Chlorine and fluorine partitioning between apatite and sediment melt at 2.5 GPa, 800 °C: A new experimentally derived thermodynamic model

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ABSTRACT

The partitioning behavior of Cl and F between apatite and sediment melt has been investigated by performing piston-cylinder experiments at 2.5 GPa, 800 °C using a hydrous experimental pelite staring material (EPSM) with ~7 wt% H_2O and variable Cl (~0, 500, 1000, 2000, or 3000 ppm) and F (~0, 700, or 1500 ppm) contents, relevant for subduction zone conditions. Cl and F partitioning between apatite and melt is non-Nernstian, with $D_{Cl}^{Ap-melt}$ varying from 1.9–10.6 and $D_{F}^{Ap-melt}$ varying from 16–72. In contrast, Cl and F partition coefficients between phengite/biotite and melt ($D_{Cl}^{Phen-melt}$, $D_{Cl}^{Bi-melt}$, $D_{F}^{Phen-melt}$, and $D_{F}^{Bi-melt}$) were determined to be 0.24 ± 0.01, 0.86 ± 0.05, 1.4 ± 0.1, and 3.7 ± 0.4, respectively. The Nernstian partitioning of Cl and F between phengite/biotite and melt suggests ideal mixing of F, Cl, and OH in phengite, biotite, and melt.

Exchange coefficients for F, Cl, and OH partitioning between apatite and melt were determined, with $K_{d_{Cl-OH}}^{Ap-melt}$ = 19–49, $K_{d_{Cl-OH}}^{Ap-melt}$ = 164–512, and $K_{d_{F-Cl}}^{Ap-melt}$ = 7–21. The evident variation of K_d values was attributed to non-ideal mixing of F, Cl, and OH in apatite. A regular ternary solution model for apatite was developed by modeling the variation of K_d values for experiments from this study and those from Webster et al. (2009) and Doherty et al. (2014). Positive values (~15 to ~25 kJ/mol) obtained for Margules parameters W_{Cl-OH}^{Ap}, W_{F-Cl}^{Ap}, and W_{F-OH}^{Ap} at low-pressure conditions (0.2 GPa, 0.05 GPa, and 900 °C) are in contrast to zero or negative values at 2.5 GPa, 800 °C. Based on a thermodynamic framework for F, Cl, and OH exchange between apatite and melt, using values for $-\Delta_r G_{Cl-OH}^{o}(P,T)$, $-\Delta_r G_{F-OH}^{o}(P,T)$, $-\Delta_r G_{F-Cl}^{o}(P,T)$, W_{Cl-OH}^{Ap}, W_{F-Cl}^{Ap}, and W_{F-OH}^{Ap} obtained through regression, F and Cl contents in melt can be derived from apatite compositions.

Keywords: Apatite, chlorine, exchange coefficient, fluorine, melt, partitioning, piston-cylinder experiments, regular solution model, subduction