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Rebuilding isotope fractionation theory for evaporation of silicate melts in vacuum

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There is usually an inconsistency between the observed experimental isotope fractionation result of evaporation and the one predicted by a well-accepted isotope fractination theory, which is based on the Hertz-Knudsen equation. Unfortunately, according to previous works in chemical physics, the Hertz-Knudsen-equation-based theory can only be used for situations where the vaporized species is identical with the one in the melt or liquid. This important requirement cannot be met for most cases of silicate melt because the species in melts are usually complicated oxygen-bearing compounds and are not identical with the vaporized species. In other words, the Hertz-Knudsen-equation-based theory is wrong for studying evaporation processes of silicate melts.

Here, the theory of isotope fractionation for the evaporation process of silicate melts is rebuilt, and a multi-step sequential chemical reaction kinetics model (MSCKM) is proposed. The establishment of this model is based on the core understanding that the evaporation process of silicate melts essentially proceeds through a stepwise bond-breaking mechanism.

The isotope fractionation between the vapor and the residual silicate melt can hence be predicted precisely via the analyzing of bond-breaking steps in the melt. MSCKM can explain very well the experimental results of Mg, K, Si, Fe, Ti and Ca isotope systems and so on. For O isotope systems, because the involved O-bearing species can be changed along the evaporation process, its results can be explained by MSCKM by considering the different evaporation stages. For available Cu and Zn isotope fractionation experimental data, MSCKM cannot explain them because they are not vaporization processes under vacuum conditions. In brief, this study provides a new theoretical framework to deal with isotope fractionations of silicate-melt evaporating in vacuum and bring insights into the molecular level mechanisms of vaporization processes under high temperature.