Modeling the Sticky Rouse Model with Periodic Boundary Conditions

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Abstract. The existence of the reversible noncovalent bonds, such as hydrogen bonds, π-π stacking, metal-ligand and ionic interactions in the polymers makes it possible to form transient networks. On the other hand, the presence of covalent bonds can lead to the formulation of permanent networks. While the transient networks are reversible, easily processable and recyclable, the permanent networks are able to resist flow and creep, and to swell without losing their coherence. The co-existence of these two kinds of networks in polymers makes them ideal for applications, such as high mechanical strength, large reversible deformability in shear and extension, substantial reversible swelling, and self-healing properties. We are aiming at unveiling the mechanisms behind these unique properties by modeling so that they can be fully exploited.

Since Rubinstein et al. firstly proposed the sticky Rouse model, many improvements have been done to this model. However, most of the models are single chain model and it has inborn shortcomings. For one thing, single chain model can not predict the structure of associating polymers. For another, in single chain model system, the interactions between different chains are simulated through virtual (not real) coupling. Differently, we adopt multi-chain sticky Rouse model to simulate the associating polymers. Additionally, periodic boundary conditions are utilized, which allows us to simulate the macroscopic phenomena from the mesoscopic scale.