Molecular Dynamics Simulations of SiO2-B2O3-Na2O Glasses

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Abstract

Oxide glasses have many advantageous properties, including optical transparency, low thermal expansion coefficients, thermally insulating, etc. As such, they have a number of applications in the world today (windows in buildings, dishes, protection panels for plasma screens and solar panels, etc.). Optimizing a wide range of physical, thermodynamic and mechanical properties is necessary to ensure their best performance in each use. However, literature focuses on a select number of compositions; making optimization of the glass as a whole unreachable. This is in part due to sample lost between different tests, multiple batches, expense of sample fabrication, etc.
Recently, the development of complex interatomic empirical potentials modeling simultaneously multiple oxides makes way for capturing various physical, thermodynamic and mechanical properties. Hence, a systematic approach to capture a large numbers of different chemical compositions is feasible. This work concerns molecular dynamics simulations based on two simple and reliable empirical potentials. This presentation will focus on select physical, thermodynamic and mechanical properties presented in (1).
(1) M. B. Mama Toulou, P. C. M. Fossati, C. L. Rountree, "Systematic approach to thermophysical and mechanical properties of SiO2–B2O3–Na2O glasses using molecular dynamics simulations," Journal of Non-Crystalline Solids, 603(2023):122099.

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