Light element partitioning between silicates, oxides and metallic melts

Insights into the formation and composition of Earth's core

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MOTIVATION

- The Earth's core is an iron-nickel alloy which contains several weight percent of one or more unknown light elements. Likely candidates include Si, O, S, C (and perhaps H and Mg).
- The formation of Earth's core involved iron segregation through a silicate magma ocean and underlying solids after impacts between planetesimals and planetary embryos.
- Light elements were partitioned between the metallic alloy and the surrounding silicates during segregation.
- These early processes had a dominant effect on the oxygen and carbon budget of the shallow Earth.

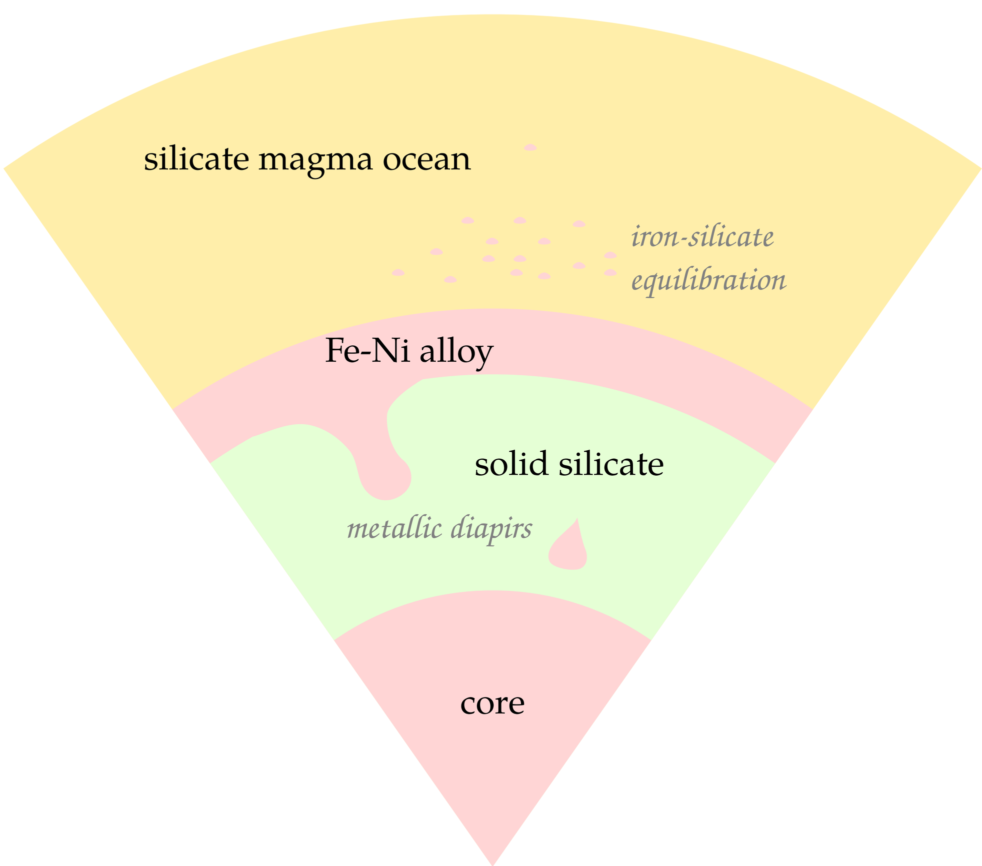

Figure 1: Schematic diagram of the proto-Earth after the impact of a large differentiated planetesimal.

The aims of this study:

- Create a self-consistent thermodynamic model of iron-rich solids and liquids within the software *burnman* [1].
- Predict the chemical evolution of the Earth and other planetary bodies during planetary growth, core-mantle differentiation and magma ocean crystallisation.
- Provide estimates of seismic velocities and densities in planetary cores.

