Application of reptation model on Brownian dynamics simulation for electrophoresis of single DNA molecule in polymer solution

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We use the Brownian dynamics(BD) model for dynamics of DNA molecule. The BD models used in previous studies are based on the assumption that intermolecular interactions are negligible. When a DNA molecule is forced to pass through pores in polymer solution by electric field, the motion of DNA is influenced strongly by surrounding polymer molecules. We follow the concept in the reptation model to represent the dynamic of DNA in polymer solution. Using the cubic Bezier spline, we manifest the contour of DNA to apply the constraint force from polymer molecules surrounding the DNA. The electrophoretic motion of DNA in polymer solution is analyzed applying the constraint force on the bead-spring model. U-shaped and I-shaped migration of DNA corresponding to each concentration of polymer solution under DC electric field, and the dynamics of DNA under AC electric field are simulated. We derive electrophoretic mobility of BD model with the constraint force to compare with experiment. We find the empirical correlation of the constraint force with concentration of polymer solution and show the validness for applying the constraint force on BD simulation.