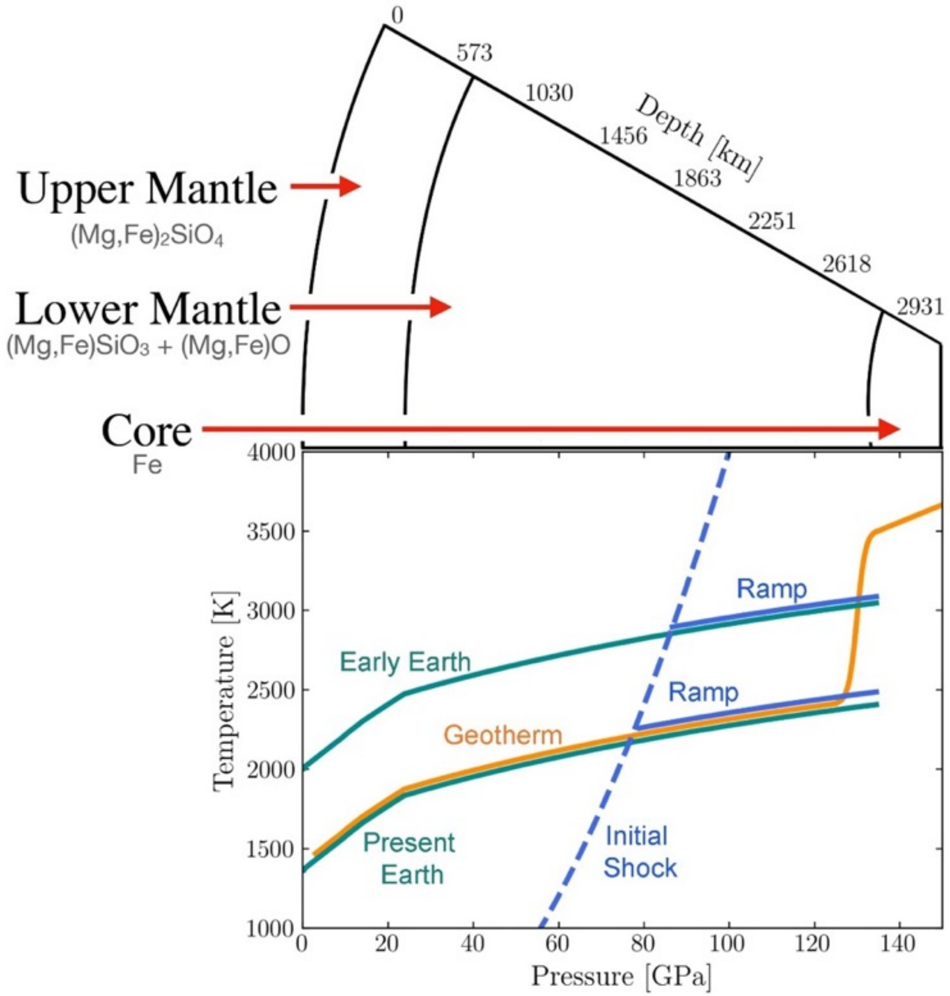

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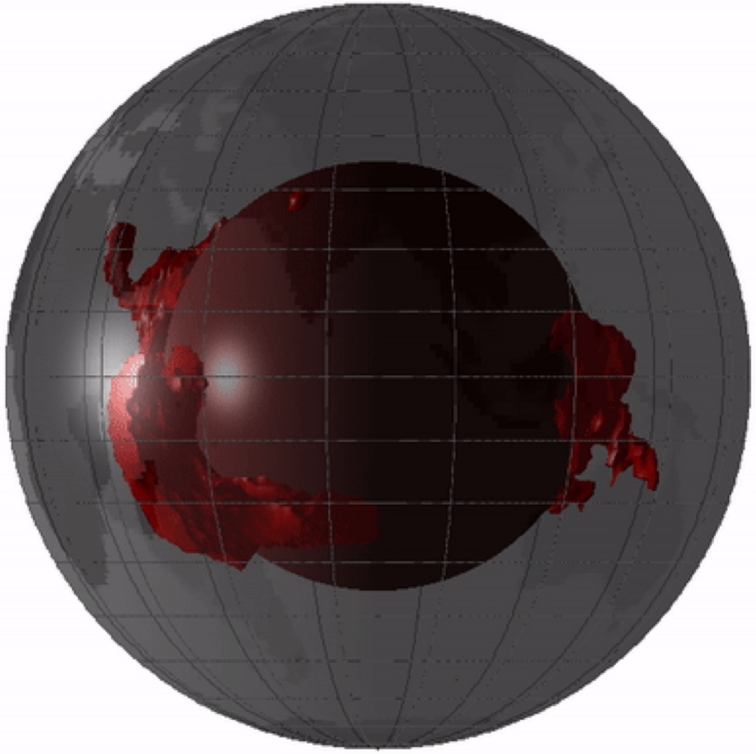
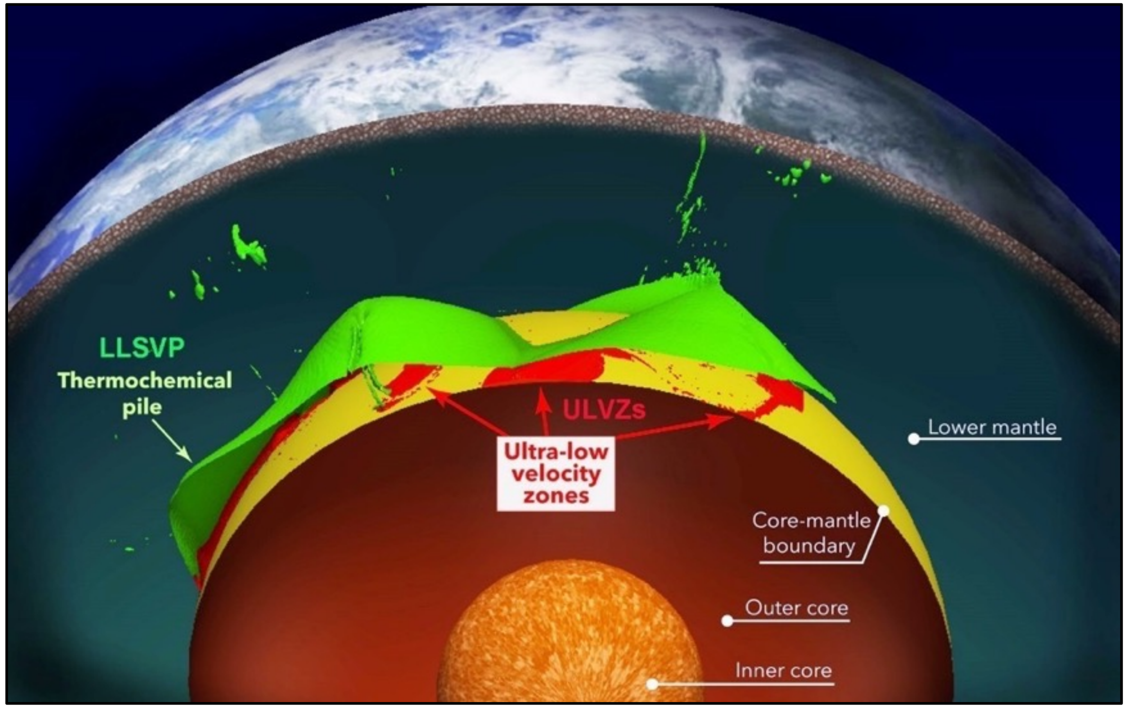
Ultra-low velocity zones



