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**Molecular Dynamics Simulations of Multilayer Polyelectrolyte Films** PRITESH PATEL, Macromolecular Science and Engineering, Case Western Reserve University, JUNHWAN JEON, Polymer Program, Institute of Materials Science, University of Connecticut, PATRICK MATHER, Macromolecular Science and Engineering, Case Western Reserve University, ANDREY DOBRYNIN, Polymer Program, Institute of Materials Science and Department of Physics, University of Connecticut — We have performed molecular dynamics simulations of multilayer assembly of oppositely charged polyelectrolytes at charged surfaces. The multilayer build-up was achieved through sequential adsorption of charged polymers in a layer-by-layer fashion from dilute polyelectrolyte solutions. The strong electrostatic attraction between oppositely charged polyelectrolytes at each deposition step is a driving force behind the nanometer-scale multilayer growth. Our simulations have shown that a charge reversal after each deposition step is critical for steady multilayer growth and that there is a linear increase in amount of polymer adsorbed after the first few deposition steps. There is substantial intermixing between chains adsorbed during different deposition steps within multilayer film. Despite significant chain intermixing, however, there are almost perfect periodic oscillations in local composition of positively and negatively charged polymers in the adsorbed film. We show that the film thickness, polymer surface coverage exhibit strong correlation with the strength of electrostatic and short-range interactions.

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