Structural and Dynamical Properties of Linear Polymer Melts in Strict and Quasi Two Dimensions using Computer Simulations

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In this study, we investigate microstructural and dynamical properties of strict and quasi 2D linear polyethylene (PE) melts using atomistic and coarse-grained molecular dynamics (MD) simulations. The Kremer-Grest (KG) model and united atom (UA) model were adopted to simulate the strict and quasi 2D melt systems, respectively. As chain length increases, strict 2D chains display compact and segregated structure, whereas quasi 2D chains exhibit elongated and interpenetrated structure. Through detailed analysis, this study has revealed the microscopic origins of the similarities and differences between two systems in terms of mean-square of radius of gyration, mean-square displacement, diffusion coefficient, and relaxation time, and so on.