Parameterized lattice strain models for REE partitioning between amphibole and silicate melt

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ABSTRACT

The distribution of rare earth elements (REEs) between amphibole and silicate melt is important for understanding a wide variety of igneous and metamorphic processes in the lithosphere. In this study, we used published experimental REE and Y partitioning data between amphibole and silicate melt, the lattice strain model, and nonlinear least-squares regression method to parameterize key partitioning parameters in the lattice strain model \((D_0, r_0, \text{and } E)\) as a function of pressure, temperature, and both amphibole and melt compositions. Two models, which give nearly identical results, are obtained in this study. In the first model, \(D_0\) depends on temperature and amphibole composition: it positively correlates with Ti content and negative correlates with temperature and Mg, Na, and K contents in the amphibole. In the second model, \(D_0\) depends solely on the melt composition: it positively correlates with Si content and negatively correlates with Ti and Ca contents in the melt. In both the mineral and melt composition models, \(r_0\) negatively correlates with the ferromagnesian content in the M4 site of the amphibole, and \(E\) is a constant. The very similar coefficients in the equations for \(r_0\) and best-fit values for \(E\) in the two models allow us to connect the two models through amphibole-melt phase equilibria. An application of our model to amphiboles in mantle xenoliths shows that observed major element compositional variations in amphibole alone can give rise to order of magnitude variations in amphibole-melt REE partition coefficients. Together with experimental data simulating fractional crystallization of arc magmas, our models suggest that: (1) REE partition coefficients between amphibole and melt can vary by an order of magnitude during arc magma crystallization due to variation in the temperature and composition of the amphibole and melt, and that (2) amphibole fractional crystallization plays a key role in depleting the middle REEs relative to heavy REEs and light REEs in arc magmas.

Keywords: REE and Y partition coefficients, amphibole, amphibole melting in the mantle, amphibole fractional crystallization

INTRODUCTION

Amphibole is ubiquitous in the Earth’s lithosphere, occurring in a wide variety of igneous and metamorphic rocks. As an inosilicate, amphibole has three main structural sites (A, M4, and M1–M3) that can accommodate cations of a range of size and charge. The general chemical formula of amphiboles may be described by the expression

\[
\text{A}_2\text{B}_2\text{C}_3\text{T}_4\text{O}_{22} \text{(OH, F, Cl)}_2
\]

where \(A = \text{Na}, \text{K}, \text{or vacant (}) \text{in A site; B = Ca, Na, Mn, Fe}^{2+}, \text{Mg in M4 site; C = Fe}^{3+}, \text{Fe}^{2+}, \text{Mg, Al, Mn, Ti, Cr in M1, M2, and M3 sites; T} = \text{Si, Al in tetrahedral site (Hawthorne 1983). The smaller M1–M3 sites are in sixfold coordination, while the larger M4 site is in eightfold coordination. The latter can accommodate larger cations such as the trivalent rare earth elements (REE) and Y [ionic radii 0.977–1.16 Å, eightfold coordination, Shannon (1976)], while the smaller M1–M3 sites can accommodate smaller cations such as high field strength elements.}

The subject of the present study is REE partitioning between amphibole and silicate melt, which is important to understand the generation and differentiation of hydrous magmas. According to the lattice strain model (Blundy and Wood 1994; Brice 1975; Wood and Blundy 1997), the partition coefficients of trivalent REEs between amphibole and silicate melt vary systematically with their ionic radii:

\[
D_j^{\text{amph-melt}} = D_0 \exp \left( -\frac{4 \pi E}{R T} \left( \frac{r_j}{2} - \frac{\rho_j}{3} r_j \right)^3 \right)
\]

where \(D_0\) is the amphibole-melt partition coefficient for the strain-free substitution; \(r_0\) is the radius of a hypothetical cation that substitutes into the site with zero strain; \(r_j\) is the ionic radius of the element of interest; \(E\) is the effective Young’s modulus for the lattice site; \(N_j\) is Avogadro’s number; \(R \approx 8.3145 \text{ J/(mol·K)}\) is the gas constant; and \(T\) is temperature in Kelvin. The lattice strain parameters \((D_0, r_0, E)\) are, in general, a function of pressure \((P)\), temperature \((T)\), and composition \((X)\).

Amphibole-melt REE partition coefficients have been shown to negatively correlate with \(T\) (Green and Pearson 1985; Klei et al. 1997; Nandedkar et al. 2016; Nicholls and Harris 1980) and \(P\)

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