Abstract

Molecular dynamics simulations are used to study the dynamics of polymers in an implicit solvent, imposed by a Brownian thermostat. The dynamics of the system is reduced to its normal coordinates, and its conformation to the model proposed by Rouse is confirmed by analysing the scaling of normal coordinate correlation relaxation times with monomer and mode number. The scaling is analysed for single Gaussian chains of flexible and semiflexible polymers, with point mass monomers and harmonic bonds. The semiflexible polymer chain is subjected to a normal coordinate decomposition identical to that employed in the flexible case, which has been found to hold in the limit of low bending rigidity. It is also found that the introduction of explicit solvent particles and implementation of a dissipative particle dynamics (DPD) thermostat shifts the scaling of normal coordinate relaxation times towards the theoretical value predicted by the Zimm model, suggesting the introduction of effective hydrodynamic interactions. The clustering effects induced by introducing type-dependent deep potential wells(patches) along a heterogeneous polymer chain is also studied. Attractive patches have also been introduced randomly along rigid semiflexible polymer chains, which has been found to result in the decrease of the chain's persistence length.