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Mixtures of SiO_2 with alkali oxides and aluminium oxides: computer simulation studies

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We use molecular dynamics (MD) computer simulations to investigate the atomic transport in multicomponent silicate melts. The detailed information as obtained by MD allows to elucidate the interplay between structure, dynamics and phase behavior of liquid mixtures. We present simulation results for realistic models of ion-conducting alkali silicate melts and aluminium silicates. These systems exhibit intermediate range order that is reflected by prepeaks in static structure factors $S_{\alpha\beta}(q)$.

In aluminium silicate melts, we find the emergence of triclusters in conjunction with two-membered rings. This finding is supported by *ab initio* calculations that use small clusters from the MD simulations as an input [1]. Moreover, a prepeak is found, e.g., in $S_{\mathrm{AlAl}}(q)$ and $S_{\mathrm{SiSi}}(q)$ due to a microphase separation into Al rich and Si rich percolating regions [2]. We discuss the importance of this structure for diffusion dynamics and phase behavior.

The intermediate range order in the alkali silicates provides the presence of diffusion channels for the fast alkali ion motion. The interplay of the latter channel stucture with non-trivial transport phenomena such as the mixed alkali effect in ternary alkali silicates is demonstrated. The existence of intermediate range order in sodium silicates is verified by a comparison to inelelastic neutron scattering results by A. Meyer *et al.* [3,4]

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