LLSVPs

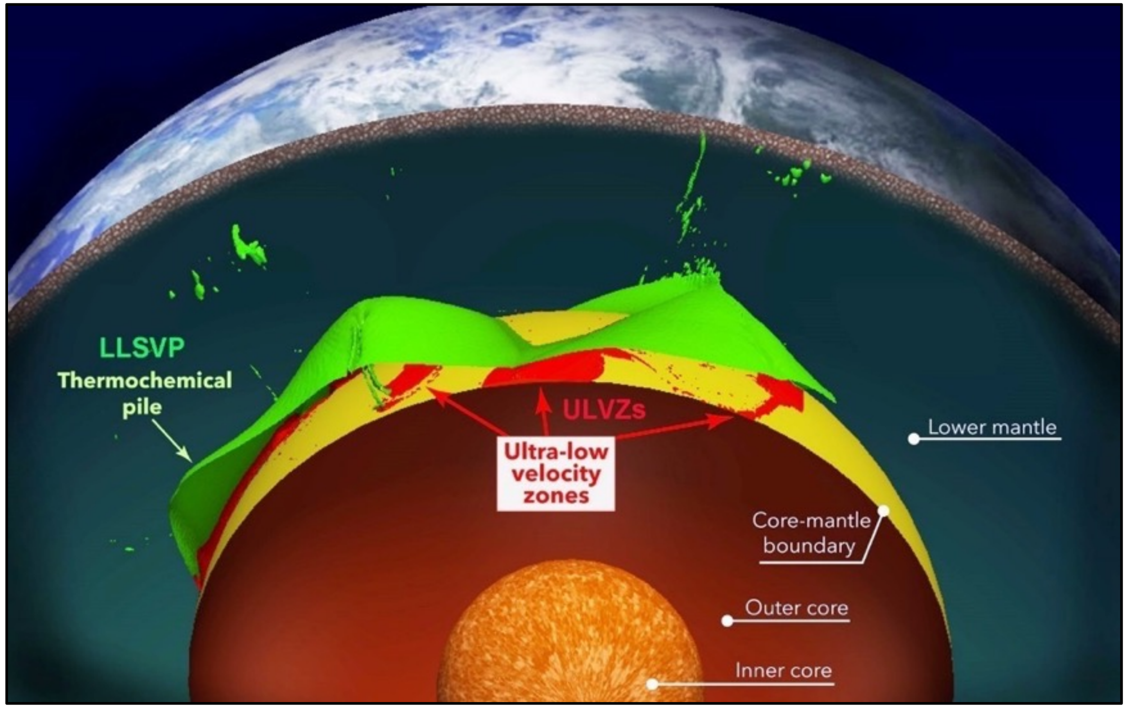


S. Cottaar and V. Lekic

E. Garnero and M. Li

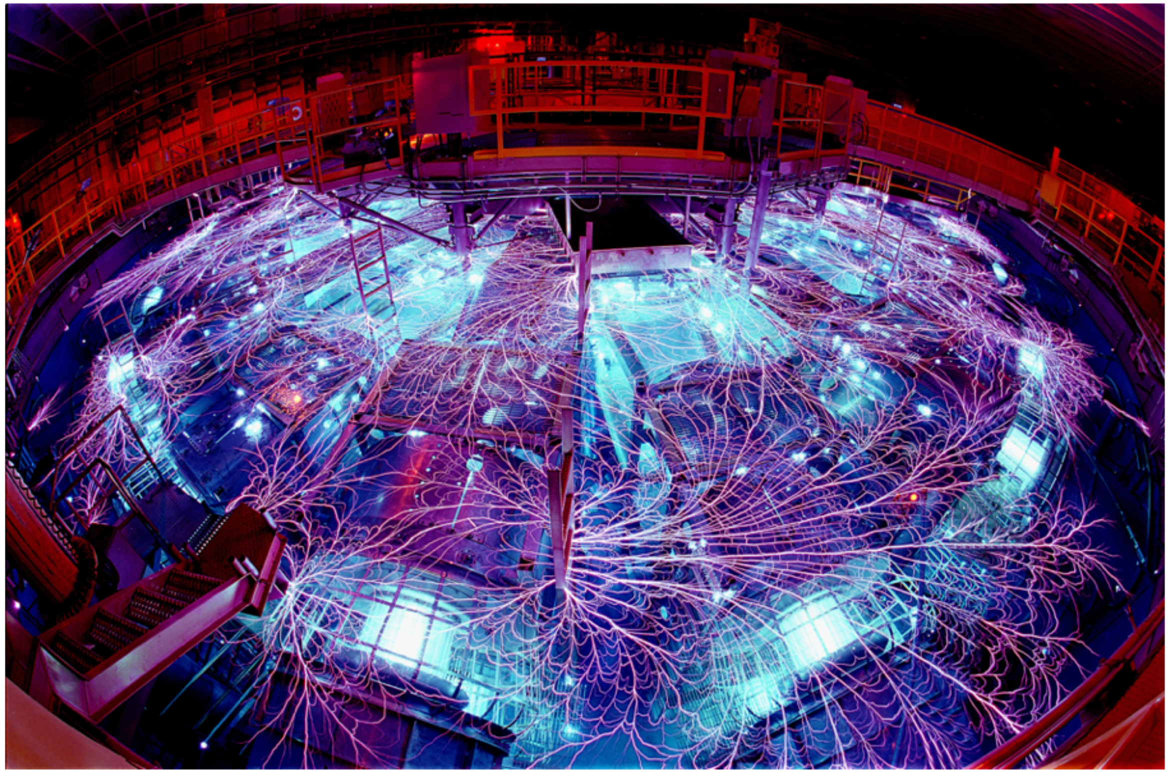
Ultra-low velocity zones

- ULVZ P- and S-wave velocities are up to 30% slower than surrounding mantle, while being up to 10% denser
- Very Fe-rich (Mg,Fe)O is a possible explanation for ULVZs
- Thermodynamic properties of Fe-rich (Mg,Fe)O at near-core conditions of both pressure and temperature remain poorly constrained

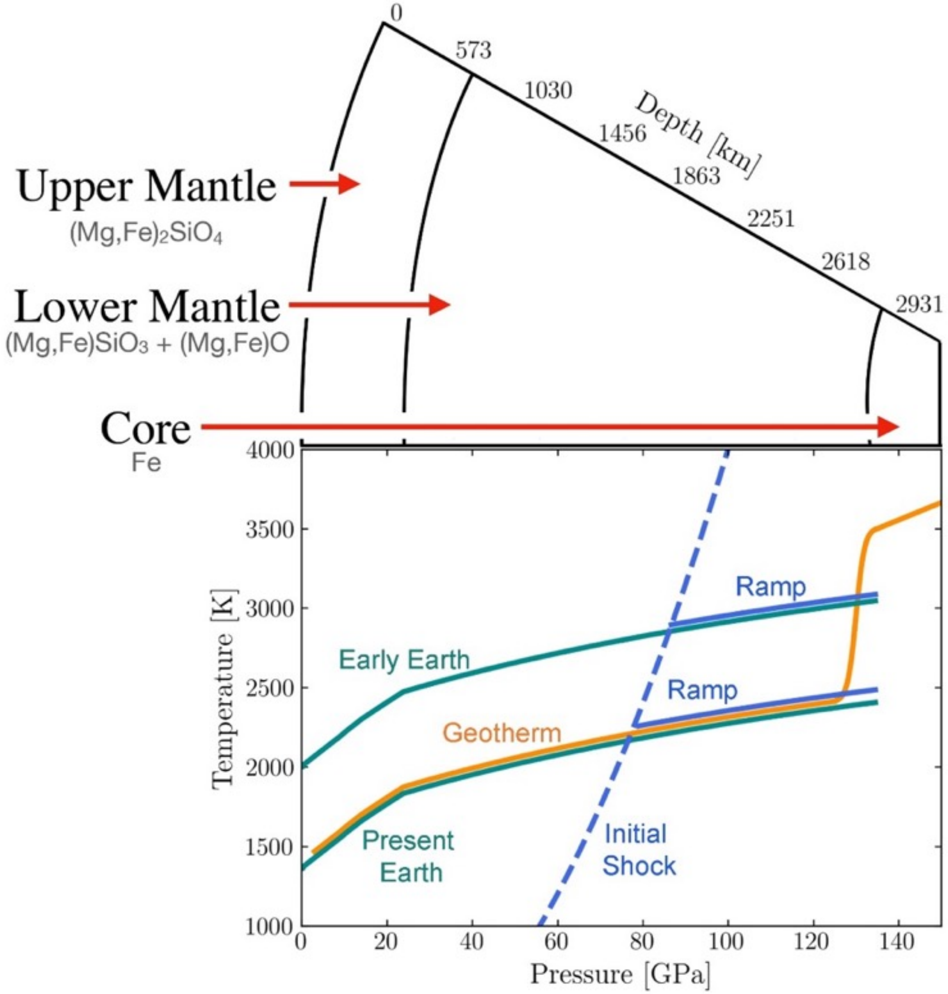


E. Garnero and M. Li

Utilizing unique shock-ramp capabilities of Z machine to reach core-mantle boundary conditions

