Self-Consistent Field Theory of Directed Self-Assembly on CH Pitch Division

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1. Introduction

The semiconductor industry has been developing technologies and has extended Moore's Law over 40 years [1]. According to Rayleigh's equation, shorter exposure wavelength and higher numerical aperture caused the higher resolution of lithography process [2]. When the exposure wavelength reached 193nm and the NA went up to 1.35 with water immersion ArF lithography, the improvement of exposure wavelength and NA came to a temporary standstill. Further improvement of resolution was achieved with double patterning techniques, e.g. Self Aligned Double Patterning [3] for 3x nm and 2x nm. Further size reduction requires triple or quadruple patterning, and it causes huge increase of CoO and the difficulty of overlay [4].

Extreme ultraviolet (EUV) lithography has been the favorite candidate of successor of immersion ArF [5]. Except EUV lithography, other lithography candidates, i.e., multi patterning, nanoimprint, mask less lithography, and DSA are also investigated. DSA appeared at ITRS road map in 2007 as lithography technology candidate [6]. A lot of work has been reported about DSA materials as sub-20nm or even sub-10nm patterning materials. DSA is expected not only as the resist materials but also as the resist support material [7].

Not only experimental approach but also computer simulation has been employed for the DSA development because micro phase separation of diblock copolymer can be predicted by DPD (Dissipative Particle Dynamics) and SCFT (Self Consistent Field Theory) simulations. Then several theoretical and computational studies have been investigated for block copolymer films forming lamellae, cylinders and contact holes [8]. For the

development of hole shrink by DSA, the choice of guide pattern is very important [7,8], namely, guide pattern CDX/CDY/film thickness size, surface condition of side wall and substrate. In this paper, we also report SCFT calculations of the stability of various hole shrink condition for DSA patterning.

2. Self-Consistent Field Theory Simulation

CH pitch division simulations are conducted using SCFT simulation code developed by the Fredrickson research group at University of California, Santa Barbara. It has been applied for many kinds of DSA simulations, such as line and space pitch division, contact hole shrink, and chemoepitaxy.

We will consider the AB diblock copolymers composed of N monomers with a fraction f of monomers of type B. The interaction between monomers of different types is described using a Flory parameter χ . To relate our simulations to experiments with poly(styrene-*b*-methylmethacrylate) (PS-*b*-PMMA) diblock copolymers, the A block denotes polystyrene and the B block refers to polymethylmethacrylate. We assume $f = 0.3$ and a segregation strength $\chi N = 25$, corresponding to experimentally relevant PS-*b*-PMMA molecular weights 55-22 K g/mol.

The oval prepattern with minor radius L_x , major radius L_y and thickness L_z is considered. SCFT simulations have been done with minor radius $7R_g$ and $11R_g$, major radius $14R_g$, $22R_g$ and $28R_g$, and thickness $2R_g$, $4R_g$ and $6R_g$. The wetting conditions at the sidewall are assumed to be neutral for the A block ($\chi_w N_A = 0$) and attractive for the B block

($\chi_w N_B = -25$). The interaction between substrate and the B block changes from neutral to attractive while the A block is neutral to substrate. The surface of block copolymers is in contact with air, assumed neutral to both blocks.

3. Results and Discussions

The characteristic length L_0 of diblock copolymers with $f = 0.3$ is the distance between cylinders in a hexagonal closed-pack phase. In order to estimate L_0 of BCPs used in the SCFT simulations, we have done bulk simulations. Figure 1 shows two-dimensional PMMA density profiles for various lengths $2L$ of rectangular cross section perpendicular to cylinders. Figure 2 shows the intensive Hamiltonian (open circle) against $2L$ and the best fit (line) by a quadratic function. This gives $L_0 = 4.46R_g$.

Fig. 1 Two-dimensional PMMA density profiles of a hexagonal closed-pack phase. For each density profile, the top panel represents a cross section in the xy plane at the middle of z -direction and the bottom panel is a cross section in yz plane at the middle of x -direction.

Fig. 2 The intensive Hamiltonian obtained by SCFT simulation (open circle) and the best fit (line) by a quadratic function.

We have done CH pitch division simulations with different prepattern thickness L_z . First $L_z = 2R_g$ where $L_z < L_0$, second $L_z = 4R_g$ where $L_z \sim L_0$, and finally $L_z = 6R_g$, where $L_z > L_0$ and L_z is not commensurate with L_0 . In order to examine structural change by L_x , L_y , and L_z , we will consider simple case with neutral substrate to both blocks.

