

## Calibrating Ti concentrations in quartz on the SIMS using NIST silicate glasses with applications to the TitaniQ geothermobarometer

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The recently developed titanium-in-quartz (TitaniQ) geothermobarometer of Wark and Watson (2006) and Thomas *et al.* (in press) has the potential to be applied to a wide range of igneous and metamorphic rocks. For Ti concentrations >20 ppm, corresponding to temperatures >600 °C, Ti concentrations can be measured using an electron microprobe, but lower concentrations are below detection levels and require techniques such as laser ablation 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 content by electron probe (18-800 ppm Ti) and compared this calibration with one obtained on the commonly-available NIST 61X glasses to evaluate the effect of changing matrix on the yield of Ti ions. We used a primary beam of <sup>16</sup>O ions and detected positive secondary ions. The mass spectrometer was operated at a mass resolving power (M $\Delta$ M) of ~2000 to separate molecular ions from elemental Ti peaks. Measurements of the titanian quartz and NIST glasses reveal general homogeneity and a linear increase in Ti<sup>+</sup>Si<sup>+</sup> ion ratios with increasing Ti contents. Background signals represent  $\leq$  0-0.3 ppm. When corrected for differences in silica, NIST 612 and 614 show 10% higher ion yield than the quartz materials, while NIST 610 is 60% higher. The former samples can thus be used as standards for Ti in quartz (given the 10% correction), and we present a demonstration of applying this calibration to a suite of natural quartz crystals.

## Results of simulated weathering of coal stockpiles and coal refuse disposal areas

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Coal mining and processing generates stockpiles of coal and processing waste (fine and coarse refuse). Weathering of these materials can increase sulphate discharge. A series of laboratory columns were constructed in 2008 to simulate the impact of weathering of these materials with the goal of improved material handling. Six leaching columns were constructed to compare coarse refuse with a blend of coarse refuse and dewatered fine refuse. Two additional columns were constructed to evaluate coal stockpiles.

The coal columns produced net alkaline drainage for the first seven months. Sodium and chloride levels were initially high (>1,900 and 800 mg/L, respectively) in all columns but declined rapidly due to the high solubility of NaCl. Similarly, sulphate levels were initially > 6,000 mg/L then diminished to <4,000 mg/L as weathering dissolves water-soluble iron sulphates and/or gypsum. Generation of acidic drainage in the coal columns was accompanied by a rapid increase in metals (i.e. aluminium <2.0 to >250 m/L and iron <1 to >3,000 mg/L in 4 months). Sulphate increased from 4,000 to 5,400 mg/L in one month. Manganese remained at a constant level of between 4 and 6 mg/L then increased during lower pH conditions to between 87 and 91.5 mg/L.

The refuse columns discharged net alkaline drainage throughout the first 9 months of simulated weathering. However, sulphate discharge from these columns declined somewhat from >6,200 mg/L to between 3,590 and 5,403 mg/L. Again, sodium and chloride levels were initially high (>1,900 and 900 mg/L, respectively) but declined rapidly as NaCl flushed from the system. In summary, laboratory-scale kinetic tests indicate that both sulphate and chloride levels decrease during simulated weathering. However, upon exhaustion of the availability of alkalinity the pH decreases rapidly. This is accompanied by increase in sulphate and metals, presumably from an increase in pyrite weathering. Additional research is needed to evaluate the mineralogy of these columns.