Raman fitting of the high frequency NBO bands in alkali silicate glasses

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Abstract

Raman spectra of the SiO4 symmetric stretch region (800-1200 cm-1) for low alkali (M) silicate glasses (5 and 10 mol% M2O) yield intense well-resolved Q3 peaks at _˜1100 cm-1 with mostly Lorentzian character (> 90% at 298K), in contrast to previous Gaussian fits for silicate glasses. Fits to the Q0 peak of a Li3PO4 melt at 1550K also yields a predominantly Lorentzian peak. The spectra of both Na and Li glasses show an additional Q3 peak. It results from close approach of alkalis (M) to BO, which alters Raman shifts of the Q species to somewhat lower frequencies. The linewidths (FWHM) of fitted Q1, Q2 and Q3 species peaks are similar (35-55 cm-1) at 298K for all alkali silicate glasses. The Q species FWHM of 5 and 10 mol% Cs2O silicate glasses show a T dependence similar to those of crystal silicate spectra: both increase by 35-45 cm-1 from 298K to 1200K. The T dependence and the Lorentzian lineshapes can be explained on theoretical grounds considering Heisenberg lifetime linewidths and the Balkanski formulation. The 30 mol% K2O glass and the 50 mol% Na2O spectra are then readily fit with two or three Q2 or Q3 peaks of mainly Lorentzian character, which yield reasonable linewidths and separations between peaks. The 50 mol% Na2O spectrum shows that Q3> > Q1, and the free oxygen content is 4.5 (±1.5) mol%, in good agreement with previous 29Si NMR and O 1s XPS results.

Keywords: Structure, Raman, fitting, Q species, Lorentzian, Gaussian, NBO

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