Dynamical heterogeneity in glass-forming toluene: Comparison of bulk and confined conditions by quasielastic neutron scattering and molecular dynamics simulations

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Résumé en anglais	We investigate the presence of dynamical heterogeneities and their consequences on the incoherent intermediate scattering function Fs(Q,t) of a molecular glass-forming liquid, toluene, in bulk and confined conditions. We show that the dynamical heterogeneity deeply affects the shape (stretching and plateau height) of the function Fs(Q,t) and the mean square displacement when the slowest or the fastest populations are considered. Owing to the rigid character of the molecule and the remarkable agreement of the MD simulations with the quasielastic neutron scattering experiments, we extend our analysis to the interplay of translational and rotational motions in the relaxation processes. Since the existence of dynamical heterogeneities and a related cooperative length in the supercooled regime are postulated in many theoretical approaches of the glass transition phenomenon, the liquid is then confined into a pore of a few nano-meter diameter, where this characteristic length cannot extend beyond the pore size. The dynamics slow down when the size of the pore becomes smaller than the correlation length evaluated in the bulk with different methods (size effect on the diffusion coefficient, size of dynamical heterogeneities). An important increase of the stretching of the intermediate incoherent scattering function Fs(Q,t) also appears. We show that the heterogeneous character of the dynamics increases when the liquid is confined due to the presence of a rigid surface.
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