
Raman spectroscopy and structure of selected Ga₂O₃-CaO-P₂O₅ glasses

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Abstract

The structure of $x\text{Ga}_2\text{O}_3 \cdot (50-x)\text{CaO} \cdot 50\text{P}_2\text{O}_5$ ($x = 0, 5, 10, 15, \text{ and } 20$) glasses was investigated by ^{31}P MAS NMR and Raman spectroscopy. With increasing content of Ga_2O_3 the shift from metaphosphate (Q2) to pyrophosphate (Q1) Q-units was found by the ^{31}P MAS NMR. Only small amount (approx. 3%) of orthophosphate Q0 units was observed for $x = 15, \text{ and } 20$. The principal component analysis of experimental Raman spectra identified two independent components. Multivariate Curve Resolution analysis (MCR) of experimental Raman spectra performed for two components resulted in corresponding loadings and scores. Spectral decomposition by the method of Malfait was performed using the molar amount of Q2 and Q1 units as composition data. Such way the partial Raman (PRS) spectra of Q2 and Q1 structural units were obtained. In both cases (i.e. MCR and Malfait decomposition) the experimental spectra were reproduced with excellent accuracy. Moreover the normalized PRS are practically identical with the corresponding normalized loadings obtained by MCR. As far as the scores obtained by MCR are not unique, the method of scores adjustment was proposed. This way the good coincidence between the adjusted scores and molar amounts of considered Q-units (i.e. Q2 and Q1) was obtained. The obtained results confirmed the structural information acquired from ^{31}P MAS NMR.

Keywords: glass structure, MAS NMR, Raman spectra, phosphate glasses, MCR

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