SOLID ENDMEMBERS

- Popular thermodynamic models for minerals use a Debye-type lattice model [2] or polynomial parameterisation [3] for thermal properties.
- We adopt the Debye model approach, with additional terms to account for magnetic, order-disorder, electronic and anharmonic contributions to the thermal pressure.

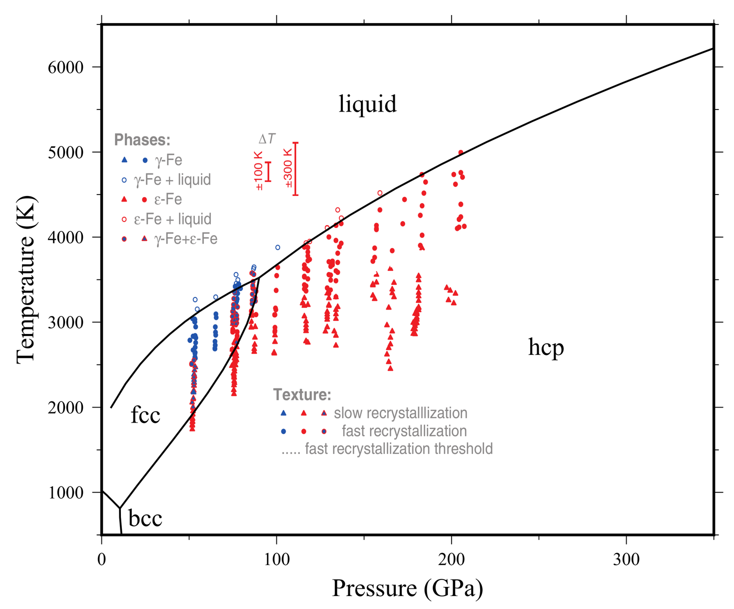

Figure 2: The phase diagram of iron. The experimental data are from [4].

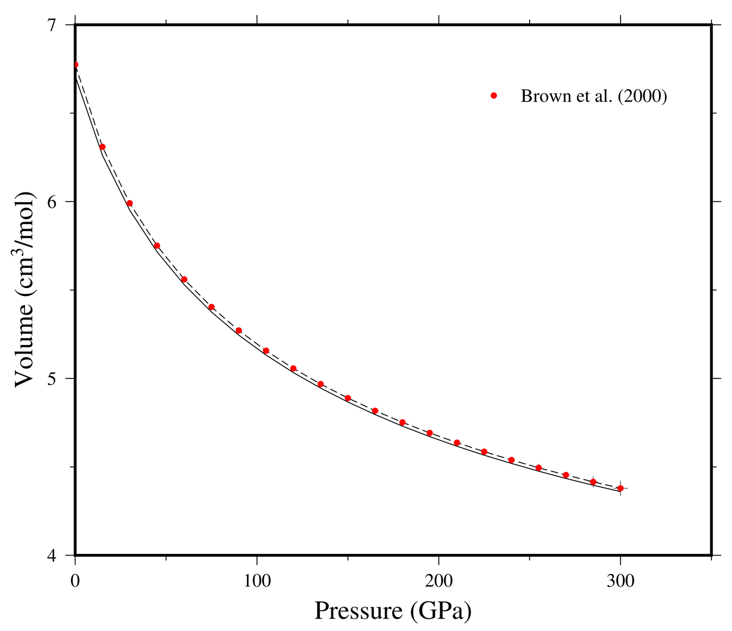

Figure 3: The volume of HCP iron along the Hugoniot. Red dots are experimental data [5].

MELT ENDMEMBERS

- There is significant disagreement on the properties of melts reported in the literature.
- We use the constraints provided by the volume, heat capacity and thermal expansivity at 1 bar, and use the piston-cylinder/multianvil-constrained melting curve.
- To extrapolate to high pressures, we attempt to satisfy the following equations [6]: $\Delta S_{melt} = R \ln 2 / (1 - \alpha K_T\, dT/dP)$; $\Delta V_{melt} = \Delta S_{melt}\, dT/dP$.

