MOLECULAR RELAXATIONS IN POLYETHYLENE: A COMPARATIVE STUDY OF COMPUTER SIMULATION AND EXPERIMENTAL OBSERVATIONS

Javier Martínez-Salazar, Javier Ramos and JF Vega
Dep of Macromolecular Physics. Instituto de Estructura de la Materia. CSIC. Spain
# email: jmsalazar@iem.cfmac.csic.es

A full atomistic computer simulation of the molecular structure and dynamics of entangled linear and branched polyethylene chains in the melt is reported. The work has been carried out by using a number of equilibrated molecules in all length scales by advanced Monte Carlo moves. This strategy allows us to evaluate the density and the intermolecular local packing (chain size) in the melt, by a convenient mapping of the Monte Carlo atomistic simulations on the packing length model. We have found a striking agreement between the simulated chain dimensions and the corresponding entanglement features obtained from rheological measurements. Furthermore, a description of the full atomistic chain dynamics in a range of hundreds of nanoseconds is also possible. The time evolution of the mean-squared inner segments displacement is in perfect agreement with the experimental results obtained in incoherent neutron spin echo experiments by Wischnewski et al for a monodisperse polyethylene sample with a similar molecular architecture, which follows the well-known transition from free 3D-Rouse relaxation to the local 1D-reptation regime.

1 Ramos, J.; Peristeanu, L.D.; Theodorou, D. Macromolecules 2007, 40, 9640