Equilibrium inter-mineral titanium isotope fractionation: Implication for Ti isotope behaviors during magmatic differentiation

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With the advancement in analytical techniques, Ti isotopes become an important cosmochemical and geochemical tracer. Recently, large mass-dependent Ti isotope variations have been observed in terrestrial rocks and used to trace magma differentiation processes (Millet et al., 2016; Deng et al., 2019). They found that the mass-dependent Ti isotope composition ($\delta^{49}Ti$) is positively correlated with SiO_2 content and speculated that Ti isotope behaviors are controlled by the fractional crystallization of Ti-Fe oxides. Therefore, the equilibrium Ti isotope fractionation factors among major Ti-oxides and silicate minerals are key for understanding those reported $\delta^{49}Ti$ variations. However, such data do not exist in the literature.

Here we present the first-principles investigation of equilibrium inter-mineral Ti isotope fractionation factors ($10^3ln\alpha$) among Ti-doped clinopyroxene, orthopyroxene, olivine, and pyrope, geikielite-ilmenite solid solutions, and rutile based on the density functional theory (DFT). Our calculations suggest the enrichment of light Ti isotopes in ilmenite and rutile relative to the Ti^{4+}-doped silicate minerals but no significant Ti isotope fractionation among Ti^{4+}-doped silicate minerals. Large equilibrium Ti isotope fractionation between Fe-Ti oxides and silicates supports that Fe-Ti oxides are important fractionating phases during magma differentiation. In particular, the Fe/(Mg+Fe) ratio in ilmenite significantly affects the $10^3ln\alpha$ between ilmenite and silicates, suggesting that the chemical composition of Fe-Ti oxides crystallized from magma also controls Ti isotopic fractionation during magma differentiation.

Millet M. et al. (2016) Earth Planet. Sci. Lett. 449, 197–205.

Deng Z. et al. (2019) Proc. Natl. Acad. Sci., 201809164.