Worm-Like Polyelectrolyte in Confined Spaces: Brownian Dynamics Simulations

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A coarse-grained modeling of the polysaccharide xanthan, which finds wide industrial applications, is described and its structure and dynamics under confinement are examined with Brownian dynamics (BD) simulations. The BD model of xanthan is based on a bead-spring model with the finitely extensible nonlinear elastic (FENE) spring, the Debye-Hückel electrostatic interaction, and the Rotne-Prager hydrodynamic interaction. The long-range interaction between the beads and the confining solid wall is also taken into account. The model parameters are determined from the Yamakawa-Fujii interpretation of experimental viscosity data according to Chun and Park [Macromol. Chem. Phys. 195, 701 (1994)]. The effects of the confinement, modulated by the wall-to-wall distance and the wall surface charge density, on the structural and diffusive properties of xanthan are characterized with BD simulations. The implication of the findings is discussed in relation to the transport of polyelectrolyte complex fluids in micro/nanofluidic channels. (This work was supported by the Basic Research Funds R01-2004-000-10944-0 from the Korea Science and Engineering Foundations.)