Statistical Mechanical Approach to Predict the Structure Evolution in Borosilicate Glasses

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Predicting the compositional evolution of the atomic-scale structure and properties of oxide glasses is important for designing new materials for advanced applications. In borosilicate glasses, addition of network modifiers will simultaneously alter the local structure around silicon and boron atoms in the glass based on the competition among various possibilities for modifier/former interaction. Based on both nuclear magnetic resonance (NMR) spectroscopy and molecular dynamics (MD) data, we here develop a statistical mechanical model to predict the compositional evolution of structure in borosilicate glasses by accounting for the relative enthalpic and entropic contributions to the modifier/former interactions. By using previously established parameters for binary silicate and binary borate glass systems, the number of free parameters can be reduced significantly. We discuss the possibilities for transferring established model parameters from systems with different modifiers, with the long-term goal of predicting structural evolutions in oxide glasses without any free parameters.