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

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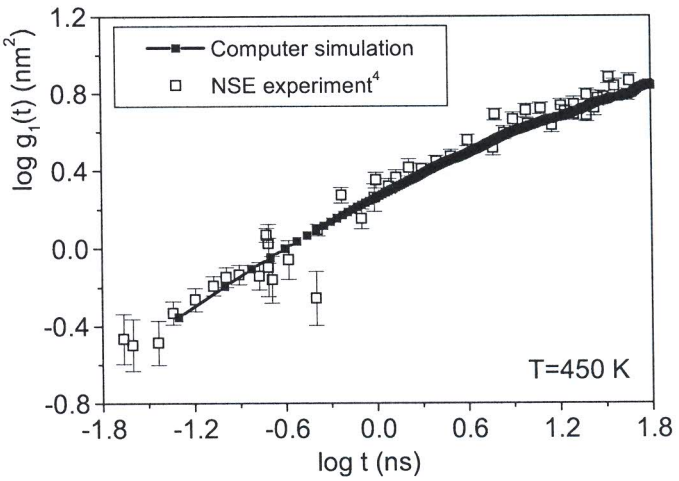
A full atomistic computer simulation of the molecular structure and dynamics of entangled linear and branched polyethylene chains in the melt is reported. The work has been carried out by using a number of equilibrated molecules in all length scales by advanced Monte Carlo moves.[1] This strategy allows 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.[2] We have found a striking agreement between the simulated chain dimensions and the corresponding entanglement features obtained from rheological measurements.[3] 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[4] 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.



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