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Calibration of zircon as a Raman spectroscopic pressure sensor to high temperatures and application to water-silicate melt systems

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Abstract

The shifts in wavenumber of the $\nu_3(SiO_4)$ (~1008 cm^{-1}) Raman band of fully crystalline synthetic zircon with changing pressure (P) and temperature (T) were calibrated for application as a Raman spectroscopic pressure sensor in optical cells to about 1000 °C and 10 GPa. The relationship between wavenumber (ν) of this band and T from 22 to 950 °C is described by the equation ν (cm^{-1}) = $7.54 \cdot 10^{-9} \cdot T^3 - 1.61 \cdot 10^{-5} \cdot T^2 - 2.89 \cdot 10^{-2} \cdot T + 1008.9$, where T is given in °C.

The pressure dependence is nearly linear over the studied range in P. At ~25 °C, the $\partial\nu/\partial P$ slope to 6.6 GPa is 5.69 cm^{-1}/GPa, and that to 2 GPa is 5.77 cm^{-1}/GPa. The $\partial\nu/\partial P$ slope does not significantly change with temperature, as determined from experiments conducted along isotherms up to 700 °C. Therefore, this pressure sensor has the advantage that a constant $\partial\nu/\partial P$ slope of 5.8 ± 0.1 cm^{-1}/GPa can be applied in experiments to pressures of at least about 6.6 GPa without introducing a significant error. The pressure sensor was tested to determine isochores in experiments with H_2O+$Na_2Si_3O_7$ and H_2O+$NaAlSi_3O_8$ fluids to 803 °C and 1.65 GPa. These pressures were compared to pressures calculated from the equation of state (EoS) of H_2O based on the measured vapor dissolution or ice melting temperature for the same experiment. Pressures determined from the zircon sensor in runs in which $NaAlSi_3O_8$ melt dissolved in aqueous fluid were close to or lower than the pressure calculated from the EoS of H_2O using the vapor dissolution or ice melting temperature. In experiments with H_2O+Na_2O+SiO_2 fluids, however, the pressure obtained from the Raman spectrum of zircon was often significantly higher than that estimated from the EoS of H_2O. This suggests that the pressures along some critical curves of water–silicate melt pseudobinary systems should be revised.

Keywords: Zircon, Raman spectroscopy, temperature, pressure sensor, diamond-anvil cell