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Coarse-Grained Kinetic Modeling of Polymer Networks with Non-Affine Slip-Tube Behavior and Heterogeneous Microstructure BRIAN PASQUINI, FERNANDO ESCOBEDO, YONG LAK JOO, Department of Chemical and Biomolecular Engineering, Cornell University — Elements of existing entanglement network models have been extended to better account for non-affice slip-tube behavior and to incorporate the effect of heterogeneous spatial domains. Starting with the Density Cloud Model (DCM) framework from Terzis et. al., an entanglement bond potential acting at each entanglement point is introduced. This potential mimics the non-affine tethering from network theories, and in combination with slippage accurately reproduces Non-Affine Slip-Tube behavior. This framework can easily be extended to study the effect of polymer architecture on the mechanical response of the resulting networks. Secondly, the temporary bond from the model of Termonia and Smith is combined with the DCM framework to simulate rigid domains within a matrix of soft polymer network. The modulus of the additional bonds sets the elastic properties of the rigid domain, while DCM entanglement relaxation assures that local deformation remains consistent with the bulk polymer density. The effect of rigid domain size on initial modulus is reported.

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