Toward Understanding Polyelectrolyte Multilayers

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Polyelectrolyte multilayers (PEMs) is composed of alternate layers of oppositely charged polyelectrolytes (PEs). They can be built by using the simple Layer-by-Layer (LbL) technique proposed by Decher et al. in the early of last decade. By dipping the charged substrate into oppositely charged PE solution followed by a rinsing step, and repeating the dipping and rinsing steps, hundreds of alternating charged layers can be built into a PEM. PEMs have adsorbed great interests both from academic researchers and industries due to its potential usage.

Despite the big amount of experimental literatures, the publications in theoretical and computer simulational method are relatively scare. Our recent work [1] found that the formation of stable PEMs is not as simple as the researchers previously thought. Given long enough equilibration time in the simulations, PECs come to occur by dissolving the previously adsorbed PEs, thus the previously stable-like PEM is disrupted consequently. On the other hand, the atomistic simulations, with all atoms and solvent (*e.g.*, water) explicitly used, can be used to refine the parameters used in the coarse grained simulations, so that the experimental condition can be better mimiced. To that end, the atomistic simulation is performed by us to try to improve the coarse-grained simulations by providing more realistic potential.

Poly(styrene sulfonate)(PSS)/poly(diallyldimethylammonium)(PDADMA) PEM has been investigated based on atomistic simulations. Given the experimental reports that PSS/PDADMA PEM has similar structure as polyelectrolyte complex (PEC), the PSS/PDADMA PECs are studied alternatively, which can decrease the requirement for the computer resourses. The ion-pairing, hydration and glassy behavior are investigated

References

[1] Cerdà, J. J.; Qiao, B.; Holm, C. *Soft Matter* **2009**, DOI: 10.1039/B912800J.