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Composition-Structure-Liquid Fragility Relationships in Phosphorous Oxynitride Glasses

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Oxynitride glasses are mixed-anion glasses in which the oxygen atoms have been partially substituted by either two-fold or three-fold coordinated nitrogen atoms, introducing additional bonds and thereby constraining the glass network and enhancing the atomic packing density¹. Phosphorus oxynitride glasses may be suitable for making solid-state glass electrolytes. But, while the physical properties of these glasses (e.g., mechanical properties, chemical durability and electrical conductivity), have been thoroughly studied, the dynamics remains unexplored. By studying the dynamics, we could obtain insights into the structural dependence of liquid fragility index (m), glass forming ability, and transport phenomena.

In this work, we therefore study the dynamics of oxynitride mixed alkali metaphosphate and phosphosilicate glasses with varying nitrogen (N/P ratio) and SiO₂ content. In detail, we investigate the compositional dependence of glass transition temperature (T_g) and thermodynamic and kinetic fragility by means of differential scanning calorimetry (DSC) measurements. In addition to the indirect determination of m through DSC measurements with varying heating/cooling rate, we also directly access the temperature dependence of viscosity by beam-bending measurements in the low-temperature range under controlled atmosphere for selected samples. The effects of nitridation on the atomic packing and mechanical properties are also investigated. The observed changes in the dynamics and macroscopic properties are correlated with changes in the local structural environments, as followed by Raman and ³¹P NMR spectroscopy to obtain the distribution of PO_{4-x}N_x (x=1,2) and silicate species. Finally, x-ray photoelectron (XPS) spectroscopy is used as a tool to quantify the oxygen bonding environments and the ratio of bridging to non-bridging oxygens (BO/NBO). Based on these systematic studies, we have revealed the composition-structure-dynamics relationships in the phosphorous oxynitride glasses. Our findings could contribute to seeking the structural sources of liquid fragility in general.

1). Muñoz, F., Durán, A., Pascual, L. & Marchand, R. Compositional and viscosity influence on the nitrogen / oxygen substitution reactions in phosphate melts. *Phys. Chem. Glas.* **46**, 39–45 (2005).