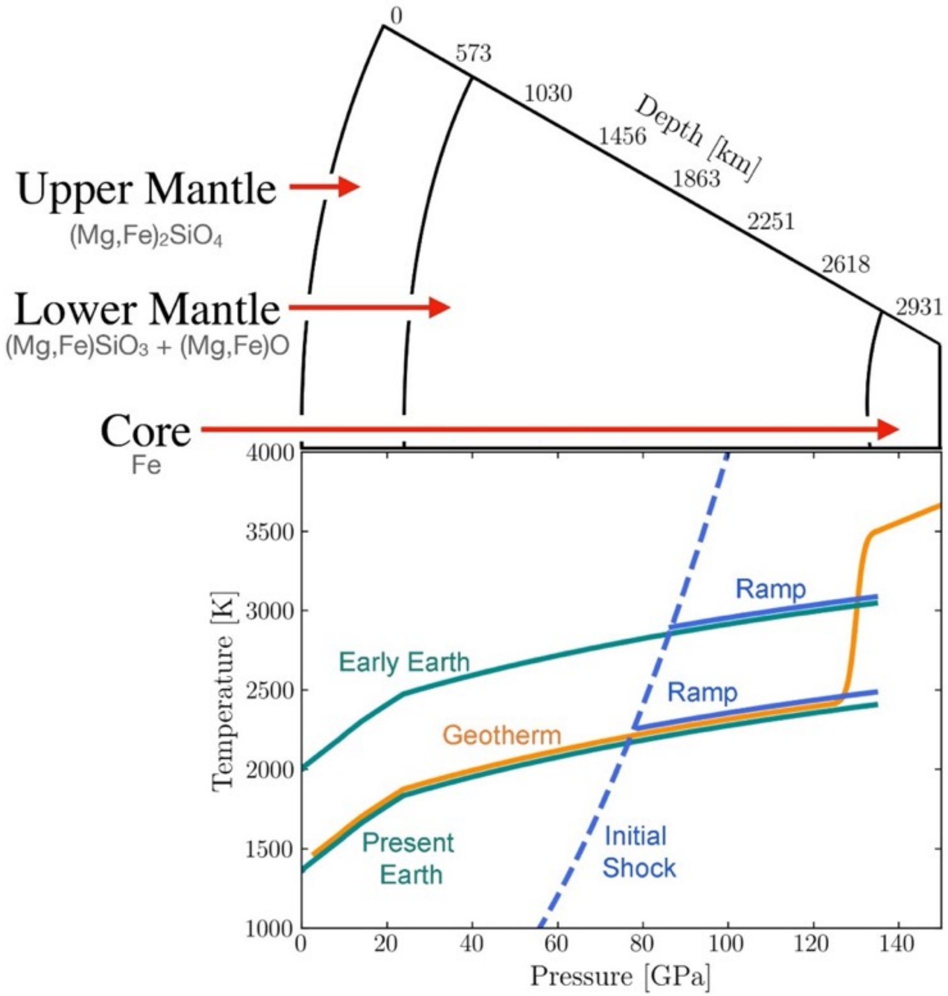


Z machine, Sandia National Lab



Utilizing unique shock-ramp capabilities of Z machine to reach core-mantle boundary conditions

- *Planned experiments*: shock-ramp compression on (Mg,Fe)O with X_{Fe} = 25% and X_{Fe} = 50% along isentropes at shock states relevant to Earth's core-mantle boundary
- *Experiment goals*: first direct measurements of sound speeds of (Mg,Fe)O following isentropic paths similar to the geotherm



DFT calculations guiding shock and ramp

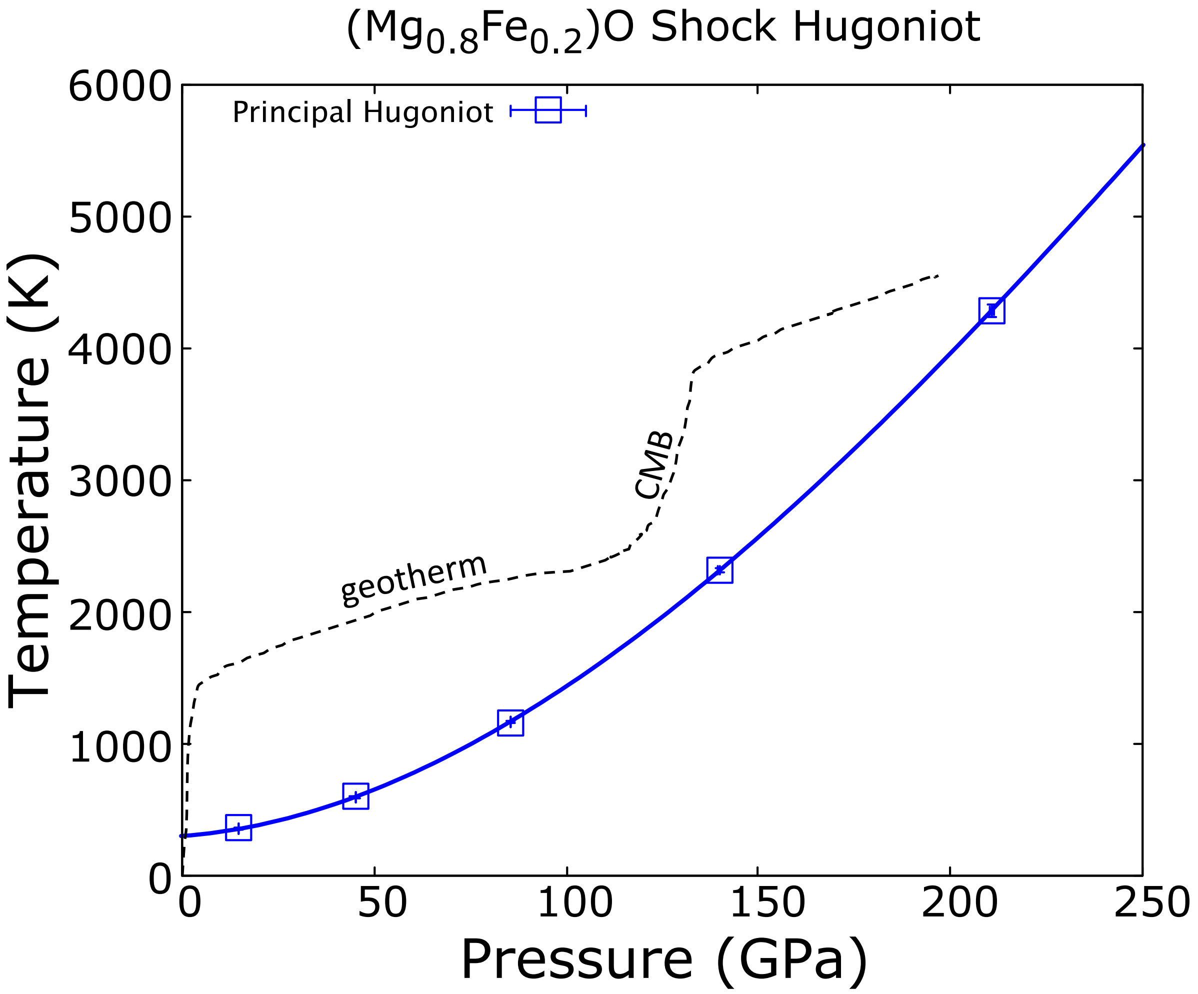
- $(Mg_{0.8}Fe_{0.2})O$ B1
- PBE calculations using Quantum Espresso
- Reference density = 4.099g/cc

