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Dynamic Heterogeneity in Highly Cross-linked Epoxy in the Vicinity of Glass Transition PO-HAN LIN, RAJESH KHARE, Texas Tech University — Cross-linked epoxy has been widely used in aerospace and electronics industries. The highly cross-linked nature of these systems leads to different chain dynamics as compared to the linear polymeric systems. In this work, we have used molecular dynamics (MD) simulations to study the dynamic heterogeneity in cross-linked epoxy near the glass transition temperature. Well-relaxed atomistic models of cross-linked epoxy were first created by employing the simulated annealing polymerization approach. The specific epoxy system studied consisted of diglycidyl ether of bisphenol-A (DGEBA) as the epoxy monomer and trimethylene glycol di-p-aminobenzoate (TMAB) as the cross-linker. The glass transition temperature of these model structures was determined from MD simulation by monitoring their volume-temperature behaviour in a stepwise cooling run. The chain dynamics of these systems were characterized by their local translational and orientational mobility. Furthermore, dynamic heterogeneity was studied by analyzing the spatial distribution of the mobile and immobile atoms in the system near the glass transition temperature.

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