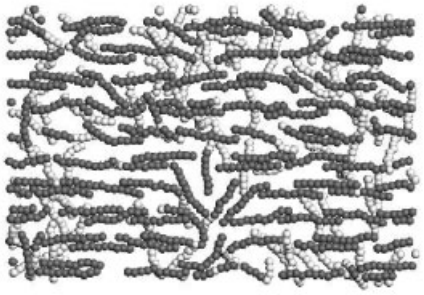
Adsorption of Semiflexible Chains on Nanostriped Surfaces: Monte Carlo Simulations

Abdullah AlSunaidi

Monte Carlo simulations were carried out to investigate the adsorption of semiflexible chains from a semidilute solution to substrates with periodic stripes of width w. The chains are made of fused $N = 10$ monomers of diameter σ interacting with each other through excluded volume interactions and with the stripes via a square-well potential of depth ε and width σ. The surface coverage was found to increase upon increasing the chain stiffness and decreases on increasing the width of the stripes. At small w, more flexible chains are adsorbed than stiff chains. Analysis of the radius of gyration for the chains showed that when $w < 8\sigma$, the component along the stripe direction is significantly larger than the others. Orientational order parameter reveals that, for small w, chains have preference to align along the stripe direction.



Introduction

Adsorption of macromolecules to solid surfaces has been a topic of intense research due to its wide application in industrial and biological processes including coating, lubrication, and protein adsorption. With the emergence of the nanotechnology era, experimentalists were able to design two-dimensional surfaces to which macromolecules would adsorb and self-assemble to form nanostructures that might be functionally useful. Fabricating such solid surfaces with nanopatterns would help in the control and manipulation of macromolecules at nanolength scales. Several experimental studies have reported on the effect of the pattern size on the conformation and the orientation of the adsorbed macromolecules. For example, Rockford et al.[1] have investigated the adsorption of polystyrene on striped substrates made of periodically varying polar (silicon oxide) and non-polar (gold) interactions where the period and width of the stripes are designed to be comparable to the size of the individual polymer chain. The polymer is repelled from the silicon oxide and adsorb to the gold stripes. It was found that low molecular weight chains would produce more uniform but thinner stripe coverage. Pallandre et al.[2] have studied the adsorption of a globular protein (antigen 69k) on protein-repellent hydrophobic (ethylene oxide) stripes periodically spaced by hydrophobic (alkylsilane) stripes favoring protein adsorption. The stripe widths were between 20 and 160 nm. The adsorption of the globular proteins on nanostriped templates can be selectively and locally adsorbed down to extremely small dimensions, and their orientation can be tuned by reducing the size of the adsorbing region. Stripes wider than 90 nm, display features typical of the proteins absorbed onto a homogenous surface. The adsorption of protein collagen on ethylene oxide and

A. AlSunaidi
Department of Physics, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia
Fax: (+00966) 3 860 2293; E-mail: asunaidi@kfupm.edu.sa

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