

Thermodynamic constraints on the mineralogy of the lower mantle

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Phase equilibria experiments are challenging at lower mantle conditions due to difficulties in characterising small recovered samples, the large thermal gradients in experimental devices, slow cation diffusion in the mineral phases of interest and problems in accurately determining the pressure. Thermodynamic treatments are consequently essential as they allow different types of data to be incorporated in a single model that then allows inconsistencies to be identified and permits the results to be interpolated and extrapolated. In particular if the volume behaviour of mineral end members can be determined the speciation of such components can be rigorously extrapolated in pressure.

Bridgmanite, the dominant lower mantle mineral, is a relatively complex solid solution particularly considering that trivalent cations can substitute through both a coupled substitution mechanism, and through the creation of oxygen vacancies. We have synthesized single crystals of bridgmanite in the system Fe-Mg-Al-Si-O through high pressure experiments in order to principally study the incorporation mechanism of trivalent cations. Samples recovered from experiments performed at different oxygen fugacities and silica activities have been characterised using single crystal x-ray diffraction. Using the determinations of cation site occupancies and unit cell volumes in addition to further Fe-Mg partitioning data a thermodynamic model has been derived to describe bridgmanite composition as a function of pressure, temperature and oxygen fugacity. We use this model to examine the structure of the 660 km seismic discontinuity and explore the implications for the redox state and volatile speciation throughout the lower mantle.