P.28 Passive and active microrheology of a polymer melt studied by molecular dynamics simulation

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The rheological behaviour of a material is determined by the relaxation of its stress autocorrelation [1]. In simulation studies the stress tensor can explicitely be calculated and serves as a reference for the microrheological results, that are based on the behaviour of suspended particles [2]. The system under study is the well established bead-spring polymer melt model [3] including one or two nanoscopic particles.

Passive microrheology yields linear response properties of the polymer melt by looking at the thermal motion of the nanoparticles. From the mean squared displacement of the nanoparticles the complex modulus $G^*(\omega)$ of the melt is determined by using a generalized Stokes-Einstein equation. Results for different particle sizes, monomer-particle interaction strengths and temperatures are compared to the real microscopic moduli. With regard to hydrodynamic effects, a more complete form of the analysis is discussed [4].

For a comparison to recent experimental results from X-ray photon correlation spectroscopy [5], the temperature dependence of the incoherent intermediate scattering function is shown.

Furthermore the linear and nonlinear response of the polymer melt is investigated by applying forces to the melt (active microrheology). Here a nanoparticle-oscillator is used; i.e. two nanoparticles are connected by a harmonic potential and the compressed oscillator is put into the polymer melt. The resulting oscillation of the nanoparticles is studied for different melt temperatures and different spring constants.

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