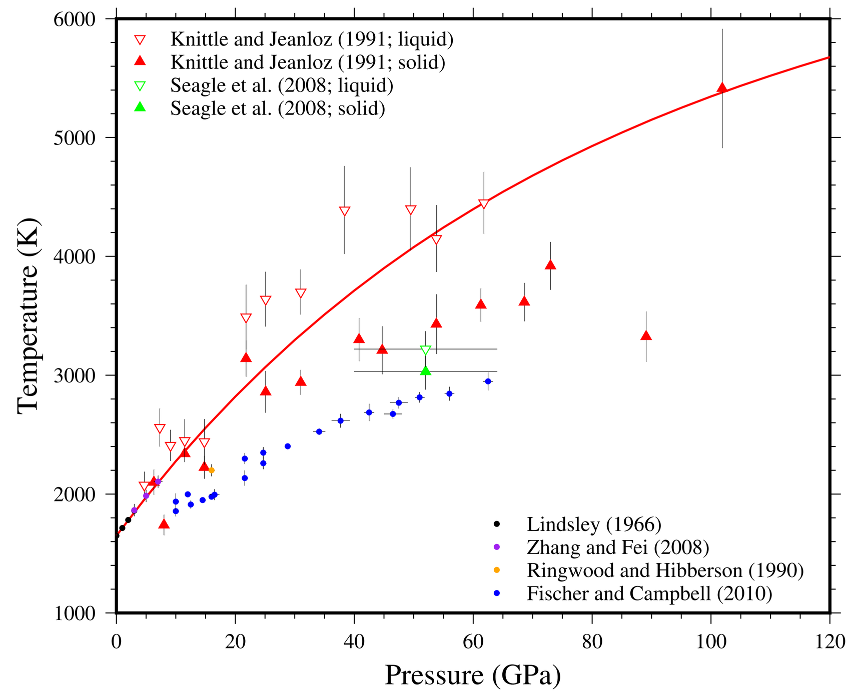

Figure 4: The melting curve of Fe_xO ($0.94 \leqslant x < 1$). Model curve for FeO in red. Constraints are from PC [7], MA [8, 9] and LH-DAC experiments [10, 11, 12].

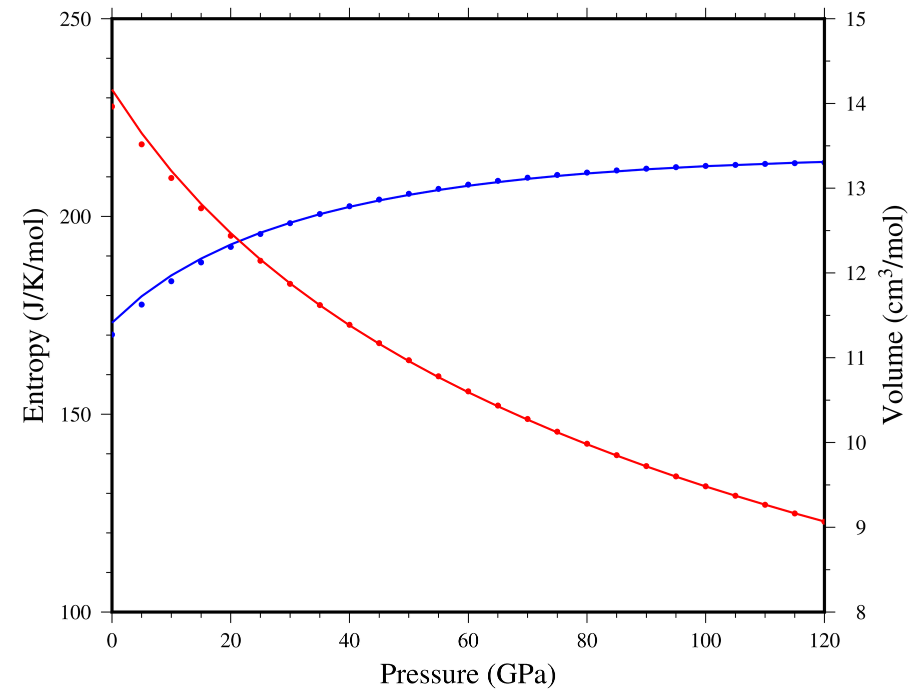

Figure 5: Liquid properties along the FeO melting curve. The dots correspond to the predicted properties based on a model for simple melting [6].

