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Morphological Similarities between Single-Walled Nanotubes and Tubelike Structures of Polymers with Strong Adsorption Affinity to Nanowires

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Abstract. In their tubelike phase, nanowire-adsorbed polymers exhibit strong structural similarities to morphologies known from single-walled carbon (hexagonal) and boron (triangular) nanotubes. Since boron/boron nitride tubes require some disorder for stability the triangular polymer tubes provide a closer analog to the carbon tubes. By means of computer simulations of both two and three dimensional versions of a coarse-grained bead-spring model for the polymers, we investigate their structural properties and make a detailed comparison with structures of carbon nanotubes.

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1 Introduction

In a recent computational study, it could be shown that flexible polymers interacting with a wirelike substrate possess a barrellike phase [1]. Optimally packed, the monomers form a cylindrical polymer tube, reminiscent of a triangular lattice which wraps around the wire. Depending on the competition between steric constraints and monomer-substrate

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attraction, other structural phases can also form. These phases were also found in previous, related studies of polymers interacting with nanocylinders [2,3].

Tubelike structures formed by atoms or molecules possess interesting physical properties such as amazing mechanical stability, which make them potential candidates for nanotechnological applications. Recently, tin nanowires have been coated with atomic nanotube structures in order to stabilize them for conducting superconductivity experiments, i.e., protect them from shape fragmentation as well as from oxidation [4]. The understanding of the wetting behavior of atomic nanotubes with polymeric materials has been claimed to be the key to carbon nanotube-polymer composites [5]. Biological cells require a stable cytoskeleton which consists of tubelike myosin fibers.

The most prominent examples of tubes on atomistic scales are carbon nanotubes [6,7] which can be thought of as "rolled-up" and "zipped" sheets of graphene, sharing its hexagonal honeycomb lattice structure and sp^2 hybridized atoms [8–11]. Specifically, single-walled carbon nanotubes (SWCNTs) have been extensively studied on different levels of approximation. While nanotube models are typically based on continuum approximations, it has recently been shown that their atomistic nature is crucial for correct estimation of nanotube parameters [12,13].

As well as carbon nanotubes, boron and boron nitride tubes have also been created [14] and modeled. A review of boron tube modeling is given in [15]. The salient differences between boron and carbon tubes are that the boron tubes form a triangular lattice structure (as do the polymer tubes) but the boron tubes appear to require either puckering, substitution with nitrogen or regular vacant sites for stability, unlike both polymer and carbon tubes. Thus the polymer tubes share one feature – the underlying lattice – with single-walled boron nanotubes (SWBNTs) and another – non-buckled, translationally invariant surfaces – with the carbon tubes.

From a formal point of view the hexagonal nanotube atomic lattice is dual [16] to the triangular lattice, suggesting there may be a deeper connection. This has been extensively explored for idealized single-walled boron nanotubes [15], but the buckling or regular vacancies in real boron tube structures complicate a precise modeling. The polymer tubes we investigate in this study are complete, unbuckled triangulations of single-walled tubes and thus we can directly adopt the theory introduced in [15] for idealized boron tubes to link our results for polymer tubes with known atomic boron and carbon nanotube structures.

This paper is structured as follows. The description of the hybrid polymer-wire model leading to monolayer polymer tube conformations for certain parameters, and a summary of our previous findings on those systems, is given in Section 2. In Section 3 we present details of typical nanotube configurations and quantify their characterization. Since the correct treatment of discrete tube structures is indispensable for our discussion and was introduced quite recently, we also review the polyhedral model for the description of ideal nanotubes in detail. In Sections 4 and 5 we will present a detailed discussion of our mappings and simulations based on Monte Carlo simulations in the full three dimensional space (Section 5.1). These simulations indicate that it is indeed adequate to