Computer Simulation Studies of Glasses: Structure and Transport Mechanisms

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Molecular dynamics (MD) simulations are now an accepted part of the toolbox used to probe the structure of glasses. The information obtained from MD simulations has shed considerable light on both the structure and structure-related properties, such as alkali ion transport. In this presentation, we will review briefly the technique and discuss some recent applications, particularly to the question of alkali ion transport processes. These transport mechanisms are, ultimately, controlled by the local structure of the alkali ions. Although difficult to obtain experimentally, they emerge naturally from the simulations. We have followed the jump mechanisms of some alkali ions in a couple of different alkali silicate glasses and will describe in some detail our observations, which lead to the conclusion that there is some degree of similarity with traditional vacancy mechanisms found in crystalline materials.