Structure of Nb_2O_5-$NaPO_3$ glasses by X-ray and neutron diffraction

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Main facets of the structure of mixed Nb_2O_5-$NaPO_3$ glasses were already studied thoroughly by spectroscopic methods such as ^{31}P, ^{17}O, ^{93}Nb nuclear magnetic resonance (NMR), O1s X-ray photoelectron spectroscopy and Raman scattering. Here, X-ray and neutron diffraction results are added to extract the detailed numbers and lengths of the first-neighbor bonds. The P–O distances of the PO_4 units change in accordance with the rupture of P–O–P bridges due to Nb_2O_5 additions as it was determined by ^{31}P NMR. The NbO_6 units possess three different lengths of Nb–O bonds for glasses of Nb_2O_5 content up to 20 mol%. The changes of these Nb–O bonds for glasses of greater Nb_2O_5 contents result from an increasing number of distances in Nb–O–Nb bridges. The medium-range order of the glasses is compared with that of GeO_2-KPO_3 glasses of equivalent compositions. A characteristic length of ~1.0 nm was determined from the first sharp diffraction peak for the GeO_2-KPO_3 glasses which was interpreted with the micro-segregation into K phosphate and Ge phosphate sub-networks. Similar features are widely missing for the Nb_2O_5-$NaPO_3$ glasses. The different behavior is attributed to the different valence and structural variability of the Ge^{4+} and Nb^{5+} ions.