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Spring-block approach for nanobristle patterns

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ABSTRACT

A two dimensional spring-block type model is used to model capillarity driven self-organization of nanobristles. The model reveals the role of capillarity and electrostatic forces in the pattern formation mechanism. By taking into account the relevant interactions several type of experimentally observed patterns are qualitatively well reproduced. The model offers the possibility to generate on computer novel nanobristle based structures, offering hints for designing further experiments. In order to allow for experimental validation of the model through future experiments, the cell-size distribution of the simulated cellular pattern is also studied and an exponential form is predicted.

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Reproducible nanoscale patterns and structures are of wide interest nowadays for engineering components in modern small-scale electronic, optical and magnetic devices [1]. The so-called *bottom up* approach for the fabrication of these nanostructures uses nanoparticles as elementary building blocks. Under some specific conditions the nanoparticles self-organize into the desired structures [2]. A well-known and widely explored possibility to induce this self-organization is to use the capillarity forces which appear during the drying of a liquid suspension of nanoparticles [3,4]. For instance, regular and irregular two-dimensional polystyrene nanosphere arrays on silica substrates are generated by such methods [5]. These patterns are used then as a convenient mask in the NanoSphere Litography (NSL) method.

Carbon nanotubes (CNT) are attractive materials for nanotechnology because of their interesting physico-chemical properties and molecular symmetries. In order to make them appropriate for certain applications, proper initial CNT configurations have to be built, and specific conditions have to be found which enable their controlled self-organization [6–8]. This is a very ambitious and challenging task, which can be made easier by elaborating working computer models for the self-organization of CNTs on substrates. Therefore, not only experimental, but also computational studies can advance the field of nanoengineering.

In the work of Chakrapani et al. [9] an experimental procedure is presented in which capillary self-organization of nanobristles (or so called 'CNT forrests') leads to puzzling cellular patterns. As pointed out by the authors, crack formation results from the reassembling of highly ordered, elastic CNTs. The obtained remarkable cellular patterns are extraordinarily stable.

The experimental procedure [9] may be shortly summarized as follows. Multi-walled nanotube arrays are grown on rigid silica surface by chemical vapor deposition (CVD) based on the decomposition of ferrocene and xylene. The resulting nanotubes have a wall thickness of ca. 10 nm and a diameter of ca. 30 nm. The average distance between two nanotubes is ca. 50 nm. The obtained nanotube bristle is oxidized in an oxygen plasma at room temperature and 133 Pa pressure for 10 min and immersed in a wetting fluid. After the liquid evaporates, characteristic cellular type patterns are formed as the ends of nanotubes self-organize in compact walls.

Figure 1 shows scanning electron microscope images of some typical structures. From the figures we deduce that a wide variety of structures are engineered in such manner. Both statistically symmetric polygonal cells and rather elongated ones can be obtained by changing the experimental conditions.

These micrometer scale structures have many advantageous features. They can be elastically deformed, transferred to other substrates or used for producing free-standing macroscopic fabrics. Thus, they might find potential applications as shock absorbent reinforcement in nanofiltration devices, elastic membranes and fabrics, and containers for storage or growth of biological cells.

Despite of its applications and the existence of well elaborated production protocols, the exact mechanisms responsible for self-organization of CNTs into vertically aligned cellular structures is not clearly understood. Recently, it has been argued that although we lack some basic information regarding the self-organization of CNTs within a bristle, this process can be approximated with the self-organization of arrays of CNT micropillars of micron-scale diameters [10] each consisting of thousands of CNTs. This observation enables the construction of a computationally tractable model which operates instead of stand-alone CNTs with micropillars.

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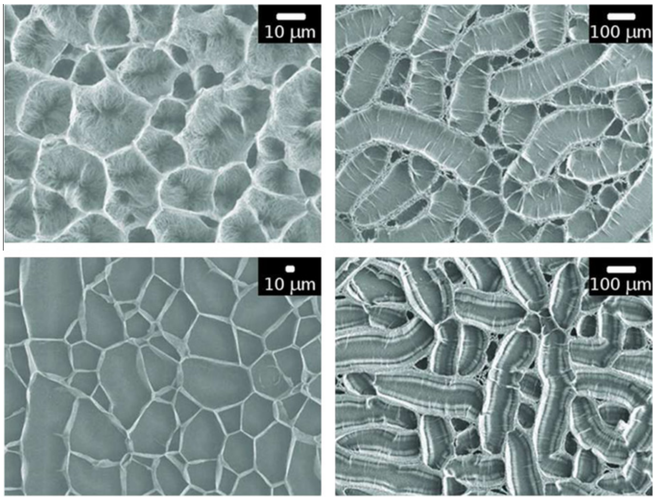

Figure 1. Scanning electron microscope images of the structures obtained in drying nanobristles.

In the present work a simple mechanical spring-block type model defined at mesoscopic micropillar level is considered for understanding the capillarity driven self-organization of nanobristles.