<u>Rankine-Hugoniot relations</u>

$$\rho_0 U_s = \rho(U_s - u_p)$$

$$P - P_0 = \rho_0(U_s - u_0)(u_p - u_0)$$

$$E - E_0 = 1/2(P + P_0)(V - V_0)$$



DFT calculations guiding shock and ramp

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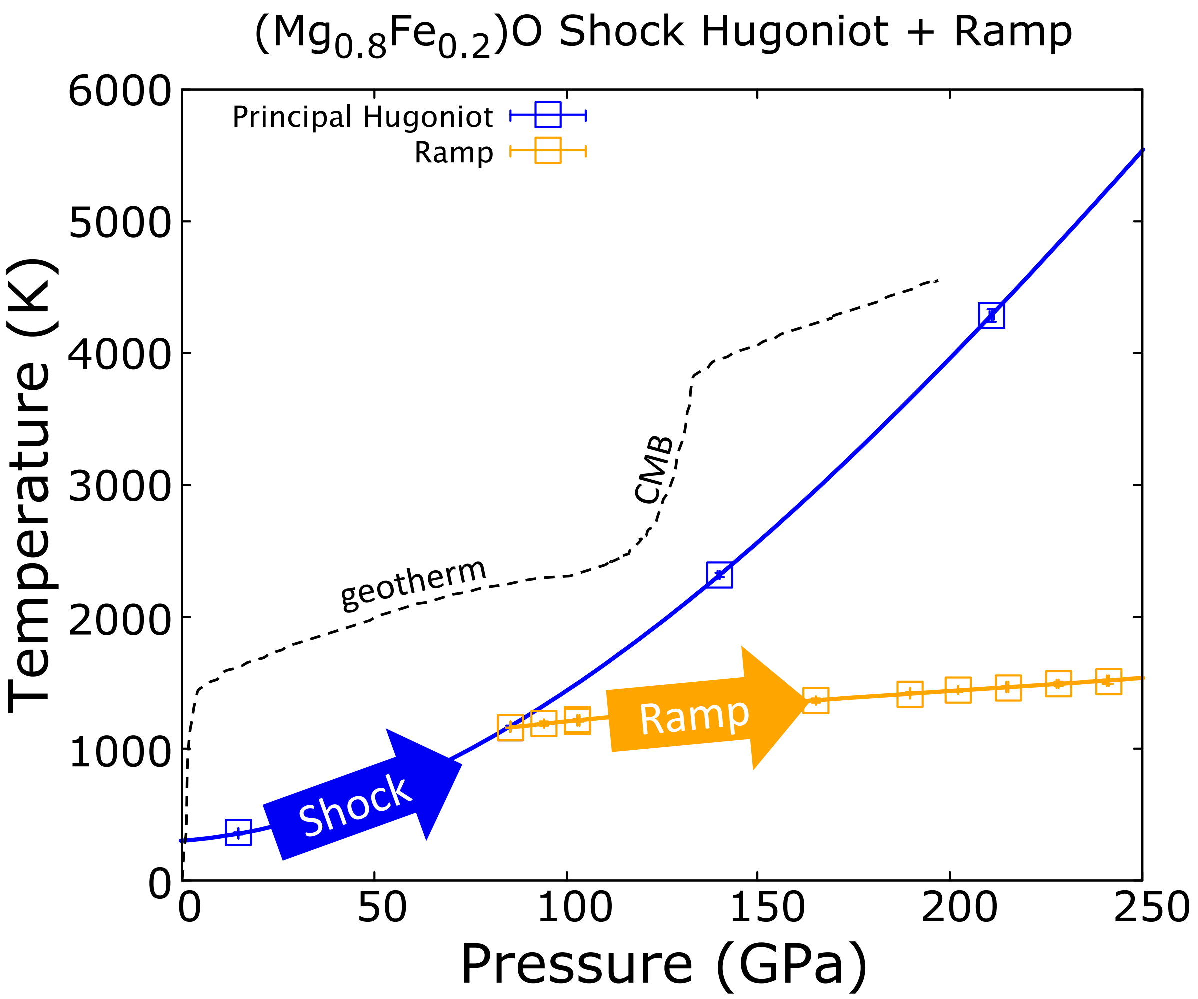
<u>Rankine-Hugoniot relations</u>

