Goldschmidt2017 Abstract

Lithium defects and diffusivity in forsterite and its high pressure phases - wadsleyite and ringwoodite

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The distribution of trace elements in the mantle forming minerals plays important role in understanding the thermal and chemical processes occurring in the Earth's mantle over geological time. As a geochemical tracer, the two isotopes of Lithium (^{6}Li and ^{7}Li) have a large relative mass difference and its fractionation leads to compositional variations at low temperatures. It was evidenced that Li isotopic fractionation is temperature dependence and the diffusion driven isotopic fractionation can aslo be significant at high temperatures.

In order to determine the point defect chemistry responsible for Li isotope fractionation and to constrain the isotope fractionation factors as a function of temperature and pressure, we conducted computational and theoritical methods to investigate the details of the Li diffusion and its isotopic fraction between the lattice sites in forsterite, wadsleyite and ringwoodite.

Our simulations show that Li can diffuse out of forsterite and its high-pressure polymorphs via substitutional mechanism with Mg vacancies around in the lattice. This migration progress is mainly controlled by the concentration of Mg vacancies and Li-Mg exchange rate. The Li diffusion activation energy is 0.254 eV (α-phase), 0.110 eV (β-phase) and 0.257 eV (γ-phase) respectively in all three phases. Pressure has less effect on the Li isotope partition, however, there will be temperature dependent fractionation of its two isotopes between the lattice sites (interstitial and substitutional). The fractionation decreases dramatically from 300 K to 2500 K: 49.50 ‰ to 0.85 ‰ (α-phase), 58.98‰ to 1.21‰ (β-phase) and 135.73‰ to 2.62‰ (γ-phase), respectively.

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