

Equilibrium Ag isotopes fractionation between minerals and aqueous solutions: Insight from ab-initio calculations and equilibrium experimental

YUAN FANG, DR. ZICONG XIAO, PHD. AND FANG HUANG

University of Science and Technology of China

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

Mineral-fluid reactions are critical processes during ore formation. In recent years, the silver (Ag) isotope compositions of Ag-bearing minerals have been measured precisely, making them potential tracers of deposit evolution. However, the tracing of liquid-related processes by Ag isotope is hindered by the lack of equilibrium isotope fractionation factors between minerals and fluids.

In this study, we estimated the equilibrium Ag isotope fractionation factors between Ag-bearing minerals and aqueous solutions with various compositions in two independent ways. Equilibrium dissolution experiments and *ab initio* calculations were employed. Excess solid AgNO₃ and AgCl were dissolved in aqueous solutions, which were subsequently sampled until the isotope compositions plateaued. The offset of $\delta^{109}\text{Ag}$ between saturated AgNO₃ aqueous solutions and coexisting solids is less than 0.05 ‰ at 25°C. The $\delta^{109}\text{Ag}$ of the AgCl aqueous solution was 0.27‰ heavier than that of the AgCl solid. Moreover, molecular dynamics simulations of deep potential models trained by DFT data were conducted to estimate the equilibrium Ag isotope fractionation factors between different aqueous solutions and Ag-bearing minerals. The results are consistent with the observations, suggesting an equilibrium state of isotope exchange in the experiment in an independent way. The parameters estimated in this study provide insights for Ag isotope applications to trace fluid-related silver ore-forming processes.