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Diffusion-Driven Neon Isotope Fractionation in MORB Melts: Insights from Molecular Dynamics Simulations

JEHIEL NTEME AND MANUEL MOREIRA

Institut des Sciences de la Terre d'Orléans (ISTO), Université d'Orléans, CNRS, BRGM

The origin of volatile elements on Earth remains a central question in planetary science, as these elements originate from diverse sources in the Solar System, and their chemical and isotopic signatures can be altered by various processes. A key aspect of this puzzle is understanding how volatile elements behave during magma degassing. Recent experimental studies, using a bubble-by-bubble extraction technique, have demonstrated that neon isotopes undergo diffusional fractionation during the early stages of bubble formation, growth, and coalescence [1]. However, the rates at which neon isotopes diffuse in magmatic systems remain poorly constrained. To address this, we conducted classical molecular dynamics simulations to investigate the influence of isotopic mass on neon diffusion in a mid-ocean ridge basalt (MORB) melt. This influence is typically expressed by the relationship $D_i/D_j = (m_j/m_i)^{\beta}$, where D_i and D_j are diffusion coefficients of two isotopes whose masses are m_i and m_j. Using the pseudo-isotope method, we found that at ambient pressure, the β factor for neon isotopes decreases linearly with temperature, ranging from 0.291 ± 0.039 at 3500 K to 0.204 ± 0.038 at 2500 K. Furthermore, under increasing pressure along the 3500 K isotherm, β shows a linear decline, dropping from 0.291 ± 0.039 at 0 kbar to 0.147 ± 0.041 at 20 kbar. These results provide new constraints on diffusion-driven neon isotope fractionation, offering a framework to better quantify neon loss during magmatic degassing and to reconstruct the original isotopic composition and concentration of neon in magma source regions.

[1] Núñez-Guerrero, E., Moreira, M., Scaillet, B.(2025) Isotopic fractionation of neon during magma degassing. Geochem. Persp. Let. 34, 1–5.