Smart Materials: Methods and Applications – 2017 (SMMA-2017)
PP37

Kinetics of Swelling and Collapse of a Single Polyelectrolyte Chain

Soumik Mitra[1] and Arindam Kundagrami[1,2]

(1)Department of Physical Sciences and (2)Centre for Advanced Functional Materials, Indian Institute of Science Education and Research Kolkata, Mohanpur 741246,India

Kinetics of swelling and collapse of a single, isolated, flexible polyelectrolyte (PE) is described by a theoretical model considering uniform spherical expansion along with charge regularization. The equation of motion resulting from the osmotic and viscous forces is first solved numerically to obtain the temporal profiles for size and charge of the PE for swelling and deswelling in good solvent and collapse in poor solvent. Further, simpler analytical expressions for the equation of motion are obtained in the high- and low-salt limits. Finally, asymptotic analytical expressions for the time evolution of the size of the PE are derived. Of three major effects, like-charge repulsion of monomers, entropic force, and two-body attraction dominate respectively the processes of swelling, deswelling, and collapse. In general, the profiles show that the chain swells faster and farther for higher temperatures, lower dielectric mismatch, and lower concentrations of monovalent salt and deswells faster to smaller sizes for reverse trends of the same parameters. The kinetics is faster for lower molecular weights. Deswelling, followed by collapse, along with condensation of counterions, occurs in sufficiently poor solvents. For all configurational changes, charge of the PE chain decreases with decreasing size. Our results are in qualitative agreement with those available from simulations and experiments.