
1D/2D NMR analysis of Al₂O₃-NaPO₃ glasses

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Abstract

Phosphate based glasses have attracted much attention during the last decades. Thanks to their good properties (low T_g, high TEC...), this type of glass has been used in many applications (laser glasses, low temperature sealing glasses, host matrix...). All these applications require glasses with acceptable stability and this parameter can be significantly improved by the addition of trivalent oxides (Al₂O₃, Fe₂O₃, B₂O₃). The impacts of these additions on the materials structure and properties need to be perfectly understood and many papers were devoted to this topic. In this presentation, we will show how the insertion of Al atoms in the sodium metaphosphate (NaPO₃) glass was studied by 1D/2D solid state NMR. The local order and its evolution were first analysed by 1D ²³Na, ²⁷Al and ³¹P MAS-NMR experiments. Then the presence of P-O-Al bonds was investigated by the ²⁷Al(³¹P) D-HMQC NMR technique. The set of results was used to decompose the 1D ³¹P NMR spectra and to determine the overall Q_{nm} phosphate speciation (n and m being the number of attached P and Al). The results show that the Q₂ units of the NaPO₃ structure are converted into Q₁₁Al and Q₁₂Al species at low Al₂O₃ contents and to Q₀₂ and Q₀₃ species at higher Al₂O₃ amounts. The structural model deduced from our experiments was used to understand the three-domains evolution of the T_g parameters.

Keywords: NMR, phosphate glasses

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