
MD Simulations of the melting of sodium and lithium metasilicates

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Abstract

Melting has been described as the single most important phase change in fundamental (materials) science. However, none of the theories put forward come close to explaining experimental observations, and this particularly true of the melting of silicate materials. The "reverse" reactions, crystallization and its solid-state counterpart, devitrification, also fall into the not-completely-understood category.

Whereas the timeframes associated with nucleation and growth make devitrification difficult to probe by standard atomistic simulation techniques such as molecular dynamics, melting does not suffer from such drawbacks. In this presentation, we describe the application of molecular dynamics to probe the structural changes that occur on heating crystalline sodium and lithium metasilicates to above their melting temperatures. The behavior of these two silicates is different; sodium silicate shows a pronounced pre-melting regime, associated with an excess heat capacity, whereas the lithium metasilicate does not. In melting, however, both show a change from a single distribution of Q₂ units in the crystal to a distribution of multiple Q_n units in the melt (and subsequent glass).

The simulations allow us to shed light on the role played by the alkali ions in the pre-melting regime, as well as identifying the initial mechanisms that lead to the reduction in the number of Q₂ species. It is hoped also that these results may provide some insight into the reverse process of nucleation and growth.

Keywords: Molecular Dynamics, melting, alkali silicates

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