

Self-Assembly of Nanoparticle Mixtures in Lamellar Diblock Copolymers: Multiscale Molecular modeling.

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In this paper, we present an application of the concept of multiscale molecular modelling to the simulation of the morphology of nanoparticles dispersed into self assembly lamellar diblock copolymers. Simulation is performed at atomistic, mesoscale and finite elements level and provides information on the morphology and the mechanical properties of the systems of interest.

Extended Abstract

Polymer nanocomposites are receiving increased attention for potential applications including magnetic storage media, high-surface-area catalysts, selective membranes, and photonic band gap materials, etc.⁽¹⁾. Their role in more conventional applications is still relevant in many different fields. Infact, this combination of polymers and nanoparticles can lead to the enhancement of mechanical, optical, thermal, fire-retardant, and ablative properties, as well as gas-transport properties compared to either of the individual components^(1,2). Furthermore, due to the ability to microphase separating into a variety of ordered structures on nanometer length scales, block copolymers can be used as ordered template to afford opportunities for controlling the spatial and orientational distribution of nanoparticles to lead to new materials with tailored microstructure-dependent properties^(1,3-5). It is of paramount importance to describe the fundamental phenomena that leads to the microstructure at nanoscale level and, for achieving this result, it is necessary to resort to multiscale molecular modelling.

Lamellar diblock copolymers micro phase behaviour may be described by mesoscale simulation methods⁽⁶⁻⁹⁾. Among the different methods, a particle based (DPD) method⁽⁷⁾ is chosen here for the description of the system since it considers beads of different types and different dimensions that allow us to simulate both the enthalpic and entropic effect of the nanoparticles embedded in the polymeric matrix. Having obtained a realistic morphology at mesoscale, it is possible to transfer the simulated mesoscopic structure to finite elements modelling tools (FEM) for calculating macroscopic properties for the systems of interest^(9,10). If all these methods are tightly integrated we obtain the multi scale molecular modelling⁽⁹⁾.

In this paper we apply this procedure to the system made up by a copolymer [symmetric poly(styrene-*b*-2 vinyl pyridine) (PS-PVP) diblock copolymer] and PS- and PVP-coated gold particles. Recently⁽¹¹⁾ an experimental investigation developed a simple procedure to incorporate nanoparticles and control their location within different diblock copolymer

domains by controlling the surface chemistry of the particles. To localize particles within the A- or B-domain of an A-B block copolymer, particles are coated with either A or B-type homopolymer, respectively. To localize particles at the interfaces between the blocks, particles are coated with a mixture of A- and B-type homopolymers. Using this approach, the particles can be localized entirely within one copolymer domain or the other, or they can be localized at the interfaces between the blocks.

Recently ⁽¹²⁾ a first attempt to simulate the system has appeared in the literature showing promising results for the morphology at mesoscale, indicating that both enthalpic and entropic effects must be considered in the modeling. We will present an integrated multiscale method that starts at atomistic level with the determination of the interaction energies between the components involved, passes this information to the mesoscale level where the morphology is simulated including the embedded particles and finally the macroscopic properties are calculated with a finite elements method. Simulated data at each single scale will be compared with experimental information to validate the methodology.

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