Lithium Diffusion and its isotopic fractionation in forsterite

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The distribution of impurities in minerals can provide important clues to thermal and chemical processes occurring in the Earth's mantle over geological time. Lithium (Li) is increasingly used as a geochemical tracer as its two isotopes (6Li and 7Li) have a large relative mass difference and thus fractionation can lead to compositional variations at low temperatures. At higher temperatures, isotopic fractionation is less pronounced, although high temperature diffusion can lead to variations in observed isotopic signatures in mantle minerals. The importance of this cooling driven process is increasingly recognized.

Knowledge of point defect chemistry and diffusion is critical for the interpretation of Li distribution in minerals. In this work, we are using quantum mechanical methods to investigate the details of the Li diffusion and its isotopic fraction in Olivine.

We found that in forsterite Li will be incorporated as bound interstitial–substitutional pairs. Furthermore, there will be temperature dependent fractionation of its two isotopes between the different sites. The fractionation decreases dramatically from 87.1 ‰ at 300 K to 1.0 ‰ at 3000 K. Diffusion is predicted to occur via two inter-related mechanisms: Mg–Li exchange, and a second, vacancy assisted interstitial mechanism. This behaviour is complex, facilitates migration of the heavier isotope and offers insights into observations of Li mobility and zoning in olivine, the most volumetrically important upper mantle mineral.

The results enhance our knowledge of the behaviour of chemical exchange, material transport and electrical con- ductivity in the Earth's upper mantle, and to interpret ob- served isotopic variations in real rocks.

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