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Self-Similar Conformations and Dynamics of Non-Concatenated Entangled Ring Polymers[1]

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A scaling model of self-similar conformations and dynamics of non-concatenated entangled ring polymers is developed. Topological constraints force these ring polymers into compact conformations with fractal dimension D=3 that we call fractal loopy globules (FLGs). This result is based on the conjecture that the overlap parameter of loops on all length scales is equal to the Kavassalis-Noolandi number 10-20. The dynamics of entangled rings is self-similar, and proceeds as loops of increasing sizes are rearranged progressively at their respective diffusion times. The topological constraints associated with smaller rearranged loops affect the dynamics of larger loops by increasing the effective friction coefficient, but have no influence on the tubes confining larger loops. Therefore, the tube diameter defined as the average spacing between relevant topological constraints increases with time, leading to "tube dilation". Analysis of the primitive paths in molecular dynamics (MD) simulations suggests complete tube dilation with the tube diameter on the order of the time-dependent characteristic loop size. A characteristic loop at time t is defined as a ring section that has diffused a distance of its size during time t. We derive dynamic scaling exponents in terms of fractal dimensions of an entangled ring and the underlying primitive path and a parameter characterizing the extent of tube dilation. The results reproduce the predictions of different dynamic models of a single non-concatenated entangled ring. We demonstrate that traditional generalization of single-ring models to multi-ring dynamics is not self-consistent and develop a FLG model with self-consistent multi-ring dynamics and complete tube dilation. Various dynamic scaling exponents predicted by the self-consistent FLG model are consistent with recent computer simulations and experiments. We also perform MD simulations of nanoparticle (NP) diffusion in melts of non-concatenated entangled ring polymers. NPs larger than the undilated tube diameter undergo power-law sub-diffusion in entangled rings in contrast to strong suppression in entangled linear chains. This result demonstrates that there is no long-lived confining tube in entangled ring polymers, which agrees with complete tube dilation in the self-consistent FLG model.

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