The model is based on the mechanical spring-block stick-slip model family. This model family appeared in 1967, when Burridge and Knopoff [11] constructed a simple mechanical model for explaining the Guttenberg-Richter law for the distribution of earthquakes after their magnitude. The basic elements of the model are blocks and springs that interconnect in a lattice-like topology. The blocks can slide with friction on a planar surface. The original model introduced by Burridge and Knopoff (BK) is one-dimensional. It can be studied numerically and it exhibits self-organized criticality [12]. The BK model gained new perspectives with the strong development of computers and computer simulation methods. Variants of the BK model proved to be useful in describing complex phenomena where avalanche-like processes are present, pattern formation phenomena and mesoscopic processes in solid-state physics or material sciences [13,14].

Recently, by using this model, we have successfully explained the patterns obtained in capillary self-organization of nanospheres [5,16]. Motivated by this success, hereby we propose to map the capillarity driven self-organization of nanotube bristles to a spring-block system, and to understand the pattern selection process by means of computer simulations.

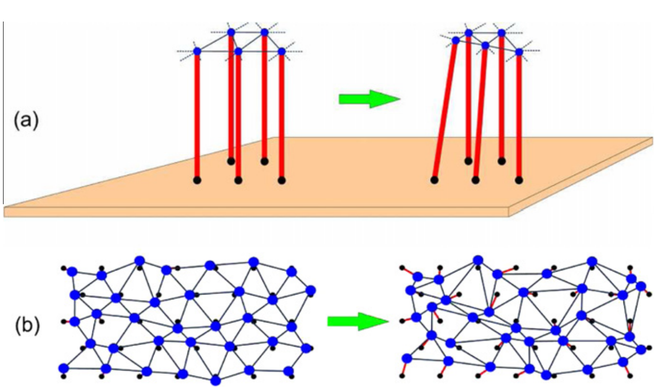

Figure 2. Main elements of the spring-block model. Panel (a) shows a schematic 3D representation of the nanobristle for the initial and a later state. Panel (b) illustrates the dynamics of the equivalent 2D model.

First, let us consider the three-dimensional (3D) model, which is very similar to the real nanotube arrangement. As sketched in Figure 2a, the micropillars composed by thousands of nanotubes having fixed bottom ends are modeled by flexible strands. Their interactions are represented by non-classical springs that connect the neighboring pillars. As motivated below, the evaporation of the liquid is simulated by the stepwise increase of tension in the springs. This will result in the agglomeration of micropillar ends creating the final structure in the studied system.

As shown in Figure 2b, this 3D model can be easily mapped into a two-dimensional (2D) one by projecting the micropillars' top ends on the surface. In the projection plane the micropillars bottom ends are represented as dots, and their positions are fixed on a predefined lattice. The movable top ends are modeled by the disk shaped blocks which can slide with friction on the 2D simulation surface. For visual purposes only, each disk is connected by an extensible string with its bottom end showing the micropillars' trunk. In our simplest approach there is no restriction imposed to the length of these extensible strings which means that nanotubes with infinite length are used. This corresponds to the real case when the nanotubes length is much grater than the linear size of the cells in the final patterns. The disks (top of micropillars) are connected with their nearest neighbors through special springs that model the resulting forces acting between the micropillars.

These special springs are one key ingredient of our computational model. They represent the resultant interaction force acting between two micropillars immersed in suspension. The tension force in the spring has a complex variation with the spring-length, i.e. the inter-pillar distance. It's form is sketched with a red line in the top panel of Figure 3. This force is the resultant of the capillary force, and the dipolar electrostatic repulsion between the micropillars.

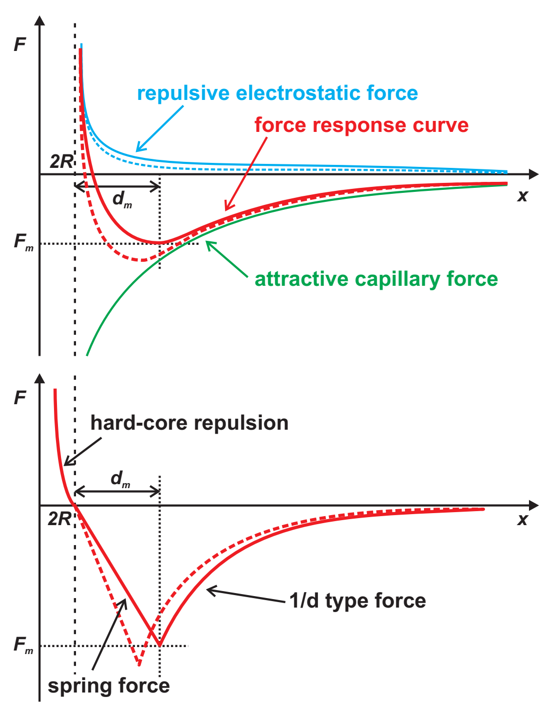

Figure 3. Forces acting between micropillars immersed into liquid (top panel). Forces are shown both at a given time step (solid line), and at a later one (dashed line). The bottom panel shows the length dependence of the net force used for modeling the resultant of the real interactions. It also contains the hard-core repulsion force between disks. Again, the shape of the force curve is shown at an earlier (solid line) and at a later stage (dashed line). The slope of the net force determines the spring-constants.

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