

Quantitative polarized infrared analysis of trace OH in populations of randomly oriented mineral grains

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ABSTRACT

Use of infrared spectroscopy as an accurate, quantitative method to measure concentrations of hydrous species in minerals requires consideration of the interactions of anisotropic crystals with infrared light. Ensuring that contributions are identified from species at all orientations in the crystal requires combining three measurements, taken with the electric field polarized along three mutually perpendicular directions. This is typically accomplished by determining the orientation of a crystal in advance, and then sectioning it perpendicular to its principal axes. In many instances, however, natural or experimental samples are not suitable for such handling. Here we demonstrate a method that instead uses at least three randomly sectioned grains, considered to be multiple samples of a homogeneous population. We explain the theory whereby: (1) the orientations of the polarization vectors of measurements taken on these grains are determined by comparison to oriented standards of the same mineral, and (2) the principal-axis spectra of the sample are synthesized from the randomly oriented spectra. By comparison to complementary electron backscatter diffraction (EBSD) data, we demonstrate that determination of orientations using the silicate overtone bands in Fourier-Transform infrared (FTIR) spectra is accurate and precise, with typical angular errors of 6°. We show that this precision is sufficient for the synthetic principal-axis spectra to be essentially indistinguishable from X-ray oriented standard spectra. We demonstrate the application of this technique to determining the OH concentrations in a population of hydrated olivine grains recovered from a high-pressure, high-temperature multi-anvil experiment.