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Structural characterization of niobium phosphate glass by solid-state nuclear magnetic resonance

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While niobium-containing oxide glasses are used in several technological applications, especially as optical glasses owing to its unique linear and non-linear optical properties Nb bestows upon oxide glasses, the exact structural role of Nb and, accordingly the correlations of physical properties of Nb-containing glasses with structural information are still ill-understood. Solid-state nuclear magnetic resonance (NMR) technique has proved quite powerful tools for the structural elucidation of glasses, due to their element-selectivity, inherently quantitative character, and focus on local order. (1) In this work we attempt to understand the influence of Nb on the structure of a phosphate-based glass network, in which all the chemical constituents involved provide NMR active structural probes. For this, a model glass system $(100-x)\text{NaPO}_3\text{-}x\text{Nb}_2\text{O}_5$ (labelled as SPNb x) was synthesized with niobium concentrations ranging from $x = 0$ up to $x = 40$ mol. To investigate the structural changes with the addition of different Nb concentrations, ^{31}P , ^{23}Na , ^{93}Nb magic-angle spinning (MAS)-NMR, spin echo decay (SED), dipolar techniques such as constant time double quantum-based dipolar recoupling effects nuclear alignment reduction (CT-DQ-DRENAR), $^{31}\text{P}\{^{93}\text{Nb}\}$ rotational echo saturation pulse double resonance (RESPDOR), $^{23}\text{Na}\{^{31}\text{P}\}$ rotational echo double resonance (REDOR) along with Raman spectroscopic were utilized. The results are discussed in relation to the concentration dependence of the glass transition temperature.

Palavras-chave: NMR; Niobium; Phosphate glass.

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