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Numerical study of dynamical properties of entangled polymer melts in terms of renormalized rouse models

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Abstract

The dynamic properties of n-renormalized Rouse models (n = 1, 2) were numerically investigated. Within two decay orders of magnitude, the damping of normal Rouse modes of a polymer chain was shown to be approximated by the stretched exponential function Cp(t) ∝ exp{- (t/τp*)βp}, where βp is the stretching parameter dependent on the number p of the Rouse mode and τp* is the characteristic decay time. The dependence of the stretching parameter on the mode number has a minimum. It was found that the nonexponential form of autocorrelation functions of the normal modes affects the dynamic characteristics of a polymer chain: the mean-square segment displacement r2(t)nRR and the autocorrelation function of the tangential vector b(t)b(0)NRR. In comparison with the Markov approximation, the r2(t)TRR and b(t)b(0)TRR values in the twice-normalized Rouse model change over time at a lesser rate: ∝t 0.31 and ∝t-0.31 at times t ≪ τ p TRR, respectively. The effect of the finite dimensions of the polymer chain on the relaxation times of the normal modes was studied.