SOLUTION MODELS

- We adapt the subregular solution model to incorporate excess bulk moduli and heat capacities, enabling accurate modelling over the *P*-*T* range of the mantle.
- Metallic melt solutions are fit to immiscibility gaps and liquidus curves.

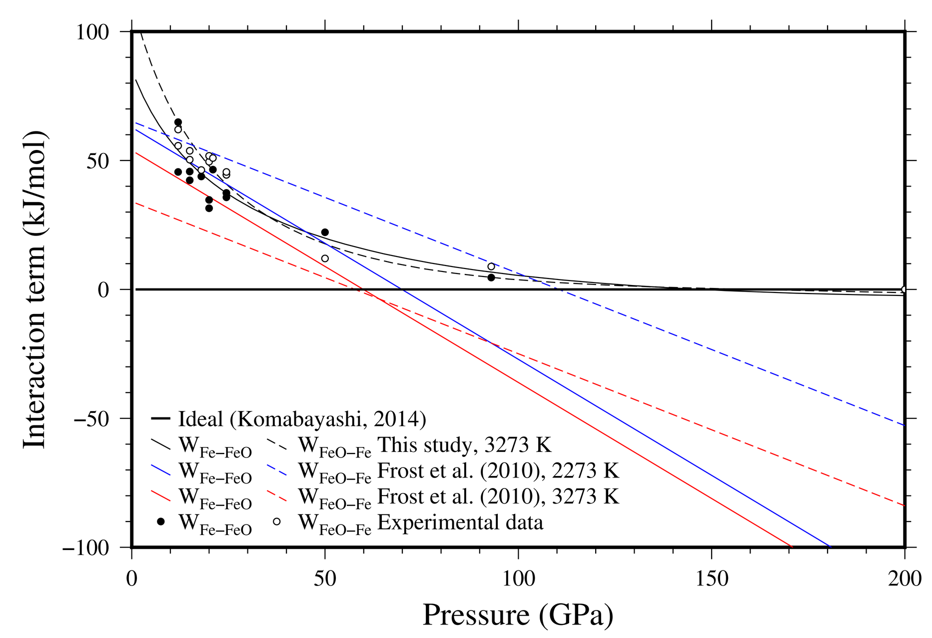

Figure 6: Interaction parameters of Fe-FeO and FeO-Fe. Also shown are extrapolations of published low pressure [13] and high pressure [14] parameterisations.

