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In-situ Raman spectroscopy of quartz: A pressure sensor for hydrothermal diamond-anvil cell experiments at elevated temperatures

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ABSTRACT

Changes in frequency and linewidth of the 206 and 464 cm^{-1} A_1 Raman modes of quartz were determined over temperatures from 23 to 800 °C and simultaneously at pressures ranging between 0.1 MPa and 2.1 GPa using a hydrothermal diamond-anvil cell (HDAC). The frequency shift of the 464 cm^{-1} peak can be used as a secondary pressure standard for SiO_2-saturated systems in HDAC experiments at temperatures up to 560 °C. The frequency of this peak depends quasilinearly on pressure in the studied pressure range. The global slope $(\partial\nu_{464}/\partial P)_T$ is 9 ± 0.5 cm^{-1}/GPa. A significant variation of this slope with temperature was not observed. Including literature data, the temperature induced frequency shift of the 464 cm^{-1} mode is described by $(\Delta\nu_T)_{464,\,P=0.1\text{ MPa}}$ (cm^{-1}) $= 2.50136\cdot10^{-11}\cdot T^4 + 1.46454\cdot10^{-8}\cdot T^3 - 1.801\cdot10^{-5}\cdot T^2 - 0.01216\cdot T + 0.29$ where $-196 \le T$ (°C) ≤ 560. The pressure dependence of the linewidth of the 464 cm^{-1} line increases with temperature. The frequency shifts and linewidths for the 206 cm^{-1} mode indicate that this line can be used as an alternative to the ruby fluorescence technique as a pressure sensor to about 5 GPa for experiments at room temperature. Both the frequency and linewidth of this mode show significant cross-derivatives $(\partial^2\nu_{206}/\partial P\partial T)$ and $(\partial^2 FWHM_{206}/\partial P\partial T)$.