Microphase Segregation within Polyelectrolyte Brushes

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Polyelectrolyte brushes (PEBs) are functionalizable surface modifiers with tunable response to stimuli. A comprehensive understanding of their conformational behavior can improve already existing applications such as anti-fouling and contribute to their development as smart materials. Our self-consistent field theory (SCFT) considers the coupling of polymer elasticity, solubility, and electrostatics, enabling the characterization of PEBs at various charge fractions and solvent qualities. Using this theory, we have found multi-layered PEB conformations in which comprising chains are permitted in only one layer each. Calculated end-point distributions are negligible between layers, indicating that multi-layered brushes are formed by collections of melted mushroom conformations grafted upon each other. To facilitate the experimental validation of our multi-layered PEB conformations, we have also calculated corresponding reflectivity spectra for PEBs with up to four layers. Finally, a good fit with an experimentally measured height profile of a protein brush suggests our model can also provide quantitative insights for future experimental collaborations.