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# Iron and silicon isotope fractionation in silicate melts using first-principles molecular dynamics

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The study of silicate melts remains one of the major challenges of the Earth Science field, especially when it comes to the determination of their isotopic composition. Experimentally, melts are often approximated by silicate glasses (e.g. [1][2]). Here, we use first-principles molecular dynamics based on density functional theory to determine iron and silicon isotopes compositions of different silicate melts, namely: iron-rich basalt, iron-depleted basalt, basanite, trachyte and phonolite. This study also allowed us to determine the structural properties of the natural-like melts. The iron isotope composition ($^{57}$Fe/$^{54}$Fe - factors) of the melts are spread over a 1‰ range at 1000K while the silicon isotope compositions ($^{30}$Si/$^{28}$Si -factors) display only a variation of 0.5‰ at the same temperature.

The main parameters controlling iron isotope fractionation in silicate melts having similar iron oxidation state, after temperature, seem to be the Fe-O bond lengths as well as the local environment of iron (i.e. Fe-Fe and Mg-Mg distances). Silicon isotope fractionation appears also to be affected, to a lesser extent, by its local environment as decreasing Si-Fe distances lead to slightly heavier isotopic composition.

These new Fe and Si -factors of silicate melts allow us to calculate precise equilibrium Fe and Si isotopes fractionation factors ($\Delta^{57}$Fe) between melts and a previously published wide variety of minerals [3]. As such, it is possible to use the new $\Delta^{57}\text{Fe}_{\text{min-melt}}$ dataset to discuss the implication of processes such as fractional crystallization and partial melting in the observed Fe and Si isotopes variations in igneous rocks.

References:

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