$\rho_{n-1} U_S = \rho_n (U_S - u_p)$

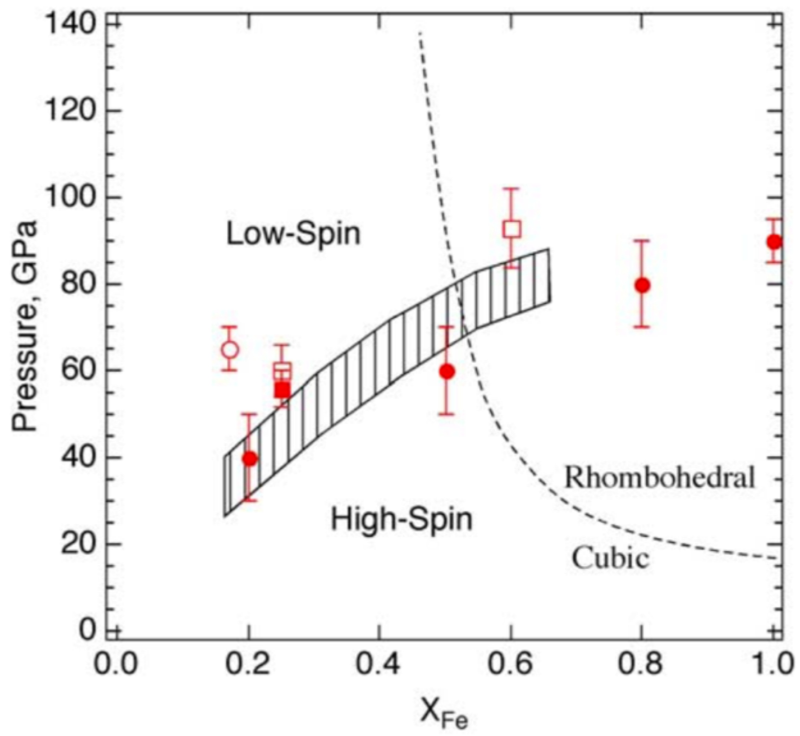
$P_n - P_{n-1} = \rho_{n-1}(U_S - u_{n-1})(u_p - u_{n-1})$

$E_n - E_{n-1} = 1/2(P_1 + P_{n-1})(V_1 - V_{n-1})$

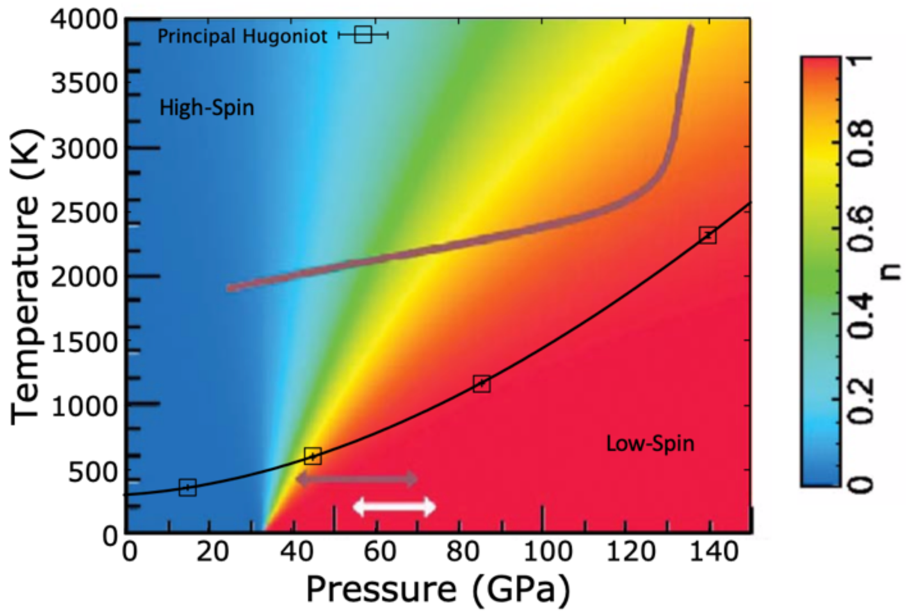


Fe spin transition

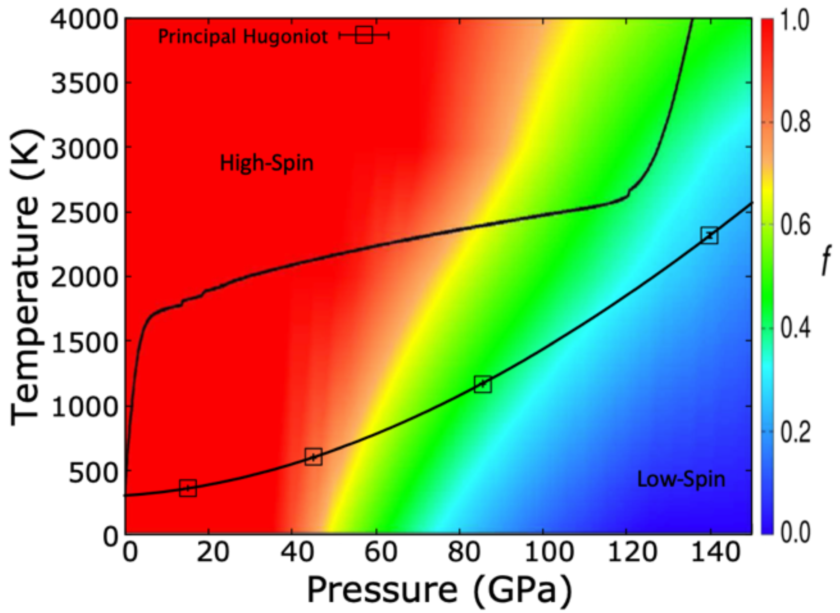
- PBE does not consider Fe spin transition



