Multi-Scale Simulation for the Adsorption of Model Polymers and Proteins on Nano-Patterned Surfaces

A. Striolo[C,S]
Department of Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK, U.S.A.
astriolo@ou.edu

The adsorption of polymers at surfaces is industrially exploited for the fabrication of coatings, adhesives, and composite materials. The surface adsorption of biopolymers is important for the fabrication of medical implants such as artificial heart valves and joint prosthesis. It has been recently shown that the adsorption of surfactants on nano-patterned solid surfaces leads to the synthesis of nano-structured materials with potential applications for the production of nano-batteries, and for quantitatively studying cell adhesion and motility [1]. The features of the resultant nano-structured materials strongly depend on the pattern dimensions. Pillars are obtained when small (~100 nm in diameter) patterns are used, honeycombs when larger patterns are used (~200 nm or larger).

To control the morphology of the final product, we require a fundamental understanding of the molecular mechanisms involved in the adsorption of polymers, surfactants, and proteins on nano-patterned surfaces. We implemented a combination of Monte Carlo (MC) and molecular dynamics (MD) simulation techniques for these purposes. Within our MC simulations, we employed a previously developed coarse-grained model [2] to study the adsorption of surfactants and proteins on nano-patterned surfaces. The attractive surface is covered by repulsive masks with different geometrical features. We will discuss the results obtained for a variety of scenarios that replicate relevant experimental conditions. Within our MD simulations, we investigated the structure of adsorbed surfactant monolayers. We will present the strategies implemented to generate coarse-grained models from our all-atom simulation results.

[1] M. Marquez, K. Patel, A.D.W. Carswell, D.W. Schmidtke, and B.P. Grady, "Fabrication of nanometer-scale polymeric structures on surfaces: pillars and honeycombs", submitted to Advanced Materials.
[2] A. Striolo, A. Jayaraman, J. Genzer, and C.K. Hall, *J. Chem. Phys.* **123**, 64710 (2005).