Two-dimensional PMMA density profiles for various L_x and L_y with $L_z = 2R_g$ is shown in Fig.3. Perpendicular cylinders are stable in this case since the system is nearly two-dimensional. The first rows represent morphologies with $L_x = 7R_g$, where liner rows of cylinders align along major radius. The number of cylinders increases from two to four by increasing L_y from $14R_g$ to $28R_g$. The second rows represent morphologies for wider ovals with $L_x = 11R_g$, where additional rows of cylinders are packed in a staggered hexagonal arrangement. The perfect HCP structure which is favorable to diblock copolymers with $f = 0.3$ could not be taken due to PMMA attractive walls.

Fig. 3 Two-dimensional PMMA density profiles for various L_x and L_y with $L_z = 2R_g$. Dimensions of L_x and L_y are A : $L_x = 7R_g$, $L_y = 14R_g$, B : $L_x = 7R_g$, $L_y = 22R_g$, C : $L_x = 7R_g$, $L_y = 28R_g$, D : $L_x = 11R_g$, $L_y = 14R_g$, E : $L_x = 11R_g$, $L_y = 22R_g$, F : $L_x = 11R_g$, $L_y = 28R_g$.

Fig. 4 Two-dimensional PMMA density profiles for various L_x and L_y with $L_z = 4R_g$. Dimensions of L_x and L_y are the same as those of Fig. 3.

Figure 4 shows two-dimensional PMMA density profile for various L_x and L_y with $L_z = 4R_g$. PMMA does not exist in the cross sectional image in the middle of film thickness because perpendicular cylinders are not stable in this case. Three-dimensional illustration of the PMMA density profiles for $L_x = 7R_g$, $L_y = 22R_g$ and $L_z = 4R_g$ is shown in Fig.5 (a). There are parallel cylinders of PMMA at the surface and interface with substrate. Since L_z is commensurate with L_0 , parallel cylinders are more stable than

perpendicular cylinders. Three-dimensional image of wider oval for $L_x = 11R_g$, $L_y = 22R_g$ and $L_z = 4R_g$ is shown in Fig.5 (b). There are rings of PMMA at the surface and interface with substrate in this case, and PMMA is not seen in the middle of film thickness.

Fig. 5 Three-dimensional illustration of PMMA density profiles for (a) $L_x = 7R_g$, $L_y = 22R_g$ and $L_z = 4R_g$, (b) $L_x = 11R_g$, $L_y = 22R_g$ and $L_z = 4R_g$.

Figure 6 shows two-dimensional PMMA density profile for various L_x and L_y with $L_z = 6R_g$. Perpendicular cylinders are stable in this case. The structural change by L_x and L_y is similar to that of $L_z = 2R_g$. Since L_z is not commensurate with L_0 , perpendicular cylinders become stable again. Thus we can conclude that perpendicular cylinders are favored when L_z is not commensurate with L_0 .

Fig. 6 Two-dimensional PMMA density profiles for various L_x and L_y with $L_z = 6R_g$. Dimensions of L_x and L_y are the same as those of Fig. 3.

We have swept the interaction between PMMA and substrate from neutral to attractive, while PS is neutral to substrate. Figure 7 shows two-dimensional PMMA density profiles for $L_x =$

$7R_g$, $L_y = 22R_g$ and $L_z = 6R_g$. While attractive interactions are weak perpendicular cylinders penetrate completely through the film, a transition to cylinders that terminate in nearly spherical caps occurs with increasing interaction. The same transition is also observed with wider ovals for $L_x = 11R_g$, $L_y = 22R_g$ and $L_z = 6R_g$, shown in Fig. 8. Thus a neutral substrate would be favorable in order to get cylinders that penetrate completely through the film.

Fig. 7 Two-dimensional PMMA density profiles for $L_x = 7R_g$, $L_y = 22R_g$ and $L_z = 6R_g$ sweeping from neutral to PMMA attractive substrates.

Fig. 8 Two-dimensional PMMA density profiles for $L_x = 11R_g$, $L_y = 22R_g$ and $L_z = 6R_g$ sweeping from neutral to PMMA attractive substrates.

4. Conclusions

We have done SCFT simulations to investigate the directed self-assembly on CH pitch division. The structural change by the thickness L_z of oval prepattern reveals that perpendicular cylinders are favored when L_z is not commensurate with the distance between cylinders L_0 . In this case linear rows of cylinders are along major radius for narrow ovals, and wider ovals tend to pack additional rows of cylinders in a staggered hexagonal arrangement. Sweeping from neutral to PMMA attractive substrates causes a transition from cylinders that penetrate completely through

the film, to cylinders that terminate in nearly spherical caps. Thus a neutral substrate would be favorable in order to get cylinders that penetrate completely through the film.

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