Yingwei Fei et al. 2007



***X_{Fe}* = 18.75%** (T. Tsuchiya et al. 2006)

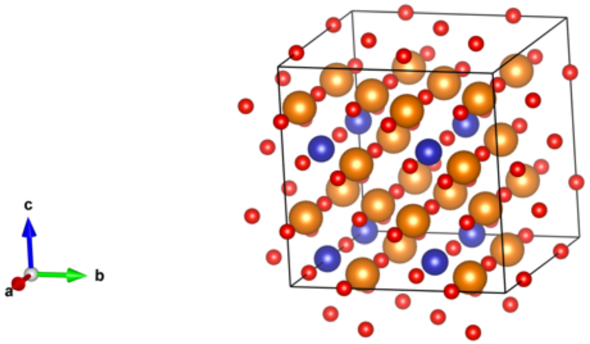


***X_{Fe}* = 25%** (E. Holmström and L. Stixrude 2015)

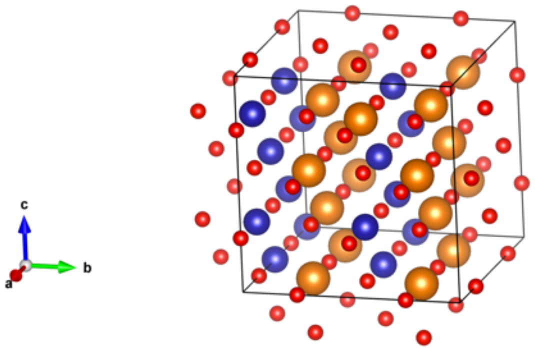
PBE + U

- $(Mg_{0.75}Fe_{0.25})O$ & $(Mg_{0.5}Fe_{0.5})O$
- PBE + U calculations using Quantum Espresso
- 64 atoms supercell

