

# Calculation of TiO<sub>2</sub> activity with phase equilibria Modeling and application to Ti-in-zircon thermometer

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Zircon has long been recognized as the best geochronometer, and Ti in zircon is sensitive to temperature. This makes zircon a particularly powerful tool for linking the U-Pb age and P-T conditions, which is essential for developing tectonic models. Being able to quantitatively determine the solubility of Ti in zircon, however, is dependent upon being able to determine the activity of TiO<sub>2</sub> in the rock during zircon growth.

Here, we implement Phase Equilibrium Modeling to determine TiO<sub>2</sub> chemical potentials of the system, projected in P-T space for pelitic and felsic composition. TiO<sub>2</sub> activities are calculated from these dependent potentials relative to that of rutile (as a standard state). With the output activity maps, corrected Ti in zircon isopleth projections can be computed. The modeling results are in good agreement with previous studies that suggest ilmenite-bearing assemblages buffer high TiO<sub>2</sub> activities. However, Rutile-, ilmenite-free and biotite-bearing assemblages may have much lower TiO<sub>2</sub> activities (even  $\leq 0.2$ ), where the projected Ti-in-Zircon temperature significant deviation (even up to 150°C) from an assumed activity of 1.0 occurs.

Corrected Ti isopleth projection based on the calculated activity map for an average pelite composition shows that 5-15 ppm Ti corresponding to temperatures of 820–860°C. This result revealed that zircons, which have 5-15 ppm Ti from most pelitic granulites, are more likely to crystallize in peak or near peak stage rather than near solidus (680-780°C if assuming fixed activities of  $\sim 1.0$ ). Thus, with zircon growth can occur on different stages of metamorphic evolution, and assuming TiO<sub>2</sub> activities associated with the metamorphic paragenesis may be misleading and result in significant errors in P-T calculations.