Parameterizing a Model of Clinopyroxene/Melt Partition Coefficients for Sodium to Higher Upper Mantle Pressures

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2018: M.Sc. Geosciences at Ruhr-University Bochum, Germany

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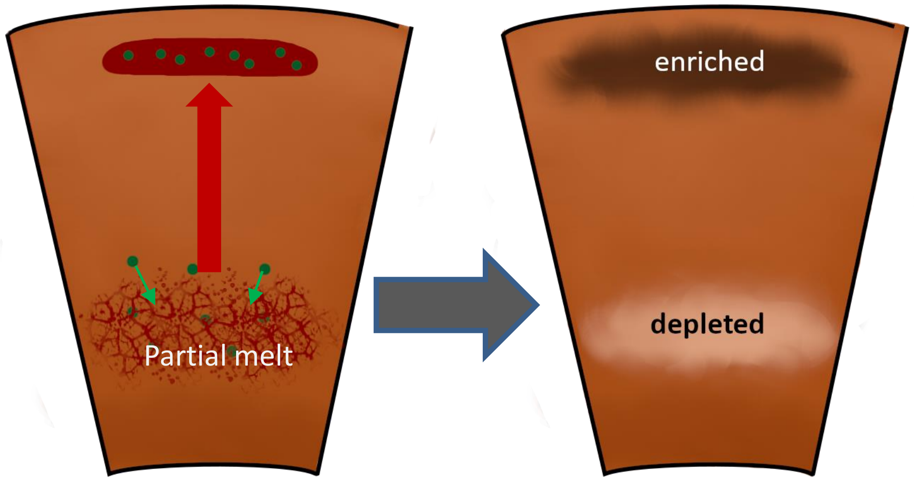
General: redistribution of trace elements

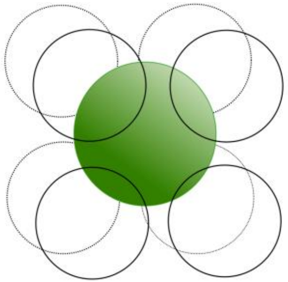
Incompatible elements are **redistributed into partial melt** and transported upwards. **Partition Coefficients** display if an element is more compatible or incompatible in the solid material.



- This results in an enriched surface and depleted upper mantle

Partition Coefficients are …

- ❖ important to comprehend the redistribution of trace elements,
- ❖ highly **Pressure** and **temperature** dependent
- ❖ crucial for **mantle evolution models**.



- ➢ But they are neglected or set constant in partial melt simulations due to **lack of high pressure models.**

Partition Coefficient Modeling

Model by Blundy et al. (1997):

$$D_i = D_0 * exp\left[\frac{-4\pi E_{M2} N_A \left[\frac{r_0}{2}(r_0 - r_i)^2 + \frac{1}{3}(r_0 - r_i)^3\right]}{RT}\right]$$

D_i=Partition Coefficient

D_0=strain-compensated partition coefficient

E_{M2}= bulk modulus of mineral‘s M2 lattice site

N_A= Avogadro‘s number

r_0=lattice site radius

r_i=element of interest‘s radius

R=Gas constant

T=Temperature

Partition Coefficient Modelling

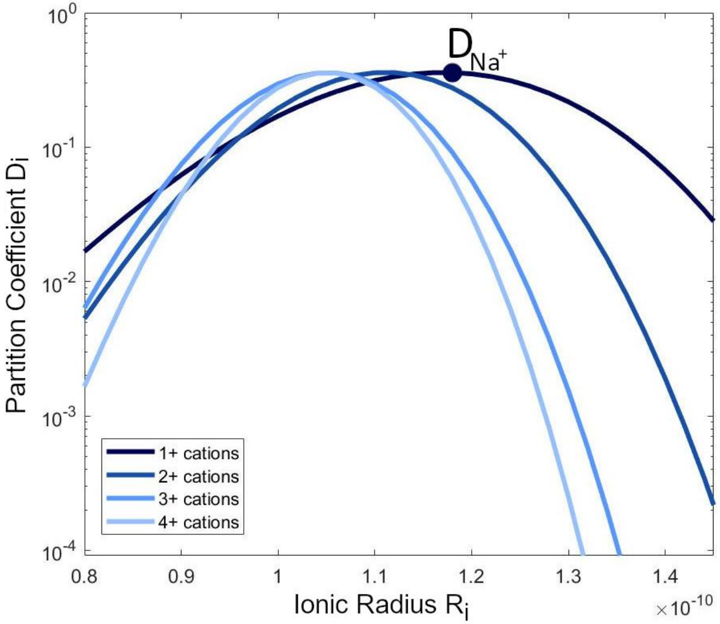
- There is a logarithmic relationship between partition coefficients of one charge.

- Partition ceofficients of different charges vary depending on E and r_0.

