Microstucture and dynamics of a coarse-grained wormlike polyelectrolyte chain in simple flows by Brownian dynamics simulation

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Recently, as the single molecule tracking has become of great attention in life science as well as nanobio technology, it is necessary to consider static and dynamic properties in flow fields. In this study, both conformation and translational diffusion of a xanthan polyelectrolyte chain in bulk solution are computed by using Brownian dynamics (BD) simulation. The coarse-grained modeling is based on the nonlinear bead-spring (i.e., FENE) with long-range electrostatic, Lennard-Jones, and hydroynamic interactions between pairs of beads. Static properties of xanthan molecule (e.g., radius of gyration, contour length) certainly depend on the solution environments such as pH, medium screening effect, an dielectric constant. In simple flows with either shear or extensional fields, conformation of xanthan molecule shows different results. we hve found that a molecule in extensional flows is more extended than in simple shear flows. Furthermore, we have tried to verify our simulation by comparing with experiental observations by means of the fluorescence microscopy.