Report

Rotation, deformation and orientation of polymer molecules

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INTRODUCTION
The deformation and orientation of chain molecules in a polymer solution or a polymer melt can be detected via the flow birefringence or by light or neutron scattering experiments which yield the radius of gyration tensor. The corresponding information can be inferred from nonequilibrium molecular dynamics (NEMD) computer simulations of polymer solutions [1] and melts [2, 3] for model systems. In the simulations, the dynamics of the rotation of molecules can be analyzed in detail (Fig. 1). This information is practically not accessible in experiments but is of importance for understanding the microscopic processes in sheared polymeric liquids.

MODELS
Here we present results on the rotation of deformable molecules of various chain length as inferred from NEMD simulations of dilute solutions. An example is given in Fig. 2. Comparison is made with simple theoretical models. Furthermore, a correlation of the average rotational velocity with a ratio of components of the gyration tensor is tested.

RESULTS
For very small shear rates, the molecules are only slightly deformed and they rotate, with a time averaged angular velocity which is equal to one half of the imposed vorticity. At intermediate and high shear rates, the average angular velocity is drastically decreased. The molecules librate (wagging mode) about a stretched and flow oriented state for a relatively long time before they contract and undergo a rather fast rotational flip to a new stretched state. Both the NEMD studies and a simple model reveal a typical chaotic behavior at intermediate shear rates.

REFERENCES