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Dynamical transition in glycerol[1] SALMAN SEYEDI, DANIEL MARTIN, DMITRY MATYUSHOV, ?Department of Physics and School of Molecular Sciences, Arizona State University???, MATYUSHOV GROUP TEAM — Mean square displacements of hydrogens reported by incoherent elastic neutron scattering show a kink in their temperature dependence. This crossover connects two approximately linear regimes and is known as the dynamical transition temperature. The dynamical transition is widely observed for glass-formers, including molecular liquids and biopolymers. It is often assigned to the dynamical freezing of subsets of molecular modes at the point of equality between the relaxation time of the system and the instrumental observation window. The origin of the dynamical transition is studied here for glass-forming glycerol by extensive molecular dynamics simulations. We found that the dynamical transition occurs for center of mass translations and molecular rotations at the same temperature insensitive to changes of the observation window. In addition, both the translational and rotational dynamics of glycerol show a dynamic crossover from the structural to a secondary relaxation at the temperature of the dynamical transition. The simulation results consistently point to a structural alteration of glycerol responsible for both the kink in the mean square displacements and the dynamic crossover, instead of the effect of the finite observation window.

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