Topological and dynamical analysis of entangled polymer using computer simulation

윤정하, 김준모, 백충기†
UNIST
(cbaig@unist.ac.kr†)

Motion of polymeric melts is hindered from the other polymers. This topological constraint is called entanglement. It is very important factor to determine the dynamics of entangled polymer. In contrast to the permanent chemical junction in rubber network, entanglements are temporary physical junction between polymers. So it is generated and removed in time. Therefore, measuring life time of individual entanglement is required to comprehensively understand the macroscopic phenomena of polymeric melts. In this study, we developed new algorithm to analysis topological and dynamical property. We get the entanglement network from the modified Z-code and track down the individual entanglement in time. Using this algorithm, we can directly calculate the segment survival probability function $\psi(s,t)$ of the linear polyethylene melts (C400H802). Also we can compute rheological properties from the survival probability function to verify present dynamic models. Through this research we evaluate basic relaxation mechanisms such as reputation, contour length fluctuation (CLF), and constraint release (CR) of entangled polymers and expand them under flowing system.