SELF-ORGANIZED MULTI-LAYERS OF NANOSTRUCTURES VIA MOLECULAR DIPOLE INTERACTION

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Self-organization is an efficient way to grow nanostructures with regular sizes and spacings on a substrate surface. As a representative system, the spontaneous domain pattern formation of adsorbate monolayers has attracted wide spread interest. An adsorbate molecule usually carries an electric dipole. Even if the molecules are non-polar, the act of binding onto a substrate breaks the symmetry and causes the formation of dipoles. A molecule can be engineered to carry a large electric dipole moment by incorporating a polar group [1]. These molecules are mobile on a surface. Domains coarsen to reduce the domain boundary energy and refine to reduce the electric dipole interaction energy. The competition leads to stable patterns.

The mechanism of monolayer pattern formation gives insight into the study of analogous phenomena in multilayers, where pertinent experiments are lacking. This paper proposes a model to simulate the self-assembly of multi-layers of molecules via electric dipole interaction [2]. Electrostatic interactions have been utilized to construct functional multilayer systems by the approach of electrostatic self-assembly (ESA) [23-25]. ESA processing involves dipping a chosen substrate into alternate aqueous solutions containing anionic and cationic molecules or nanoparticles. This leads to alternating layers of polyanion and polycation monolayers. Design of the precursor molecules and control of the sequence of the multiple molecular layers allow control over macroscopic electrical, optical, mechanical and other properties. While applications such as nano-filtration and photovoltaic devices have been demonstrated, the ESA process is generally limited to simple, laminar multilayer systems, with little or no lateral variation in the layer. We will show that for molecules carrying electric dipoles, dipole interaction can induce self-assembled patterns within each layer in a multilayer system. The capability is desirable for making complex structures, especially the formation of nanointerfaces and three dimensional nanocomposites

We consider dipole interaction between molecules within each layer, interaction between layers and the effects of dielectric substrates and embedded electrodes [2]. A phase field model is developed to simulate the molecular motion and patterning under the combined actions of dipole moments, intermolecular forces, entropy, and external electric field. The guiding effect of the underlying layers and the voltage pattern are of particular interest. Taking a two layer system as an example, we consider three situations. 1) No applied electrical field. 2) An applied electric field to guide the first layer. 3) An applied electric field to guide both layers. The study reveals self-alignment, pattern conformation and the possibility to reduce the domain sizes via a layer by layer approach. It is also shown that the pattern in a layer may define the roadway for molecules to travel on top it. This combined with electrodes embedded in the substrate provides a novel concept to construct molecular vehicles for various applications.

References

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