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SPECIAL COLLECTION: APATITE: A COMMON MINERAL, UNCOMMONLY VERSATILE

Quantification of CO_2 concentration in apatite

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Abstract

We have calibrated the infrared (IR) method for determining CO_2 concentrations in apatite with absolute concentrations obtained through nuclear reaction analysis (NRA). IR data were obtained on double-polished apatite wafers using polarized transmission IR spectroscopy. Due to the various sites and orientations of CO_3^{2-} in apatite, the IR spectra are complicated and do not have the same shape in different apatite samples. Hence, simple peak heights are not used to characterize CO_2 concentrations in apatite. The total absorbance (A_{total}) was derived using the integrated area under the curves in a given polarized spectral region. Then A_{total} is calculated as $A_{\mathbf{E}//\mathbf{c}} + 2A_{\mathbf{E}\perp\mathbf{c}}$. The calibration has been carried out for two wavenumber regions, one with high sensitivity and the other applicable to apatite with high CO_2 concentrations. The first calibration is for the fundamental asymmetric CO_3^{2-} stretching at wavenumbers of 1600–1300 cm^{-1}, and the CO_2 concentration in parts per million can be obtained as $(0.0756 \pm 0.0036)\ A_{total}/d$ where d is sample thickness in centimeters. The fundamental stretching bands are strong and hence sensitive for measuring low CO_2 concentrations in apatite, down to parts per million level. The second calibration is for the CO_3^{2-} bands at wavenumbers of 2650–2350 cm^{-1}, and the CO_2 concentration in parts per million is $(9.3 \pm 0.6)\ A_{total}/d$ where d is sample thickness in centimeters. These bands are weak and hence are useful for measuring high CO_2 concentrations in apatite without preparation of super-thin wafers. The anisotropy is significant. The difference between $A_{\mathbf{E}//\mathbf{c}}$ and $A_{\mathbf{E}\perp\mathbf{c}}$ can reach a factor of 2.73. Hence, for high accuracy, it is best to use polarized IR to determine CO_2 concentrations in apatite. For rough estimation, unpolarized IR spectra may be used by estimating $A_{total} = 3A_{unpol}$, where A_{unpol} is the integrated absorbance from unpolarized spectra.

Keywords: Carbonate in apatite, IR spectroscopy, nuclear reaction analysis, NRA