MAR07-2006-000142

Abstract for an Invited Paper
for the MAR07 Meeting of
the American Physical Society

Looking inside the tube: what molecular dynamics simulations are revealing about polymer entanglements

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Using concepts developed over the years by de Gennes, Doi, Edwards, Marrucci, Rubinstein, McLeish, Milner, and others, a kind of "standard model" for entangled polymer relaxation and rheology has been developed, which, like the "standard model" of high-energy physics, has a number of ad hoc assumptions and fitting parameters. The "standard model" of polymer relaxation is based on a phenomenological "tube" surrounding each polymer chain that represents the effect on that chain of non-crossability constraints imposed by surrounding chains. As a result of its confinement to the tube, the chain relaxes by reptation – or sliding along the tube, accordion-like fluctuations of the chain within the tube, and movement of, or dilation of, the tube due to motion of the surrounding chains creating the tube-like region. Increasing computer speed and advanced simulation methods are now making possible the direct molecular dynamics simulations of entangled polymers resolved at the monomer scale, over time scales sufficient to test the underlying assumptions of the tube model and allow direct calculation of some of the phenomenological parameters. Here we illustrate how these simulations allow us to estimate the distribution of tube lengths, the average diameter of the tube, and the mobility of the branch point in a simple "star" branched polymer. These findings confirm the validity of the tube ansatz, but suggest that some corrections to the "standard model" may be needed.