

Simulation of REE mobility and evolution of F-NaCl-CO₂-bearing fluids in hydrothermal calcite and fluorite ore-forming veins

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Rare earth element (REE) deposits are commonly associated with carbonatites and (per)alkaline rocks where hydrothermal magmatic fluids can play a significant role in REE mobilization and deposition [1]. Thermodynamic modeling permits predicting the evolution of ore-forming fluids and can be used to test different controls on hydrothermal REE mobility including temperature, pressure, the solubility of REE minerals, aqueous REE speciation and pH evolution associated with fluid-rock interaction. Previous modeling studies either focused on REE fluoride/chloride complexation in acidic aqueous fluids [2] or near neutral/alkaline fluids associated with calcite vein formation [3]. Such models were also applied to interpret field observations in REE deposits Bayan Obo in China and Bear Lodge in Wyoming [3,4]. Recent hydrothermal calcite-fluid REE partitioning experiments provide new data to simulate the solubility of REE in calcite, REE carbonates/fluorocarbonates at high temperatures [5, 6].

We studied the competing effects controlling the mobility of REE in hydrothermal fluids between 100 and 400 °C at 500 bar. Speciation calculations were carried out in the Ca-F-CO₂-Na-Cl-H₂O system using the GEMS code package [7]. The properties of minerals and aqueous species were taken from the MINEOS thermodynamic database [3,5]. The Gallinas Mountains hydrothermal REE deposit in New Mexico was used as a field analogue to compare our models with the formation of calcite-fluorite veins hosting bastnäsite. Previous fluid inclusion studies hypothesized that the REE were transported as fluoride complexes [8] but more recent modeling studies have shown that fluoride essentially acts as a depositing ligand [2]. Here we show more detailed simulations predicting the stability of fluorite, calcite and REE minerals relevant to ore-forming processes in carbonatites and alkaline systems.

[1] Gysi et al. (2016), *Econ. Geol.* 111, 1241-1276; [2] Migdisov and Williams-Jones (2014), *Mineral. Deposita* 49, 987-997. [3] Perry and Gysi (2018), *Geofluids*; [4] Liu et al. (2020), *Minerals* 10, 495; [5] Perry and Gysi (2020), *Geochim. Cosmochim. Acta* 286, 177-197; [6] Gysi and Williams-Jones (2015) *Chem. Geol.* 392, 87-101; [7] Kulik et al. (2013), *Computat. Geosci.* 17, 1-24; [8] Williams-Jones et al. (2000), *Econ. Geol.* 95, 327-341