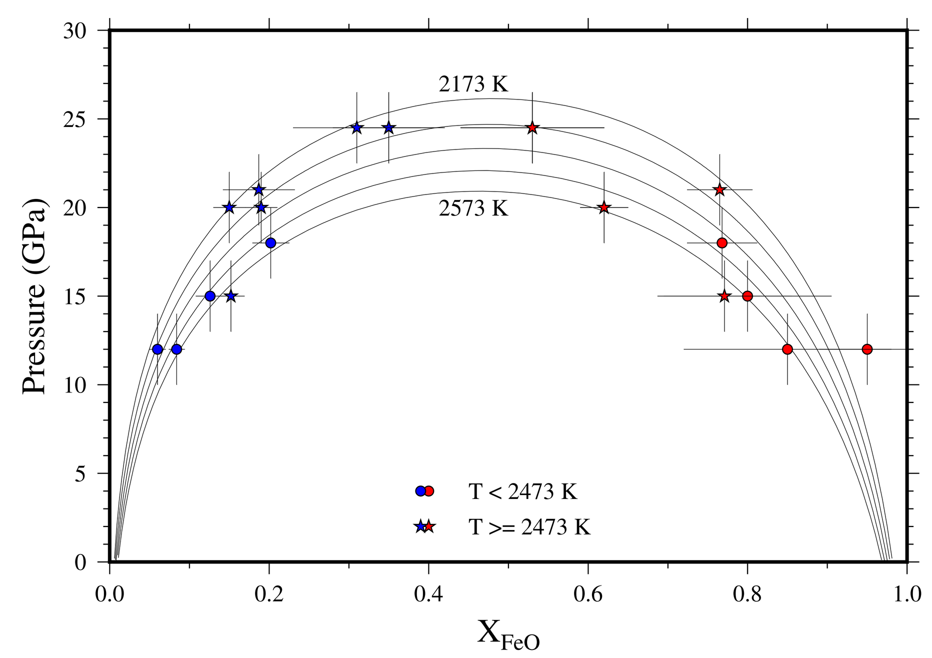

Figure 7: The Fe-FeO solvus as a function of pressure and temperature. Data points are from the published literature [13, 15].

