Electronic Supplementary Information

Hierarchical Nanostructures of Diblock Copolymer Thin Films Directed by a Saw-Toothed Substrate

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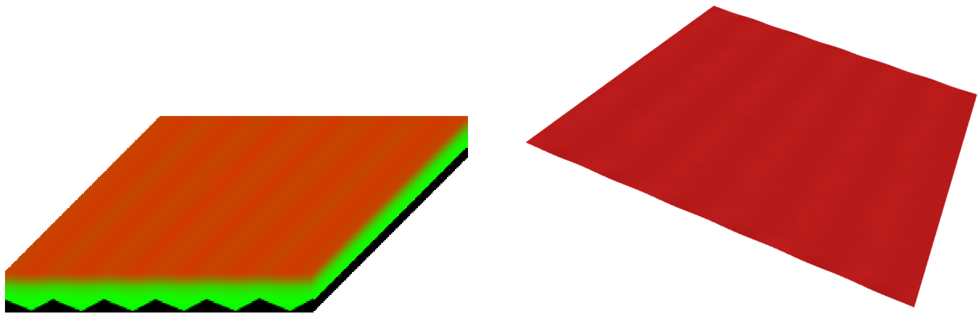
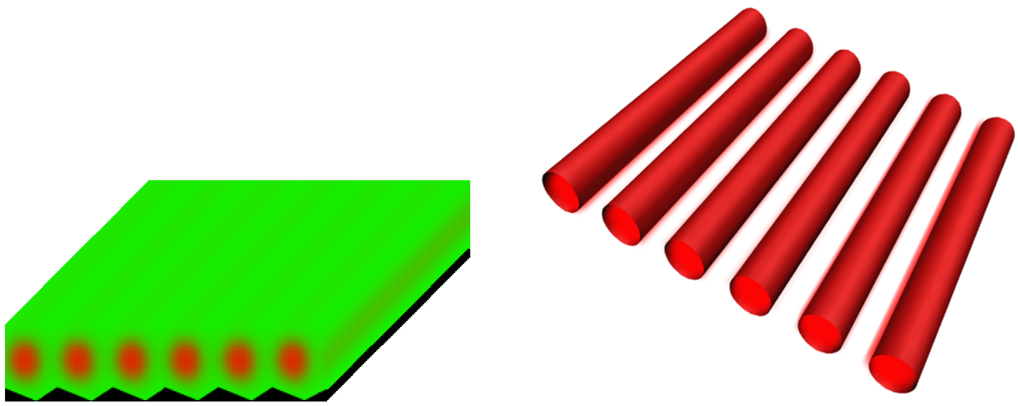
Since these two morphologies only form if there is a repulsive force between A-block and the substrate, otherwise, they do not, thus we have not put them into the Figure 2.



(a)



(b)

Figure S1. The specific structures of $L_{//}$ and $C^{az}_{//}$ formed by AB diblock copolymer thin films confined on the saw-toothed substrate. The 3D isosurface graphs are also given for a clear view beside the morphologies. The red color in isosurface graphs is assigned to A-block for a good correspondence. The black color shows the substrate. (a) $L_{//}$, (b) $C^{az}_{//}$.

