Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Finite size effects in polyelectrolyte adsorption: A simulation study MARIA SAMMALKORPI, PAUL R. VAN TASSEL, Dept. of Chemical Engineering, Yale University — In recent experiments, we have uncovered conditions where polyelectrolyte adsorption to a conducting surface may become continuous in the sense of scaling linearly with time over hours [1]. This discovery of continuous layer growth offers an enticing possibility of nanoscale thin film growth in a single step process, but also brings forth questions of the underlying mechanisms. Here, we present a molecular Monte Carlo simulation study aimed at understanding mechanistically the continuous adsorption process and, more broadly, polyelectrolyte adsorption in general. Our system consists of two parallel polymer chains composed of charged tangent spheres above a surface of variable dielectric discontinuity between the substrate and the solution, and spherical counterions and salt ions. We find that counter ion correlations act to enable the formation of stable polymer-polymer binding and aggregation. We discuss the sensitivity of the attractive regime to a Coulombic coupling parameter and to finite ion size, and the implications of finite size effects and charge distribution both in the polyelectrolytes and in the ions, and implications to experimental observations. [1] A. P. Ngankam and P. R. Van Tassel, Proc. Nac. Acad. Sci. 104, 1140-1145 (2007); C. Olsen and P. R. Van Tassel, J. Colloid and Interface Science 329, 222-227 (2009).

Maria Sammalkorpi
Yale University

Date submitted: 18 Nov 2010 Electronic form version 1.4