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Influence of Alkaline Earth Metal Fluorides (MgF_2, CaF_2, SrF_2, BaF_2) and Nb_2O_5 on the Structural and Optical Properties of Fluorophosphoniobate Glasses

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Fluorophosphoniobate glass exhibit significant technological and scientific potential as host matrices for optically active species due to their broad transparency range from the ultraviolet to the near-infrared, high solubility of RE^{3+}, chemical stability, and low phonon energy. While the effects of varying niobium concentrations on the structural, thermal, and optical properties of these glasses have been extensively studied, the role of different alkaline earth metals in modifying these matrices remains less explored. In particular, the impact of these compositional variations on the precipitation of crystalline phases requires further investigation. This study systematically examines the influence of alkaline earth metal modifiers (Mg^{2+}, Ca^{2+}, Sr^{2+}, and Ba^{2+}) on the structural and optical properties of fluorophosphoniobate glasses with the molar composition $(80\text{-}y)NaPO_3\text{-}(y)Nb_2O_5\text{-}20XF_2$. The synthesized glasses were characterized using DSC, refractive index measurements, UV-Vis absorption spectroscopy, and optical bandgap calculations. Results show that increasing Nb_2O_5 concentration enhances the covalent character of the glass network, leading to a rise in glass transition temperature, refractive index, and a redshift in the UV absorption edge due to a reduction in optical bandgap energy. ^{31}P NMR analysis revealed that increasing Nb_2O_5 content from 5 to 15 mol% promotes the depolymerization of phosphate groups, increasing the fraction of Q^0 and Q^1 species at the expense of Q^2, while simultaneously enhancing matrix connectivity through the incorporation of NbO_6 octahedral units. Additionally, varying the alkaline earth metal modifier demonstrated that cations with smaller ionic radii increase the covalent character of the glass, likely due to their stronger affinity for fluoride ions. Overall, this study provides a comprehensive understanding of how Nb_2O_5 and alkaline earth metals influence the structural and optical properties of fluorophosphoniobate glasses.

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References

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