

1.4.43

Ti substitution mechanisms in biotite: Perspectives from a biotite Ti- saturation surface

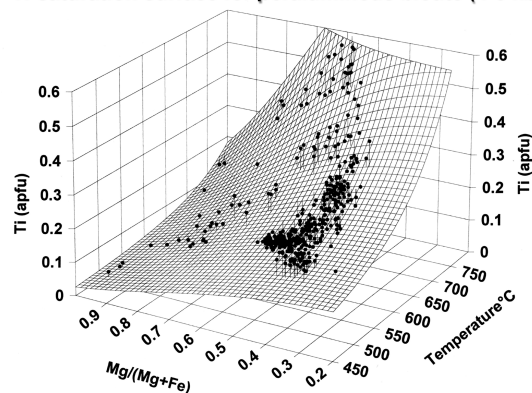
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Multiple mechanisms of Ti-substitution have been identified in different portions of a biotite Ti-saturation surface that was generated for biotite from graphitic, peraluminous metapelites that contain ilmenite or rutile and have equilibrated at roughly 4-6 kbar. The Ti-saturation surface was empirically calibrated using an extensive natural biotite data set (529 samples) from western Maine and south-central Massachusetts in combination with a calibrated petrogenetic grid. The calculated surface, best visualized in terms of the parameters $T^{\circ}\text{C}$ - $\text{Mg}/(\text{Mg}+\text{Fe})$ - Ti, is a curved surface such that for a given $\text{Mg}/(\text{Mg}+\text{Fe})$ value the Ti concentrations increase as a function of temperature in a nonlinear fashion and for a given temperature an increasing $\text{Mg}/(\text{Mg}+\text{Fe})$ ratio greatly reduces the Ti saturation limit. Detailed examination of the data used for the Ti-saturation surface establishes that the Ti-substitution at $X_{\text{Mg}} > 0.65$ is controlled by biotite crystallochemical constraints in accordance with the exchange vector $\text{TiAl}_2\text{R}_1\text{Si}_2$, where R is the sum of the divalent cations $\text{Mg}+\text{Fe}+\text{Mg}$. At intermediate X_{Mg} the $\text{TiO}_2\text{R}_1(\text{OH})_2$ exchange vector apparently controls the prominent incorporation of Ti and is primarily affected by reduction of activity of H_2O in metamorphic fluid from graphite-bearing metapelites. Analysis of isothermal biotite data from low-Al amphibolite to granulite facies samples indicate that in such low-Al compositions biotite incorporates Ti in accordance with the exchange vectors $\text{TiO}_2\text{R}_1(\text{OH})_2$ and RSiAl_2 in a roughly 4:1 ratio.

Ti-saturation surface for peraluminous biotite (4-6 kb)



1.4.P01

Modeling solid solutions with pseudo components in a diffusive system using a reactive transport model: Application to plagioclase

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Treatment of solid solutions in reactive transport models requires that the composition of the solid is treated as a variable. Since many thermodynamic models of solid solutions are highly non-linear, this can seriously impact on the stability of the transport algorithm. In addition, this can require an unreasonable amount of computational time. To improve performance, phase equilibrium calculations have been performed using pseudo components. The thermodynamic properties of a varying number of intermediate composition phases are calculated using our favourite solid solution mixing model and included in the mineral thermodynamic database for the transport calculation. The one dimensional reactive fluid transport model, IDREACT [2] was used to test this approach. We used the solid solution of plagioclase as a test case by calculating the diffusion profile that develops between an anorthite- and an albite-rich zone at hydrothermal temperatures. Several different mixing models can easily be tested since no modification of the transport code is required.

Results are compared to a skarn from the Adamello contact aureole at temperatures appropriate for hydrothermal systems. Initial speciation and concentrations of aqueous species were calculated using a geochemical speciation model (SOLUB, Baumgartner, unpub.) with input thermodynamic data of reactions calculated using SUPCRT92 [1] computer program. The fluid rock interaction simulations result in precipitation of intermediate plagioclase compositions as expected. Asymmetric diffusional profiles develop between the anorthite and albite zones due to the difference in solubility of highly charged, small aluminum and silica ions, as well as that of Na (faster) and Ca (slower). Relative aluminum immobility results in porosity reduction in the zones where anorthite is replaced, and in porosity increase where albite is replaced by the intermediate plagioclase compositions. These observations are in agreement with observations from experiments (Schliestedt, 1989, personal comm.).

References

- [1] Johnson J.W., Oelkers E.H., and Helgeson H.C. (1992) *Computers & Geosciences* **18**(7), 899-947.
[2] Steefel C.I. (1993) *IDREACT User's Manual*, p 42.