DYNAMICS OF SELF-ASSEMBLY ON SOLID SURFACES

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Advancing technologies demand solid structures of ever-decreasing length scales. During fabrication and use of these structures, atoms are mobile by diffusion or other mass transport processes. The structures may change configurations over time. Experimental evidence has accumulated in recent years that nanoscale structures can self-assemble, leading to ordered nanophase patterns in monolayers, thin films, and bulk materials. Self-assembly is a potential low-cost and high-throughput approach for nanofabrication. The following shows a few examples of self-assembled systems. 1) A binary epilayer on a substrate may separate into two phases and spontaneously organize into ordered triangular lattice of dots or stripes depending on the average concentration. The feature size is on the order of 1-100nm and stable against annealing. 2) 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. 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. 3) Subjected to continual irradiation of neutrons or heavy particles at elevated temperatures, vacancies emerge in molybdenum and agglomerate into voids. These voids form a three dimensional b.c.c lattice structure, replicating the crystal lattice of the host material. The axes of the void superlattice are parallel to those of the host crystal. 4) Polymer thin films have been demonstrated to form ordered structures via applied electric field. In the process, a polymer thin film was first spin-coated on a substrate. The film was then heated to gain enough mobility. An electric field was applied to the polymer melt, which destabilized the flat polymer-air interface and led to the formation of uniform pillars emerging out of the film.

In a structure, collective actions of photons, electrons and ions contribute to the free energy. When the configuration of the structure changes, the free energy also changes. This free energy change defines a thermodynamic force which, in its turn, motivates the configuration change of the structure. The effects of such forces may be negligible in macrostructures, but significant in nanostructures. Insight into these forces becomes increasingly valuable as the structures of technological interest miniaturize. This talk presents some of our recent work on self-organized nanostructures and guided self-assembly [1,2], including self-organized nanophase patterns on solid surfaces, guided assembly by surface chemistry and strain field, organized nanovoids and nanobubbles in a solid, patterning multilayer of molecules via dipole interaction, electric field-induced ordered polymer nanostructures, and tuning nanoparticles in nanocomposites. We have developed a thermodynamic framework to study the remarkable phenomena. Large-scale simulations have been developed to simulate the process of formation and evolution of nanostructures. The simulations reveal remarkably rich dynamics and suggest a significant degree of experimental control in growing ordered nanoscale structures.

References

[1] W. Lu and D. Salac, "Patterning multilayers of molecules via self-organization,"*Phys. Rev. Lett.* **94** Art. No. 146103, 2005.
[2] D. Kim and W. Lu, "Three-dimensional model of electrostatically induced pattern formation in thin polymer films," *Phys. Re. B* **73**, Art. No. 035206, 2006.

Keywords: self-assembly, nanostructures, evolution.