Water-speciation in silicate glass from partial Raman spectra

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Water dissolved in silicate melts and glasses is usually present in the form of two species, free molecular water H_2O_m, and OH-species. We used a mathematical approach similar to [1] to determine the H_2O_m and OH content in hydrous rhyolitic glasses from Raman spectra at 3000 cm^{-1} to 3750 cm^{-1}. The approach is based on a least-squares optimization algorithm and the key assumption that the water band can be expressed as a linear combination of two partial Raman spectra related to the two species. Our model makes no assumptions on the shape of the partial Raman spectra. Several hundreds of Raman spectra covering a water range from 0.6 to 3.1 wt. % served as input data. The key results are (Fig.1): (1) Both partial Raman spectra have strong spectral overlap. (2) Shape and position of the maxima is different, i.e., OH has a very broad and highly asymmetric band, whereas H_2O_m shows mainly a narrower more symmetric band. (3) Partial Raman spectra can be used to determine water species concentrations in hydrous glasses.

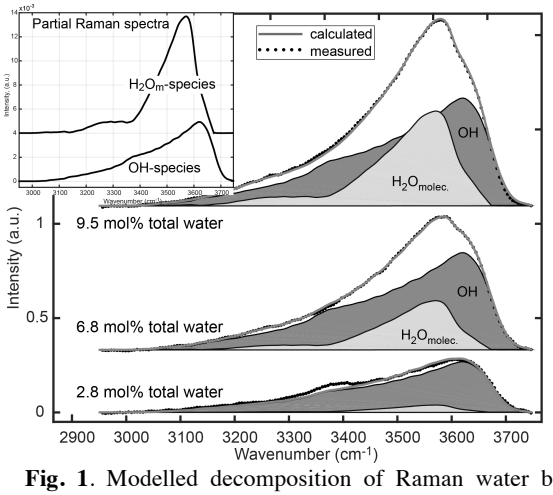

Fig. 1. Modelled decomposition of Raman water bands into their two species contributions. Inlay shows the calculated partial Raman spectra for OH and H_2O_m.

[1] Zakaznova-Herzog, V.P., Malfait, W.J., Herzog, F., and Halter, W.E. (2007), *J Non-Cryst Solids*, **353**, 4015-4028.