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Molecular dynamics simulations of electrostatic layer-by-layer assembly of polyelectrolytes near charged planar surface PRITESH PATEL, JUNHWAN JEON, Institute of Materials Science, University of Connecticut, PATRICK MATHER, Department of Macromolecular Science and Engineering, Case Western Reserve University, ANDREY DOBRYNIN, Institute of Materials Science and Department of Physics, University of Connecticut — We performed molecular dynamics simulations of multilayer assembly of flexible polyelectrolytes at a charged planar surface from dilute polyelectrolyte solutions. We have studied the effects of fraction of charged monomers on polymer backbone and the chain degree of polymerization on multilayer formation and film structure. Our simulations show that multilayer growth proceeds through surface overcharging, chain intermixing and linear increase in polymer surface coverage at each deposition step. There are almost perfect periodic oscillations of density difference between positively and negatively charged polymers in the adsorbed film despite of chain's intermixing. We have established that it usually requires more than one deposition step to complete a single layer and the ion pair formation plays an important role in multilayer stabilization.

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