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Rouse Dynamics of Polyelectrolyte Solutions: Molecular Dynamics Study ANDREY DOBRYNIN, University of Connecticut, QI LIAO, Institute of Chemistry, Chinese Academy of Sciences, MICHAEL RUBINSTEIN, University of North Carolina at Chapel Hill — We performed molecular dynamics simulations of dilute and semidilute polyelectrolyte solutions to study Rouse dynamics of polyelectrolytes. Polyelectrolyte solutions are modeled by an ensemble of bead-spring chains of charged Lennard-Jones particles with explicit counterions. We show that the simulations of the Rouse dynamics give qualitatively similar results to the experimentally observed dynamics of polyelectrolyte solutions. Our simulations showed that the chain relaxation time depends nonmonotonically on polymer concentration. The chain relaxation time decreases with increasing polymer concentration in dilute solution. This decrease in the chain relaxation time is due to counterion condensation. In the semidilute solution regime the chain relaxation time decreases with polymer concentration as inverse square root of polymer concentration. In this concentration range the chain relaxation time follows the usual Rouse scaling dependence on the chain degree of polymerization. At very high polymer concentrations the chain relaxation time begins to increase with increasing the polymer concentration. The crossover polymer concentration to the new scaling regime is independent on the chain degree of polymerization.

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