611f Spatially Heterogeneous Dynamics in Molten Silica

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Molecular dynamics simulations were carried out to study the spatially heterogeneous dynamics (SHD) in molten silica, based on a charge transfer three-body potential. In this interaction potential, the directional character of the covalent bonding in SiO2 is modeled by means of three-body terms that constrain both the Si-O-Si and O-Si-O angles. In addition, a charge transfer term controls the degree of charge polarization in a covalent bond, as well as the amount of charge transferred between atoms upon rupture or formation of such a bond. Both features have been shown to be essential for structural transformations in crystalline and amorphous silica, as well as for reproducing the short-time and long-time dynamic properties of liquid silica. In particular, the local dynamics are sensitive to the charge redistribution during bond breakage and formation. These features are not part of the BKS potential, which is commonly used for the simulation of silica near the glass transition. In this talk we compare our findings to a similar study recently carried out for BKS silica.[1,2]

[1] M.I. Vogel and S.C. Glotzer.? "Temperature dependence of spatially heterogeneous dynamics in a model of viscous silica" ?Physical Review E 70 (6): Art. No. 061504 Part 1, (2004) [2] M.I. Vogel and S.C. Glotzer.? "Spatially Heterogeneous Dynamics and Dynamic Facilitation in a Model of Viscous Silica"?Phys. Rev. Letters, 92 (25): Art. No. 255901, (2004)