Ti solubility mechanisms and their importance for understanding Ti activity

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Trace-element thermobarometry (Ti-in-quartz, Ti-in-zircon) and thermodynamic modelling of Fe-Ti oxide stability depend on our ability to estimate the activity of titania (aTiO2) in silicic systems. Whereas many metal cations (e.g., Na, K Ca, Mg) dissolved in silicate melts are incorporated through relatively simple solution mechanisms as network-modifying cations, Ti has been shown in a variety of natural and synthetic glasses to be incorporated in 4-, 5- and 6-fold coordination as a network-modifying and network-forming cation as an isolated Ti cation and as isolated clusters of Ti cations in multiple coordination states.

The complexity of Ti incorporation in silicate melts means that assumptions made about the ideal behavior of Ti used in determining aTiO2 may lead to inaccurate estimates of the value of aTiO2. To address this, we investigated Ti activity in tridymite-bearing Na-silicate melts. Tridymite was crystallized in rutile-bearing Na-silicate melts to generate a Ti-in-tridymite thermometer and determine TiO2 saturation in tridymite and coexisting melts over a range of temperatures and compositions. This thermometer enables direct comparison of aTiO2 estimated from rutile-saturation and constant activity coefficient assumptions to the actual value of aTiO2 determined via the Ti-in-tridymite saturation calibration.

The results of this study demonstrate that assuming ideal behavior of Ti in melts (constant activity coefficient and rutile-saturation modelling) can lead to an over-estimation of aTiO2. For example, whereas rutile-saturation estimates in the Na-silicate system predict aTiO2=0.6, aTiO2 observed with Ti-in-tridymite solubility record a value of 0.3. This discrepancy could under-estimate Ti-in-quartz and Ti-in-zircon temperatures by as much as 50 °C. Although this work needs to be validated in chemical systems more closely approaching natural compositions, our revised calibration for estimating could resolve some current discrepancies between Ti-based thermobarometers and other thermometric observations of natural systems.