Iron Partitioning in the Deep Mantle and Consequences for the Magma Ocean

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Abstract

The relative buoyancy of crystals and liquid is likely to exert a strong influence on the thermal and chemical evolution of the magma ocean. Theory indicates that liquids approach, but do not exceed the density of iso-chemical crystals in the deep mantle. The partitioning of heavy elements, such as Fe, is therefore likely to control whether crystals sink or float. While some experimental results exist, our knowledge of silicate liquid-crystal element partitioning is still limited in the deep mantle. We have developed a method for computing the Mg-Fe partitioning in such systems. We focused initially on (Mg,Fe)O. As a relatively simple system, the buoyancy effects of Fe partitioning are likely to be large. The method is based on molecular dynamics driven by density functional theory (spin polarized, PBEsol+U). We compute the free energy of Mg for Fe substitution in simulations of liquid and B1 crystalline phases via adiabatic switching. With the method tested fully on ferropericlase we then moved to the silicate perovskite system, (Mg,Fe)SiO3. We investigate the dependence of partitioning on pressure, temperature, and iron concentration. In the case of ferropericlase we find that the liquid becomes more dense than the crystal when the pressure increases beyond 40GPa. We also find that the high-spin to low-spin transition in the crystal and the liquid have an important influence on partitioning behavior.

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