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Topological modeling of phosphate and borophosphate glasses

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Abstract
Temperature dependent constraint theory is a powerful tool for prediction of glass properties such as glass transition temperature, liquid fragility index, heat capacity jump at the glass transition, and indentation hardness. Temperature dependent constraint theory relates properties to the number of rigid chemical bonds and bond angles at a given temperature and has mostly been applied to traditional network glasses such as chalcogenides, borates and silicates, where the properties depend largely on the network former speciation. Alkali phosphate glasses have anomalous compositional dependence of physical properties that depend on the type of alkali ion, and cannot be explained by the monotonic change in phosphorous speciation. We propose a topological model for alkali phosphate and borophosphate glass systems, which takes a modifier sub-network into account. We demonstrate that this topological model can satisfactorily predict the dynamic properties of the above-mentioned systems from chemical composition by using temperature dependent constraint theory.

Reference: