Dynamics of Polymer Melts Confined by Smooth Walls: Crossover from Non-entangled to Entangled Regime

Qi Liao, Yijie Li, Dongshan Wei, Xigao Jin, Charles Han, Institute of Chemistry, Chinese Academy of Sciences — We present the results of molecular dynamics simulations of polymer films confined by smooth walls. Simulations were performed for a wide range of chain lengths covering both non-entangled and entangled polymer dynamics, as well as film thickness crossing over the order of chain size to the bulk state. The simulation results for chain size dependence on the film thickness are compared with the prediction of the scaling model. By measuring the correlation function of the end-to-end vectors, we have determined that relaxation time of polymer chains in the different entanglement state confined in the film. It is shown that there is a minimum of relaxation time with the decrease of the film thickness in the entangled regime, which may be caused by the confinement-induced disentanglement.