EQUILIBRIUM CALCULATIONS

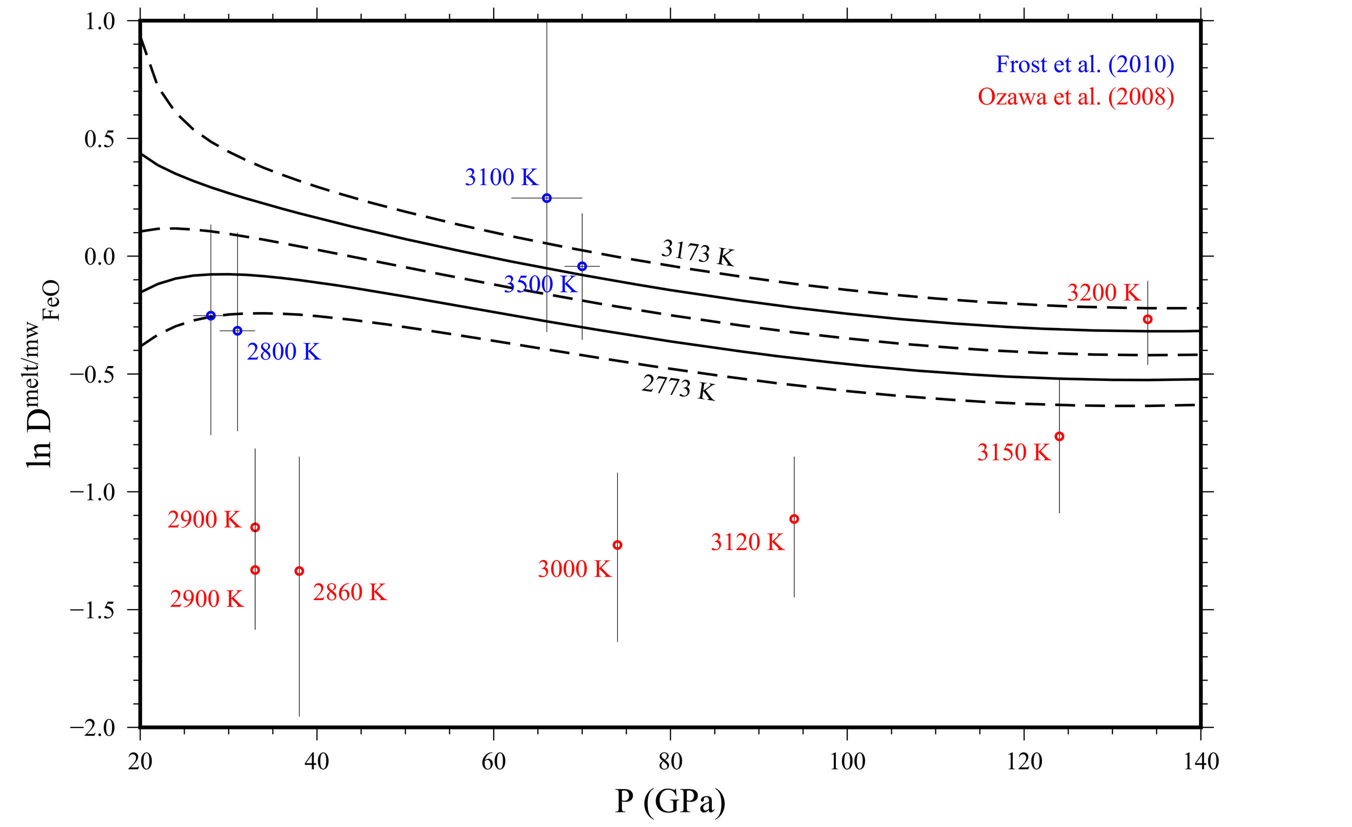

Figure 8: Model $Mg_{0.8}Fe_{0.2}O$-melt equilibria, with published experimental data [13, 16] for comparison.

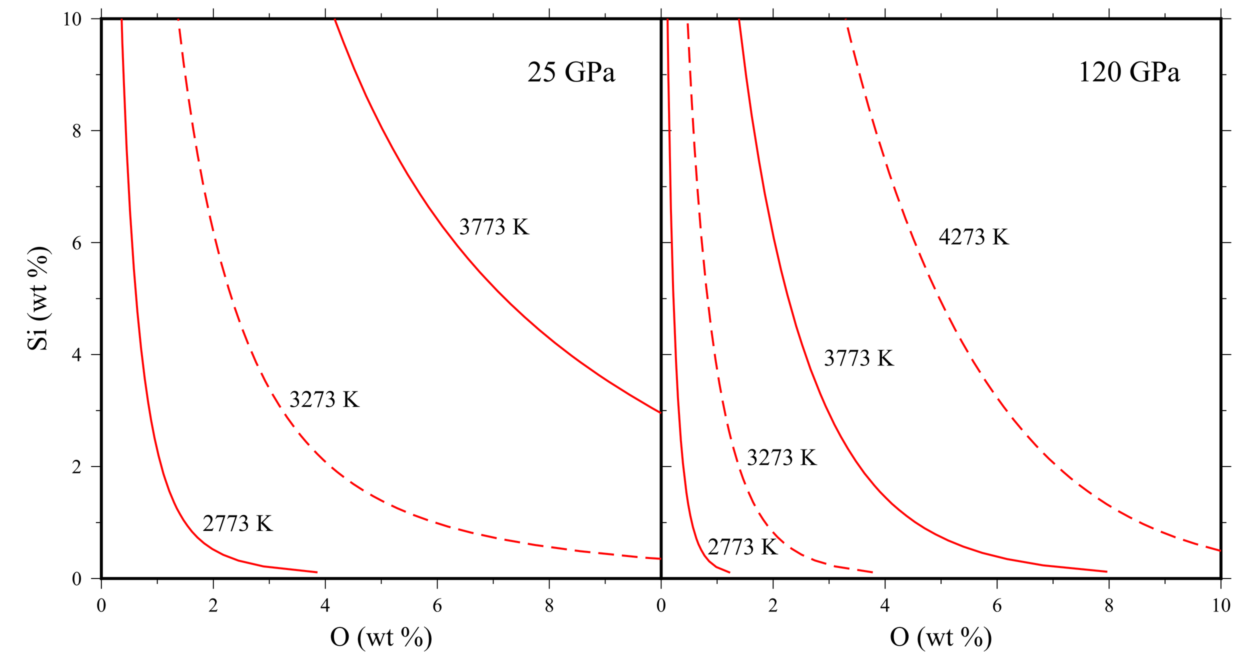

Figure 9: $Mg_{0.9}Fe_{0.1}SiO_3$ bridgmanite-melt equilibria

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