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Computer Simulations of Bottlebrush Melts and Soft Networks[1]

ZHEN CAO, Univ of Akron, JAN-MICHAEL CARRILLO, Oak Ridge National Laboratory , SERGEI SHEIKO, Univ of NC - Chapel Hill, ANDREY DOBRYNIN, Univ of Akron — We have studied dense bottlebrush systems in a melt and network state using a combination of the molecular dynamics simulations and analytical calculations. Our simulations show that the bottlebrush macromolecules in a melt behave as ideal chains with the effective Kuhn length $b_{\rm K}$. The bottlebrush induced bending rigidity is due to redistribution of the side chains upon backbone bending. Kuhn length of the bottlebrushes increases with increasing the side-chain degree of polymerization $n_{\rm sc}$ as $b_K \propto n_{sc}^{0.46}$. This model of bottlebrush macromolecules is extended to describe mechanical properties of bottlebrush networks in linear and nonlinear deformation regimes. In the linear deformation regime, the network shear modulus scales with the degree of polymerization of the side chains as $G_0 \propto (n_{sc}+1)^{-1}$as long as the ratio of the Kuhn length to the size of the fully extended bottlebrush backbone between crosslinks, $R_{\rm max}$, is smaller than unity, $b_K/R_{\rm max} << 1$. Bottlebrush networks with $b_K/R_{\rm max} \propto 1$ demonstrate behavior similar to that of networks of semiflexible chains with $G_0 \propto n_{sc}^{-0.5}$. In the nonlinear deformation regime, the deformation dependent shear modulus is a universal function of the first strain invariant I_1 and bottlebrush backbone deformation ratio β describing stretching ability of the bottlebrush backbone between crosslinks.

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