Kinetic Isotope Fractionation during Crystal Growth

YIFAN LI[1], LI ZHANG[1], ZHENXIN LI[1], HEJIU HUI[2] AND HUAIWEI NI[1]

[1]School of Earth and Space Sciences/Deep Space Exploration Laboratory, University of Science and Technology of China

[2]State Key Laboratory for Mineral Deposits Research & Lunar and Planetary Science Institute, School of the Earth Sciences and Engineering, Nanjing University

Presenting Author: liyifan0529@mail.ustc.edu.cn

Isotope fractionation between mineral crystal and its growth medium (melt or fluid) often deviates from thermodynamic equilibrium. This nonequilibrium phenomenon has been attributed to two kinetic mechanisms: (1) diffusive kinetic isotope fractionation, i.e., the light isotope diffuses faster than the heavy isotope in the growth medium; (2) reactive kinetic isotope fractionation, i.e., the light isotope is associated with higher zero-point energy and tends to be enriched in the product. Crystal growth in silicate melt involves both diffusion inside the melt and chemical reaction at the melt-crystal interface, but there is currently no model dealing with the two kinetic isotope fractionation effects together. In this study, we developed a general numerical model by treating interface reaction as short-range diffusion of constituent elements, as opposed to long-range diffusion in the melt. The soundness of model was verified by comparison with analytical solutions for two endmember scenarios (i.e., crystal growth controlled predominantly by long-range diffusion or by interface reaction). Our calculations for the major element (e.g., zirconium for zircon growth) indicate that a dimensionless parameter $f = (D/t)^{0.5}/(D^*/\lambda)$ (where D and D^* represent the long-range and short-range diffusivity of the element, respectively, t is the elapsed time, and λ is the interatomic distance similar to the diameter of the atom) governs the mechanism of kinetic isotope fractionation. At $f \leq 10^{-3}$, crystal growth is controlled by long-range diffusion, and equilibrium fractionation is maintained at the interface, but there is isotope gradient inside the melt (diffusive kinetic fractionation). At $f \geq 10^{3}$, crystal growth is controlled by interface reaction, and the light isotope is enriched in the mineral relative to equilibrium fractionation, with no isotope gradient inside the melt (reactive kinetic fractionation). At $10^{-3} < f < 10^{3}$, both diffusive and reactive kinetic isotope fractionation are in charge. Variation of parameters including relative mass difference of isotopes, partition coefficient of element, and element concentration in melt generally has little influence on modelling results. For trace elements, the more incompatible the element, the weaker kinetic isotope fractionation.