DYNAMIC NANOSTRUCTURE FORMATION IN THIN FILMS INDUCED BY ELECTROSTATIC FIELD

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Controlled formation of nanostructures in thin films has significant applications. Emerging technologies in polymer based semiconductors and functional devices, such as polymer light-emitting diodes (LEDs), printed integrated circuits, and inexpensive solar cells, rely on features of increasingly smaller dimensions. Recent experiments show that an electric field may induce self-organized morphological patterns, suggesting a potential low cost and high throughput approach for nanofabrication [1, 2]. 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 addition to the technical importance, the discoveries pose interesting scientific problems. The major issues are the mechanism by which an interface loses its stability, and how the instability leads to the final pattern of quite uniform pillars. This paper aims to address these questions and reveal the dynamic self-organization process. A three dimensional simulation is made viable via a phase field model and an efficient numerical approach.

The behavior can be explained in terms of two competing actions: surface energy and electrostatic energy. While stability analysis provides valuable insight into the early stage evolution, it is still not clear how the instability leads to the final pattern. This would require a reliable and accurate explanation of the thin film behavior in the nonlinear evolution regime. For a thin film, the self-assembly process is significantly affected by the substrate. The fast growth wavelength obtained from small perturbation analysis may not have sufficient time to develop before it meets the substrate, and thus has no direct connection to the size of the late structure. The lack of a kinetic route may essentially prevent the coarsening of pillars when the film breaks. This paper proposes a three dimensional dynamic model to reveal the detailed picture. We consider energetic components involving the interface energy and dielectric effect, and kinetics of coupled viscous flow and diffusion. Semi-implicit Fourier spectral method and preconditioned biconjugate-gradient method are applied to achieve high efficiency and numerical stability. The simulations reveal the dynamic evolution process in the nonlinear regime. The length scale is not solely determined by energy minimization, but by an interplay between the energetics and kinetics. The film thickness significantly influences the growth rate and the distance between pillars. A thinner film evolves slower due the substrate constraint. The simulations have shown that a thicker film leads to a denser pillar arrays, and the cylindrical pillars may transform into stripes after they bridge the two electrodes. This demonstrates an approach of morphology control via kinetic constraints. With patterned electrodes, we have obtained parallel stripes replicating the electrode pattern. These simulations suggest a significant degree of experimental control in directing thin film morphologies.

References

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