

Online Appendices A and B of
**Distribution of REE between amphibole and pyroxenes in the
lithospheric mantle: An assessment from the lattice strain model**

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Appendix A. Parameters in the lattice strain models for REE partitioning between amphibole, pyroxenes and silicate melts

The following equations summarize the parameters used in the lattice strain models for REE partitioning between mantle minerals (amphibole, clinopyroxene, and low-Ca pyroxene) and silicate melts of Eq. (3):

Amphibole model (Shimizu et al., 2017)

$$\ln D_0 = -4.21 + \frac{7.27 \times 10^4}{RT} + 1.52X_{\text{Ti}} - 0.35X_{\text{Mg}} - 1.83X_{\text{Na}} - 2.95X_{\text{K}}, \quad (\text{A1a})$$

$$r_0(\text{\AA}) = 1.043 - 0.039X_{\text{Fm}}^{\text{M4}}, \quad (\text{A1b})$$

$$E(\text{GPa}) = 337. \quad (\text{A1c})$$

Clinopyroxene model (Sun and Liang, 2012)

$$\ln D_0 = -7.14 + \frac{7.19 \times 10^4}{RT} + 4.37X_{\text{Al}}^{\text{T}} + 1.98X_{\text{Mg}}^{\text{M2}} - 0.91X_{\text{H}_2\text{O}}^{\text{melt}}, \quad (\text{A2a})$$

$$r_0(\text{\AA}) = 1.066 - 0.104X_{\text{Al}}^{\text{M1}} - 0.212X_{\text{Mg}}^{\text{M2}}, \quad (\text{A2b})$$

$$E(\text{GPa}) = (2.27r_0 - 2.00) \times 10^3. \quad (\text{A2c})$$

Low-Ca pyroxene model (Yao et al., 2012; Sun and Liang, 2013)

$$\ln D_0 = -5.37 + \frac{3.87 \times 10^4}{RT} + 3.54X_{\text{Al}}^{\text{T}} + 3.56X_{\text{Ca}}^{\text{M2}} - 0.84X_{\text{Ti}}^{\text{melt}}, \quad (\text{A3a})$$

$$r_0(\text{\AA}) = 0.693 + 0.432X_{\text{Ca}}^{\text{M2}} + 0.228X_{\text{Mg}}^{\text{M2}}, \quad (\text{A3b})$$

$$E(\text{GPa}) = (1.85r_0 - 1.37 - 0.53X_{\text{Ca}}^{\text{M2}}) \times 10^3. \quad (\text{A3c})$$

In Eqs. (A1a) and (A1b), X_{Ti} , X_{Mg} , X_{Na} , and X_{K} are cation numbers of Ti, Mg, Na, and K per 23-oxygen, and $X_{\text{Fm}}^{\text{M4}}$ is the total cation number of $\text{Fe}^{2+} + \text{Mn}^{2+} + \text{Mg}^{2+}$ on the M4 site. The amphibole formula is calculated using the method described in Shimizu et al. (2017). This method is simplified from that in Leake et al. (1997) by assuming all Fe to be ferrous for parameterizing the amphibole-melt REE partitioning model. The

calculation procedure is described in Text S2 of online Appendix C. In Eqs. (A2a), (A2b), and (A3a–c), X_{Al}^{T} is the cation content of the tetrahedral Al in pyroxene per 6-oxygen; $X_{\text{Al}}^{\text{M1}}$ is the cation number of Al on the M1 site in pyroxene per 6 oxygen; $X_{\text{Ca}}^{\text{M2}}$ and $X_{\text{Mg}}^{\text{M2}}$ are cation numbers of Ca and Mg, respectively, on the M2 site in pyroxene per 6 oxygen; $X_{\text{H}_2\text{O}}^{\text{melt}}$ is the molar fraction of H₂O in the melt calculated following Wood and Blundy (2002); and $X_{\text{Ti}}^{\text{melt}}$ is the cation fraction of Ti in the melt per 6 oxygen. $X_{\text{Ti}}^{\text{melt}}$ is added to correct the effect of melt TiO₂ for REE partitioning between low-Ca pyroxene and lunar basalts which have high TiO₂ concentrations, and it can be neglect in cases of Earth's mantle conditions (Yao et al., 2012; Sun and Liang, 2013). Pyroxene formulae are calculated by assuming a random distribution of Fe²⁺ and Mg²⁺ over the M1 and M2 sites (Wood and Banno, 1973) and that all iron is present as ferrous iron (Sun and Liang, 2012, 2013; Yao et al., 2012).

Appendix B. Parameters in the semi-empirical models for amphibole temperature

The following equations present the expressions of terms and in the semi-empirical models for amphibole temperature of [Eq. (5)]:

$$A_i^{\text{Opx,Amp}} = -1.16 + \frac{3.87 \times 10^4}{RT^{\text{Pyx}}} + 3.54X_{\text{Al}}^{\text{T,Opx}} + 3.56X_{\text{Ca}}^{\text{M2,Opx}} - 1.52X_{\text{Ti}}^{\text{Amp}} + 0.35X_{\text{Mg}}^{\text{Amp}} + 1.83X_{\text{Na}}^{\text{Amp}} + 2.95X_{\text{K}}^{\text{Amp}} - \frac{4\pi E^{\text{Opx}} N_A}{RT^{\text{Pyx}}} \left[\frac{r_0^{\text{Opx}}}{2} (r_0^{\text{Opx}} - r_i)^2 - \frac{1}{3} (r_0^{\text{Opx}} - r_i)^3 \right], \quad (\text{B1a})$$

$$A_i^{\text{Cpx,Amp}} = -2.93 + \frac{7.19 \times 10^4}{RT^{\text{Pyx}}} + 4.37X_{\text{Al}}^{\text{T,Cpx}} + 1.98X_{\text{Mg}}^{\text{M2,Cpx}} - 1.52X_{\text{Ti}}^{\text{Amp}} + 0.35X_{\text{Mg}}^{\text{Amp}} + 1.83X_{\text{Na}}^{\text{Amp}} + 2.95X_{\text{K}}^{\text{Amp}} - \frac{4\pi E^{\text{Cpx}} N_A}{RT^{\text{Pyx}}} \left[\frac{r_0^{\text{Cpx}}}{2} (r_0^{\text{Cpx}} - r_i)^2 - \frac{1}{3} (r_0^{\text{Cpx}} - r_i)^3 \right], \quad (\text{B1b})$$

$$B_i^{\text{Amp}} = -\frac{7.27 \times 10^4}{R} + \frac{4\pi E^{\text{Amp}} N_A}{R} \left[\frac{r_0^{\text{Amp}}}{2} (r_0^{\text{Amp}} - r_i)^2 - \frac{1}{3} (r_0^{\text{Amp}} - r_i)^3 \right]. \quad (\text{B2})$$

The lattice strain parameters r_0^{Cpx} , E^{Cpx} , r_0^{Opx} , E^{Opx} , r_0^{Amp} , and E^{Amp} are given in Appendix A.

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