Thermodynamic modeling of hydrothermal REE partitioning in critical mineral deposits

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Critical mineral deposits form through an interplay of magmatic-hydrothermal processes in carbonatites and (per)alkaline systems during their emplacement in the Earth's crust. Hydrothermal aqueous fluids can lead to the mobilization, transport, and deposition of the rare earth elements (REE) coupled to development of alteration zones at the deposit scale [1]. However, unraveling the underlying processes that affect the solubility of REE in these geologic fluids is a challenge in high temperature and pressure fluids [2]. A holistic approach is key to understand the controls of fluid-rock interaction in mobilizing REE in critical mineral deposits. Through a joint effort, we formed a new U.S. geoscience critical minerals experimental–thermodynamic research hub between New Mexico Tech, Los Alamos National Laboratory and Indiana University. The goal of this project is to conduct frontiers research on the behavior of critical elements in supercritical aqueous fluids by integration of a wide array of high temperature solubility experiments complemented by spectroscopic measurements and molecular dynamic simulations.

Here we present current advances to simulate a significant vein paragenesis of barite + fluorite +calcite +bastnäsite-(Ce) observed in many critical mineral deposits. A case study will be presented from the Gallinas Mountains REE-fluorite hydrothermal breccia deposit in New Mexico. Using the GEMS code package [3] and the MINES thermodynamic database (https://geoinfo.nmt.edu/mines-tdb), we highlight our current capabilities and limitations to simulate the behavior of REE in these hydrothermal fluids and minerals. A thermodynamic model is presented to simulate the partitioning of REE between calcite- and fluorite-fluid based on recent and ongoing experimental and thermodynamic work on the synthesis of REE doped minerals [4] and REE speciation in acidic and alkaline fluids. We further show how to integrate multiple experimental datasets and develop new thermodynamic models based on the new research efforts from the research hub and future directions to improve our prediction capabilities of REE complexation in supercritical fluids.

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[4] Perry and Gysi (2020), Geochim. Cosmochim. Acta 286, 177-197.