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Dynamics of Bottlebrush Networks: A Computational Study[1]

ANDREY DOBRYNIN, ZHEN CAO, Univ of Akron, SERGEI SHEIKO, Univ of NC - Chapel Hill — We study dynamics of deformation of bottlebrush networks using molecular dynamics simulations and theoretical calculations. Analysis of our simulation results show that the dynamics of bottlebrush network deformation can be described by a Rouse model for polydisperse networks with effective Rouse time of the bottlebrush network strand, $\tau_R = \tau_0 N_s^2 (N_{sc}+1)$ where, N_s is the number-average degree of polymerization of the bottlebrush backbone strands between crosslinks, N_{sc} is the degree of polymerization of the side chains and $\tau_0$is a characteristic monomeric relaxation time. At time scales t smaller than the Rouse time, $t < \tau_R$, the time dependent network shear modulus decays with time as $G(t) \propto \rho k_B T (\tau_0/t)^{1/2}$, where $\rho$is the monomer number density. However, at the time scale t larger than the Rouse time of the bottlebrush strands between crosslinks, the network response is pure elastic with shear modulus $G(t) = G_0$, where G_0 is the equilibrium shear modulus at small deformation. The stress evolution in the bottlebrush networks can be described by a universal function of t/τ_R.

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