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Measurement of Si—OH content in fused silica with extended dynamic range by Fourier transform infrared spectroscopy

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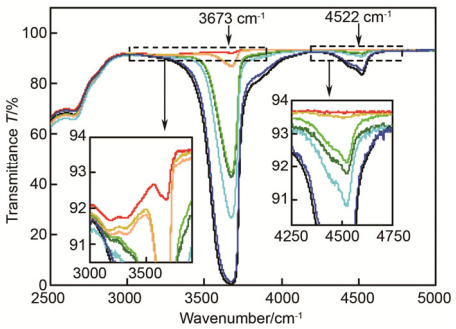

Transmittance spectra of 9 fused silica samples with 2.0 mm thickness at 2500 cm^{-1}~5000 cm^{-1} wavenumber measured 30 times. The results show Si—OH absorption bands with the absorption intensity becoming smaller: Infrasil 302, HOQ 310, Suprasil 711, Suprasil 501, Herasil 3, Suprasil 401, Herasil 102, Corning 7980, Spectrosil 2000.

Abstract: Si—OH group is the most common impurity in fused silica, which has a significant impact on the optical performance of fused silica optics from infrared to ultraviolet spectral regions. The Si—OH content can be directly measured from Si—OH stretching band at 3673 cm^{-1} with molar absorptivity of (77.5±1.5) L/(mol·cm). However, measurement range is limited by interference of absorption bands from water molecule in low Si—OH content samples and absorption saturation in high Si—OH content samples. Fourier transform infrared (FTIR) spectroscopy is employed to measure 2500 cm^{-1}~5000 cm^{-1} transmittance spectra of fused silica samples with different Si—OH contents ranging from 0.0 to 10^{-3} and thicknesses ranging from 2.0 mm to 8.0 mm. Since 3000 cm^{-1}~3100 cm^{-1} absorption bands from H_2O molecule is not covered by other infrared (IR) absorption bands, absorption at 3673 cm^{-1} from H_2O molecule can be eliminated using transmittance from 3000 cm^{-1}~3100 cm^{-1} region and line shape of H_2O band obtained by Gaussian fit from low Si—OH content samples. Compared with 4522 cm^{-1} absorption peak which is not interfered by any absorption bands, the Si—OH content calculated from 3673 cm^{-1} band without influence of water absorption band has a relative error about 2.5% lower than that directly calculated by 3673 cm^{-1} band in Suprasil 501 sample with about 5.0×10^{-5} Si—OH content and 2.0 mm thickness. After eliminating the influence of water absorption band, corresponding measurement errors and limit of detection for Si—OH content at 3673 cm^{-1} and 4522 cm^{-1} bands are calculated. Based on experimental data and Beer's law, a model to correlate Si—OH content, sample thickness, measurement error of transmittance, and measurement error of Si—OH content is established. From this model, Si—OH content measurement error is mainly influenced by logarithm of transmittance and influence of water absorption band in low Si—OH content samples, and absorption saturation in high Si—OH content samples. Since the molar absorptivity at 4522 cm^{-1} is nearly 50 times weaker than that at 3673 cm^{-1}, the corresponding transmittance at 4522 cm^{-1} is much lower than that at 3673 cm^{-1}, leading to a lower relative root mean square error for Si—OH content measurement at 4522 cm^{-1} than that at 3673 cm^{-1} in high OH content samples. With 2.0 mm thickness, a relative error less than 0.13% can be achieved in sample with 10^{-2} Si—OH content at 4522 cm^{-1} absorption band. As a result, by eliminating water absorption band at 3673 cm^{-1} for low Si—OH content samples and employing 4522 cm^{-1} band for high Si—OH content samples to measure the Si—OH content, the measurement range is increased from $(6.0\sim1810.0)\times10^{-6}$ to $(0.4\sim10000.0)\times10^{-6}$ at 2.0 mm thickness with improved measurement accuracy.

Keywords: Fourier transform infrared (FTIR) spectroscopy; fused silica; Si—OH; measurement dynamic range
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