American Mineralogist, Volume 96, pages 1100–1106, 2011

Calibrating Ti concentrations in quartz for SIMS determinations using NIST silicate glasses and application to the TitaniQ geothermobarometer

Whitney M. Behr,[1,*] Jay B. Thomas,[2] and Richard L. Hervig[3]

[1]Department of Earth Sciences, University of Southern California, 3651 Trousdale Parkway, Los Angeles, California 90089-0740, U.S.A.
[2]Department of Earth and Environmental Sciences, Rensselaer Polytechnic Institute, Jonsson-Rowland Science Center, 1W19 110 8th Street, Troy, New York 12180, U.S.A.
[3]School of Earth and Space Exploration, Arizona State University, 550 East Tyler Mall, Tempe, Arizona 85287, U.S.A.

Abstract

The recently developed titanium-in-quartz (TitaniQ) geothermobarometer of Wark and Watson (2006) and Thomas et al. (2010) has the potential to be applied to a wide range of igneous and metamorphic rocks. For Ti concentrations > ~10 ppm, the concentrations can be measured using an electron microprobe, but lower concentrations are below detection limits and require techniques such as laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) or secondary ion mass spectrometry (SIMS). SIMS is ideal for this purpose as it maximizes lateral and depth resolution. We used SIMS to analyze synthetic quartz crystals characterized for Ti concentration by electron probe (18–813 ppm Ti) and compare this calibration to the commonly available NIST 61X glasses using both high mass resolution (HMR) and conventional energy filtering (CEF) techniques. We used a primary beam of $^{16}O^-$ ions and detected positive secondary ions. During HMR sessions, the mass spectrometer was operated at a mass resolving power (M/ΔM) of ~2000 to separate molecular ions from elemental Ti peaks. For CEF analyses, the instrument detected secondary ions sputtered from the sample with excess kinetic energies of 75 ± 20 eV. Titanian quartz measurements reveal general homogeneity and a linear increase in Ti^+/Si^+ ion ratios with increasing Ti concentrations. Background signals represent 0–1 ppm. The slopes of the calibration curves for the titanian quartz crystals are ~70% of the curves constructed using NIST glasses, indicating a much higher ion yield for Ti from the glasses compared to the simple oxide of silicon. We demonstrate, however, that a simple correction factor allows NIST glasses to be used to quantitatively determine the Ti concentrations of quartz (with 3.8% error using HMR, and 8.2% error using CEF) until homogenous, well-characterized samples of SiO_2 become generally available.

Keywords: SIMS calibration, NIST silicate glass, titanium-in-quartz (TitaniQ), geothermobarometry