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Multipoint Segmental Repulsive Potential Model for Dissipative Particles Dynamics of Uncrossing Polymer Chains NOBUYUKI IWAOKA, National Institute of Technology, Tsuruoka College, KATSUMI HAGITA, Department of Applied Physics, National Defense Academy, HIROSHI TAKANO, Facluty of Science and Technology, Keio University — In scientific and industrial fields, dissipative particle dynamics (DPD) simulation is a widely used coarse-grained molecular dynamics for studying the structural and thermodynamic properties of polymeric systems. A long-standing problem in DPD polymers is that unphysical bond crossings are caused due to utilization of soft-core potential. This means that the standard DPD cannot capture entanglement effects that play a crucial role in mechanical properties of long polymers. To overcome such a drawback, a segmental repulsive potential (SRP) model has been developed by several groups. In the SRP models, repulsive potential between bonds is added to the DPD polymer as a function of the distance between nearest points or midpoints on each bond. The SRP models have been shown that bond crossings are effectively reduced and reptation-like behaviors are successfully reproduced. However, cut-off radius of the SRP d_c (thickness of bonds) is too large to maintain static properties of the standard DPD polymer. In the present study, for reducing d_c and artificial effects in SRP models, we propose a modification of the SRP model by using multipoint cites (mp-SRP) instead of single cite for bond-bond interactions.

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