Modeling Directed Self-Assembly of Block Copolymers for Lithographic Applications

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Abstract

Nano patterning for chip manufacturing has reached its limitation with 193i lithography standard process. Directed Self Assembly (DSA) of Block Co-Polymers (BCP) is envisaged as an alternative complementary technique that can reduce critical dimension and pitch with high throughput and limited cost [1]. For contact layers that require patterning of cylinders with diameter of tens nanometers, DSA with grapho-epitaxy is a good candidate for future nodes. However at these dimensions, metrology is pushed to its limitations, especially for acquiring 3D information. Complementary 3D simulations are necessary to complete the experimental data, and fully understand the physics underneath the process.

Several models are used to simulate DSA. Atomistic and coarse grained [2] models use first principles and directly compute positions of each particle into the simulation domain. Although interesting to observe interactions at the interfaces and recombination of polymers, these techniques are too computationally expensive to address systematic simulations on domain size of typically hundreds nanometers for DSA lithography. Phase field models on the other side allow simulating bigger domains by only accounting for the local concentration in each point. The Cahn-Hilliard equation implemented in COMSOL Multiphysics® software using the Phase Field physics interface is describing the phase separation of a binary mixture through a diffusion equation. Following Ohta and Kawasaki [3], we modified this equation to account for long range interactions. Equations have been modified directly into the weak formulation accessible in COMSOL. It also has been found that affinity of cavity's wall can be controlled via the wetting angle parameter.

The first 2D simulations showed really good agreement between the theoretical model and morphologies observed on silicium samples. Fig1 presents the simulation results on unpatterned surfaces compared to images obtained with Scanning Electron Microscope (SEM). We retrieve with this simulation the parameters needed in equations to match the natural properties of BCP used in the experimental procedure. We then realized 3D simulations in elliptical guides (Fig2).

The boundary conditions have been set according to the know nature of chemical interactions between BCP and surfaces. Again the model showed really good result, despite some discrepancy due to the unperfect geometries in experimental data.

These first results allow us to now use the model to determine the most suitable structures for DSA lithography, by observing the impact of different geometry parameters and wall affinities.

Reference

[1] R. Tiron et al., The potential of block copolymer's directed self-assembly for contact hole shrink and contact multiplication, Proceedings of SPIE, 8680 (2013).

[2] T. Nakano et al., Dissipative particle dynamics study on directed self-assembly in holes, Proceedings of SPIE, 8680 (2013).

[3] T. Ohta and K. Kawasaki, Equilibrium morphology of block copolymer melts, Macromolecules, 19, 2621–2632 (1986).

Figures used in the abstract

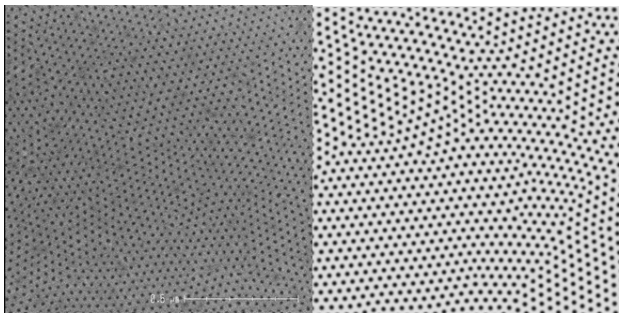

Figure 1: 2D cylindrical morphology in thin film. left: experimental (SEM image), right: simulation obtained with COMSOL

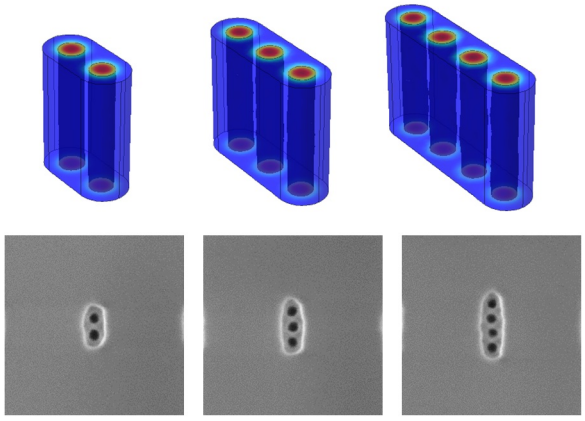

Figure 2: 3D morphologies in cavities. top: simulation in COMSOL, bottom: SEM images (cavities obtained by electron-beam lithography)

Figure 3

Figure 4