Note that for cpx/melt partition coefficients, D_{Na} is the highest 1+ charge element and can therefore be used as

➢ $D_{Na} = D_0$

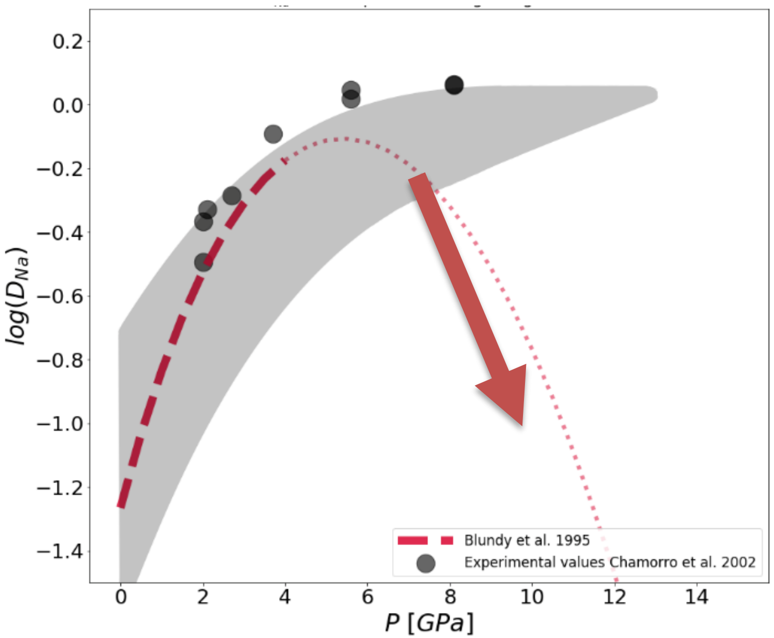
Clinopyroxene/melt partition coefficients



Schmidt and Noack (2021)

Problem with Partitioning Model

Scaling law by Blundy et al. (1995)



$$D_{Na} =$$

$$exp\left(\frac{10367 + 2100P - 165P^2}{T} - 10.27\right.$$

- ❖ Only useful for pressures up to 4 GPa!

Solution:

- ❖ Make a new scalig law based on a thermodynamic model

Thermodynamic model

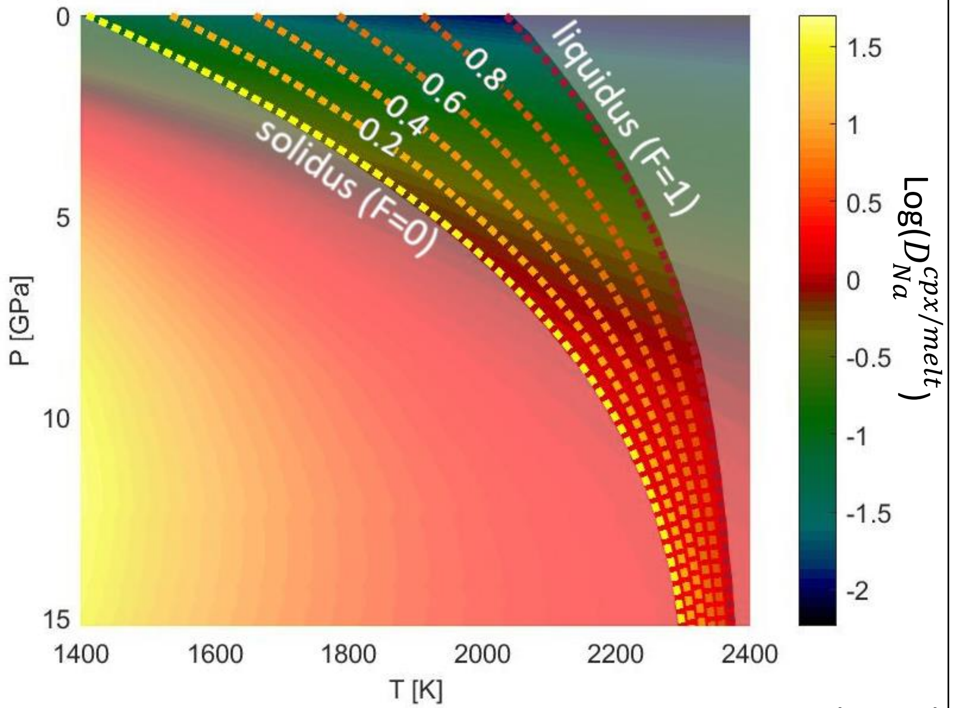
Between liquidus and solidus:

❖ Increasing partition coefficients with increasing pressure

❖ Decreasing partition coefficients with rising temperature

➢ agrees with literature!

