Block copolymers in confinements and under external fields

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Block copolymers (BCPs) are long chain molecules consisting of several chemically different blocks. Due to the chemical nature of the bond between blocks they do not macrophase, but form various structures on the nano-scale. BCP systems can be used as templates for the energy materials, advances separation templates, catalysts and for nano-electronics devises. Modern materials science uses block copolymers in solutions and mixtures of several BPCs and BCPs and homopolymers. Due to the intrinsic complexity of the systems, which have a very large physical parameter space, their experimental study is a much elaborated task. With the advances of computers, computational methods become a crucial component in the BCP research and the advances materials design. In our contribution we discuss computer simulation results for BCP systems and their relation to experimental data. Computer simulation results presented are based on two models: a Ginzburg-Landau type description and on self-consistent field theory (SCFT) for polymers. The Ginzburg-Landau model used is a basis for Cell Dynamics simulation (CDS) [1]. It is an extension of the square gradient model, which has proven to be very useful for polymer blends, while CDS is a powerful tool for BCP systems. In this talk we focus on two topics – confinements and external fields (electric, shear). In real practice BCP are often found in thin films (of the thickness of several structural domains), and most recently - in nano-pores. Confined structures are found to be very different from the bulk ones. We investigate various BCP systems: lamellae, cylindrical, spherical, and gyroid. Confinement has a profound influence on the BCP structure. In thin films non-bulk structures are formed in the layers next to the confining surfaces. In this way some such structures as perforated lamellae can be formed. In cylindrical pores helical and toroid structures are formed in various combinations. In spherical confinement the observed structures are reminiscent of knitting ball, onion, perforated spherical layer, virus-like morphology and others. Manipulation by the external electric or flow fields is a way of the nanostructure alignment. Kinetics of this process can be different depending on the field strength. We observe various phase transformations in these two types of fields. Examples include: spheres-to-cylinders and giroid-to-cylinders, as well as orientation transitions, such as changing lamellae orientation. In the case of the electric field lamellae orientation is found to depend on the strength of the electric field and the temperature. Using CDS can serve as a first part of the simulation tandem together with SCFT in a computer-aided design of novel nanostructured materials [1].

1. Pinna M., Zvelindovsky A. V. “Large scale simulation of block copolymers with Cell Dynamics”, *Eur. Phys. J. B* **85** (2012) 210, 18pp.