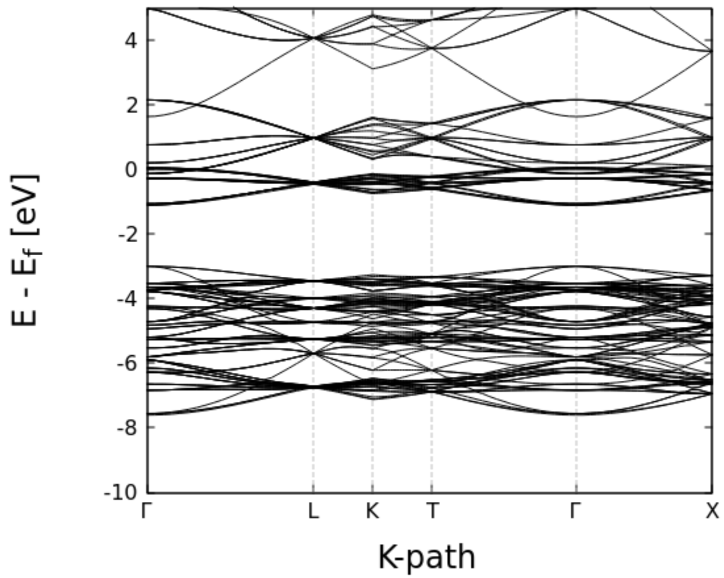
$(Mg_{0.75}Fe_{0.25})O$



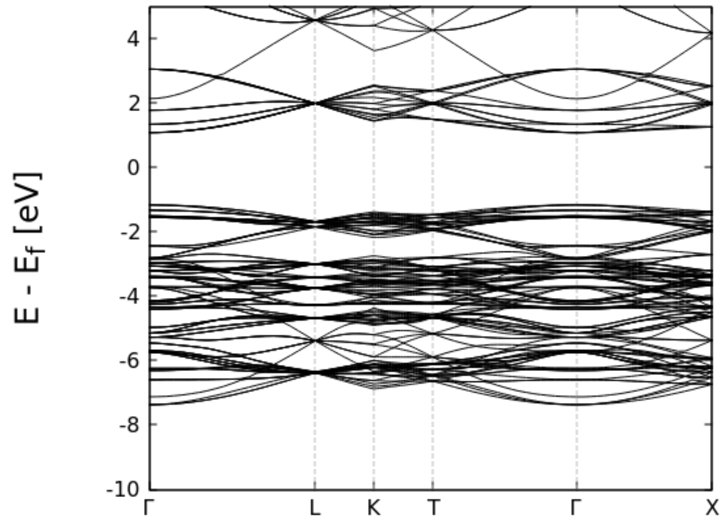
$(Mg_{0.5}Fe_{0.5})O$



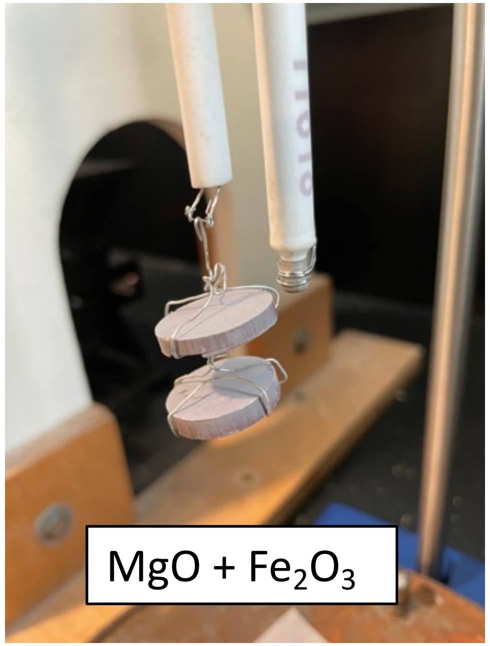
PBE

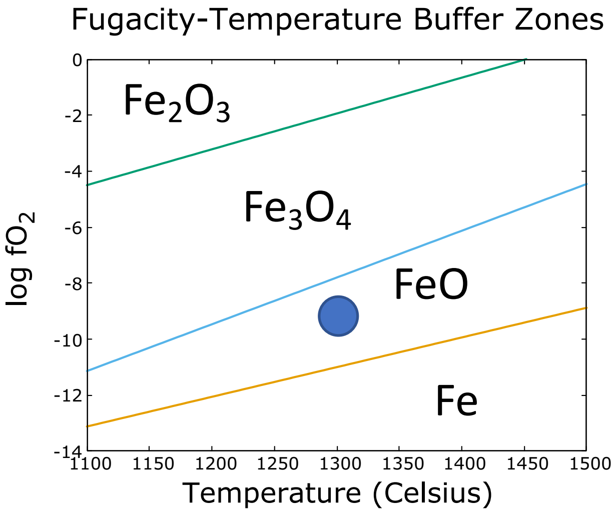


PBE + U

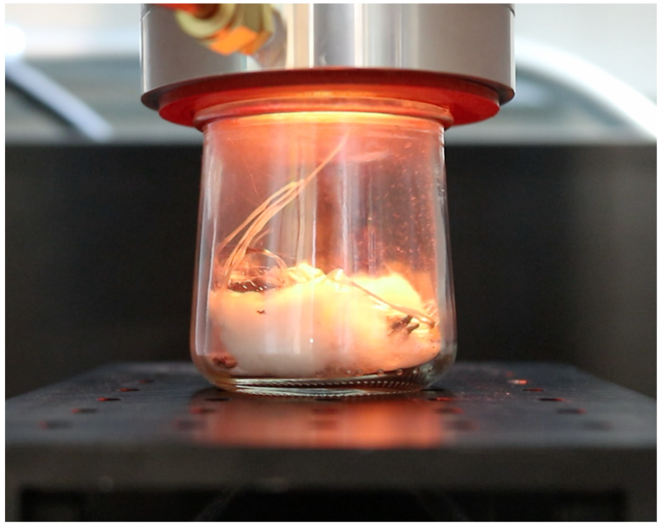


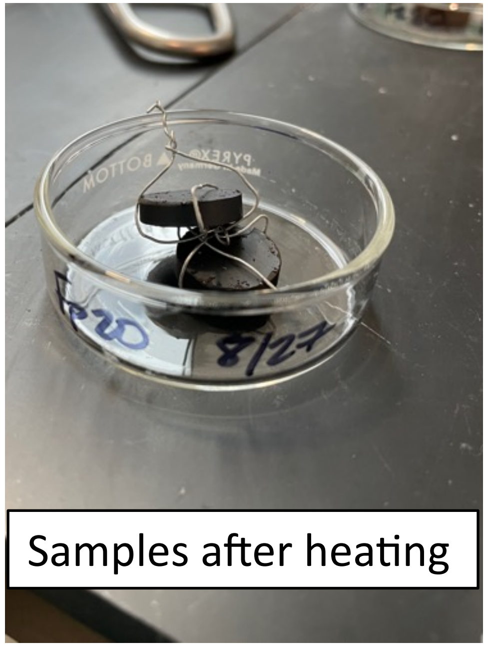
(Mg,Fe)O Sample Synthesis


MgO + Fe_2O_3

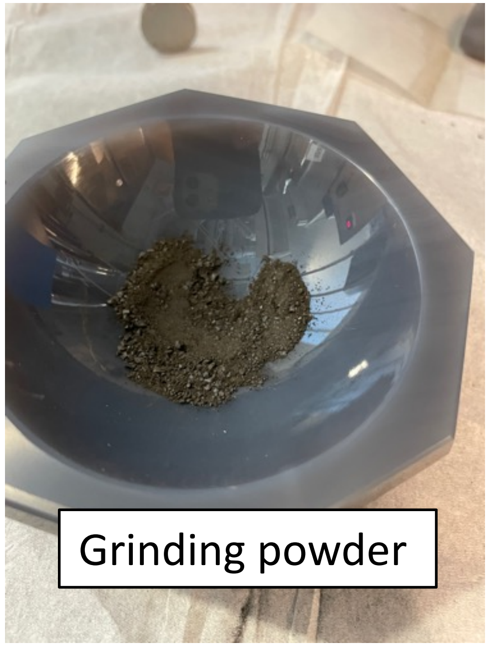


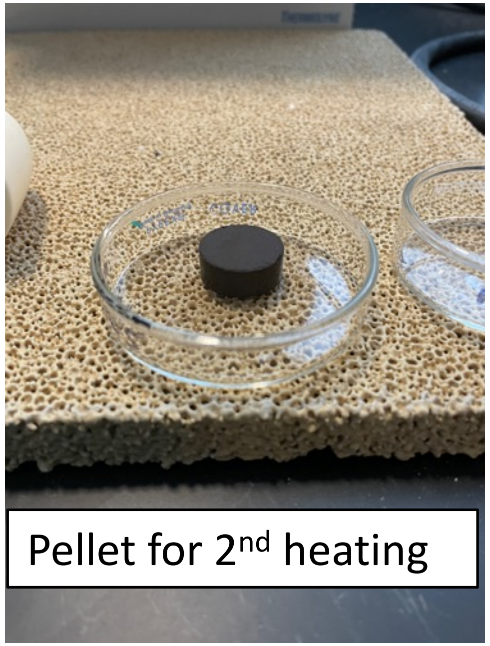
Conditions for heating


Drop quench



Samples after heating


Grinding powder


Pellet for 2nd heating

Ongoing and future work

- PBE + U (Mg,Fe)O Hugoniots
  - X_{Fe} = 25% & X_{Fe} = 50%
- Synthesis of polycrystalline samples
- Standard shock experiments
  - Ranging 70-160 GPa
- Z-machine shock-ramp experiments
  - Ramp up from 100 GPa

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Thank you

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