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Modeling Layer-by-Layer Assembly of Flexible Polyelectrolytes
QIANG WANG, Department of Chemical and Biological Engineering, Colorado State University — Using a continuum self-consistent field theory, we have modelled the sequential process of layer-by-layer assembly of flexible polyelectrolytes on flat surfaces as a series of kinetically trapped states. Up to 60 depositions of oppositely charged polyelectrolytes are performed, each followed by a washing step. The multilayer has a three-zone structure. An exponential growth is found for the first several layers, followed by a linear growth for subsequent layers evolving towards a steady state. Each layer inverts the total charge of the multilayer film (including the bare substrate charge). While adjacent layers are highly interpenetrating, stratification can be seen for every four or more layers. We have also examined the effects of surface charge density, bulk salt concentration, and solvent quality on the thickness and internal structure of the multilayer. Our results agree with most experimental findings on polyelectrolyte layer-by-layer assembly.

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