Deriving an Empirical Expression for the Partitioning of Iron between Mg-perovskite and Ferropericlase

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The major element chemical composition of the lower mantle is uncertain and its determination is important for many problems in earth and planetary sciences. The seismically derived densities and wave velocity structures for the mantle can be used to test models of mantle compositions. This involves calculating mantle densities or velocities with mineral properties from laboratory experiments to match the constraints from seismology. Mg-perovskite and ferropericlase are two major phases that comprise up to 93 vol% of the lower mantle. Iron is expected to be distributed among these two phases, affecting the density and elastic properties of the minerals. However, the distribution of Fe between ferropericlase and Mg-perovskite (K_D), especially for Al-bearing systems, shows a wide range of behavior throughout the literature and is poorly understood, limiting the extent to which the composition of the lower mantle can be constrained.

We have used a variety of empirical formulations of the excess Gibbs free energy of mixing for these two minerals, thus exploring possible expressions for the distribution of Fe among Al-Mg-perovskite and ferropericlase. The expressions are fitted to data via least squares fitting. We will further investigate whether the new formulation that is giving us the best fit can be generalized and applied to other systems that involve Fe-Mg partitioning. A formulation that is capable of explaining data in the literature may make it possible to derive K_D values suitable for the P-T conditions of the lower mantle, shedding light on its elemental composition. The figure on the right shows the mole ratio of Fe/(Fe+Mg) in ferropericlase (y-axis) plotted against the same ratio in Mg-perovskite (x-axis) for K_D at 0.4 and 0.7 using what we currently believe is our best formulation.