Title: The effect of quasi-one-dimensional confinement on dynamical heterogeneities in glass forming liquids.

Abstract:

Confined fluids display unique characteristics in comparison to bulk fluids. The geometrical constraint of the confining walls introduces incommensurate length scales in particle-particle and particle-wall interactions which lead to fundamental changes in the phase behaviour of glass forming liquids, with either enhancement or suppression of the glass transition[1], T_g, as well as re-entrant crystallization[2] with respect to the degree of confinement. Bulk liquids near the glass transition exhibit dynamical heterogeneities, where local relaxation rates that fluctuate strongly over space and time[3]. Here, we use molecular dynamics to see how confinement to long narrow channels effects dynamical heterogeneities in a 2D binary Kob-Andersen (KA) Lennard-Jones (LJ) mixture as a function of channel diameter. We investigate several dynamic and structural properties including the mean squared displacement, radial distribution function, bond-orientational order parameter and bond-breaking correlation function as the supercooled liquid approaches the glass transition as a function of channel diameter.

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[2] J. Mittal, T. M. Truskett, J. R. Errington, and G. Hummer, Layering and Position-Dependent Diffusive Dynamics of Confined Fluids, Phys. Rev. Lett. 100, 145901 (2008).

[3] Rajib K. Pandit and Horacio E. Castillo, Simple Model for Dynamic Heterogeneity in Glass-Forming Liquids, Phys. Rev. Lett. 131, 218202 (2023)