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Comparative molecular simulation study of low and high density polymer glasses: A competition between attractive and repulsive interactions[1] JALIM SINGH, PRASANTH JOSE, Indian Institute of Technology Mandi — Results of molecular dynamics simulations of a system of Kremer and Grest linear polymer melts are presented at moderate and high number density. A detailed study of molecular pair distribution function shows that potential of mean force between the molecules has form of Gaussian with an attractive tail at number density $\rho = 0.85$ (in Lennard-Jones units), which is due to the dominating attractive interactions from temperature $T = 0.7$. This system shows gelation assisted glass transition, which is interpreted from peaks of molecular structure factor at small wave-numbers. At low temperature, this system phase separate to form dense domains whose local density is high; these domains show many dynamical features of glass transition in monomer and molecular level of relaxation indicating glass transition is assisted by gelation in this system. In the same system, at $\rho = 1.0$, repulsive interactions dominate, structure does not change even at low temperatures; the system exhibits dynamic heterogeneity and known to undergo glass transition. In this work, we compare and contrast the structure and dynamics of the system near its glass transition. Also, we computed correlation length of systems from the peak value of four-point structural dynamic susceptibility.

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