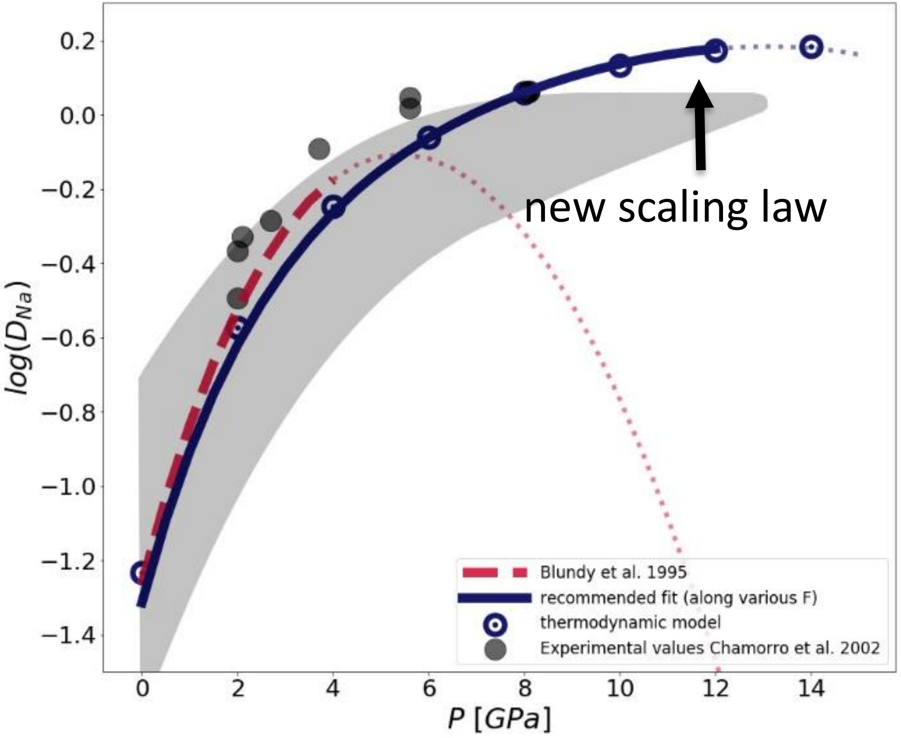
Schmidt and Noack (2021)



Liquidus and Solidus according to de Smet et al. (1999)

New scaling law

Schmidt and Noack (2021)



With our new scaling law, $D_{Na}^{cpx/melt}$ continues to **rise with increasing pressure up to 12 GPa**.

The scaling law **agrees well with experimental literature values**.

❖ Up to 4 GPa, the scaling law of Blundy et al. (1995) fits better to the thermodynamic model.

➢ From 0-4 GPa: use scaling law of Blundy et al. (1995)

➢ From 4-12 GPa: use new scaling law

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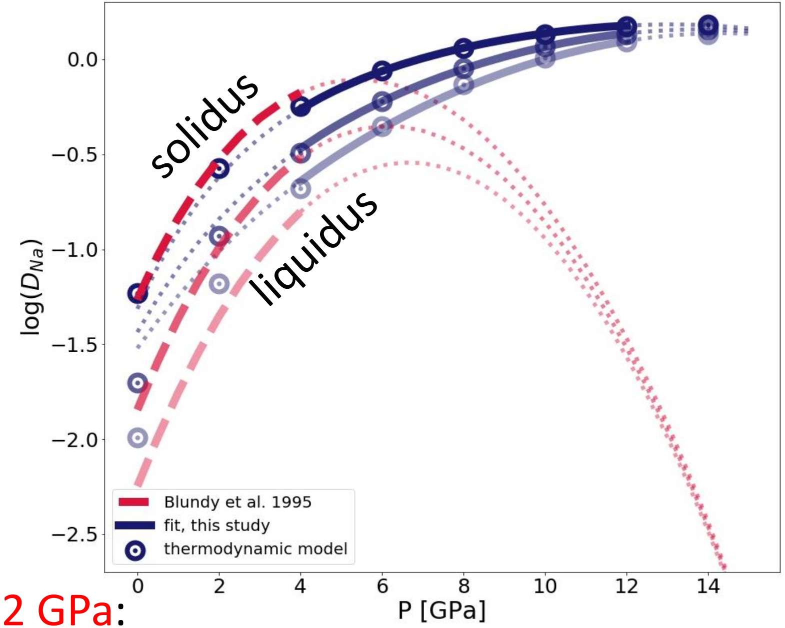

Final scaling law, to be used between 4 and 12 GPa:

$$D_{Na} = exp\left(\frac{2183 + 2517P - 157P^2}{T} - 4.575 - 0.5149P + 0.0475P^2\right)$$

Conclusions

- Now it is possible to calculate **P-T sensitive partition coefficients from 0-12 GPa** by combining the scaling laws of Blundy et al. (1995) and our study.

- D_{Na} can serve as a „reference“ coefficient to calculate **other trace elements** from.

- The results enable us to calculate the **redistribution of trace elements on Earth and other terrestrial planets** with comparable mantle compostion.

References

Bundy, J. et al. (1995): *Sodium partitioning between clinopyroxene and silicate melts*, Journal of Geophysical Research: Solid Earth, 340 100 (B8), 15501-15515

Wood, B. J., & Blundy, J. D. (1997): *A predictive model for rare earth element partitioning between clinopyroxene and anhydrous silicate melt*, Contributions to Mineralogy and Petrology, 129(2), 166-181.

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