

Molecular Dynamics Simulations of Simplified Sodium Borosilicate Glasses for Nuclear Field Applications

Fusion of valuable material properties has lent the acceptance of sodium borosilicate (NBS) glasses for nuclear waste immobilization. In spite of popularity, the mechanisms associated to these properties are yet only partially discovered and need further exploration. Bearing this in mind, the combination of experiments, molecular dynamics (MD) simulations and Dell Yuan and Bray model has been used to understand the role of composition variation for structural and physical aspects of vitrified borosilicate glasses. Experiments have been conducted to evaluate the macroscopic glass parameters: density (ρ), glass transition temperature (T_g) and thermal expansion coefficient (TEC). Experimentally observed trends for ρ , T_g and TEC with composition have been found in good agreement with the MD results. In addition, MD study provides microscopic understanding of the glass structure and phenomena associated with the change in glass composition. A detailed view of local structure and medium range connectivity for the borosilicate glasses has been explored. Owing to large B4 population, the results showed abundant presence of BO4-BO4 connections, hereby omit the generally accepted "B[4] avoidance rule" for glass. The relative propensity for connecting SiO4/BO3/BO4 structural motifs has been found in line with the predictions made by Dell Yuan and Bray model. Furthermore, the effect of composition on the mechanical integrity of NBS glasses including elastic nature, plastic distortion, yielding, breaking stress, and brittle failure has been explored by MD simulations