Conformation of a Natural Polyelectrolyte in Semidilute Solutions with No Added Salt

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We present a comprehensive study of the conformation of a model polyelectrolyte, alginate, in solutions with no added salt. We analyzed the full q dependence of small angle x-ray scattering (SAXS) plots and proposed a new model that has not been fitted to experimental scattering from polyelectrolytes yet. This model accommodates both the conformation of a chain and the electrostatic interactions between chains. Three models were examined as a way to represent the scattering from a single chain: a model of a worm-like chain, a model of a semiflexible chain without excluded volume effects, and a model of a semiflexible chain with excluded volume effects. The electrostatic interactions between chains were accounted for by using two models. We found that incorporating a Gaussian function to the model of the polymer reference interaction site (PRISM) has led to a good description of the experimental data.

Modeling the complete scattering curve allowed us to deduce information which was not available before for alginate. In particular, we found that the persistence length is not correlated with the chemical composition of the alginate. However, the electrostatic correlation length increases with the G-content. The dependence of the persistence length on the concentration was found to comply with the Odjik-Skolnick-Fixman (OSF) theory, where the persistence lengths depends on the square of the debye length. This new model has a potential to describe the scattering from other polysaccharides or polyelectrolytes.

A cross-over concentration from a string-controlled region to a bead controlled one was found in SAXS. Several rheological parameters have also changed abruptly around the same concentration.