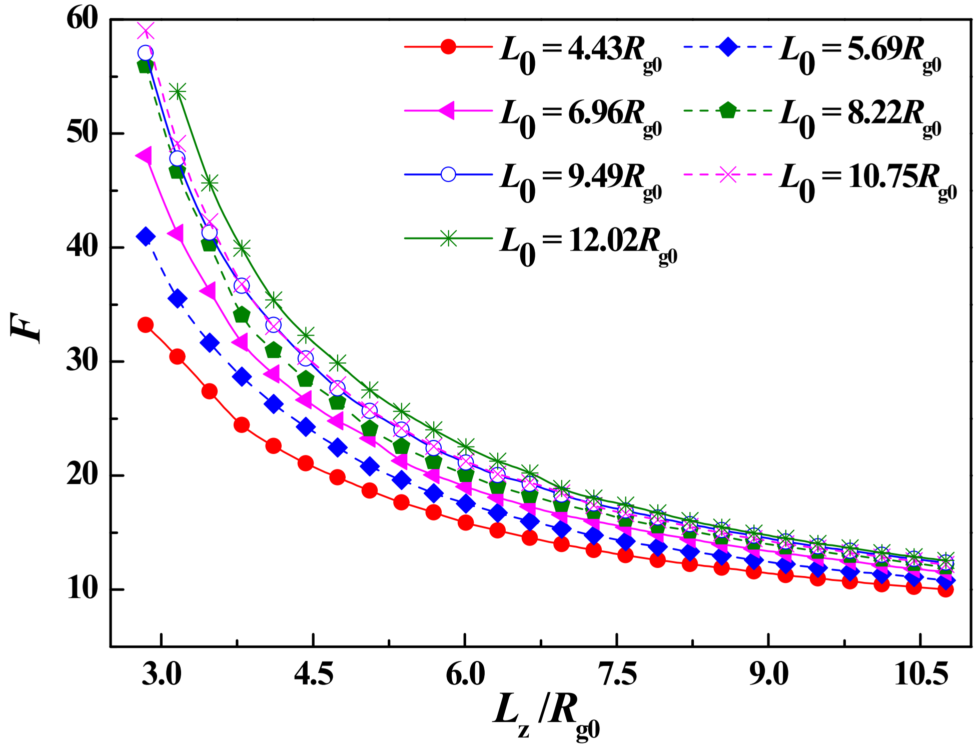
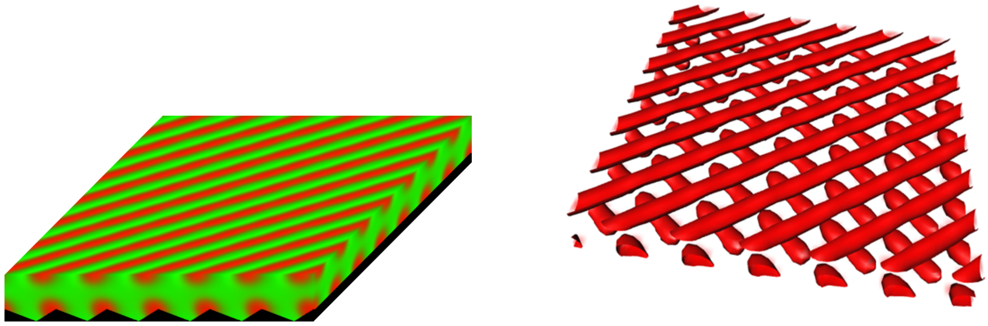
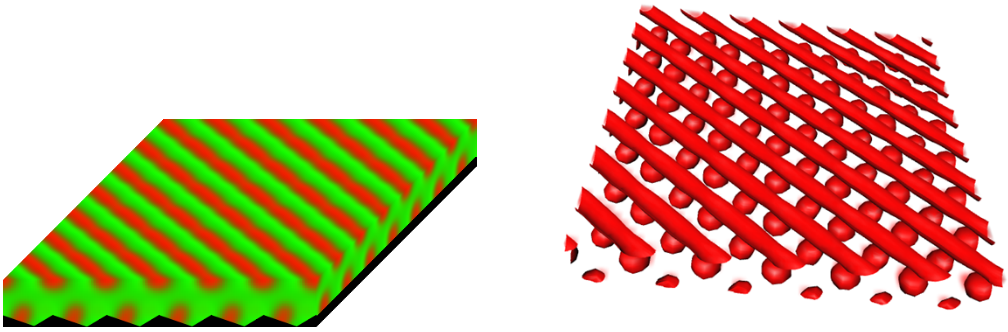


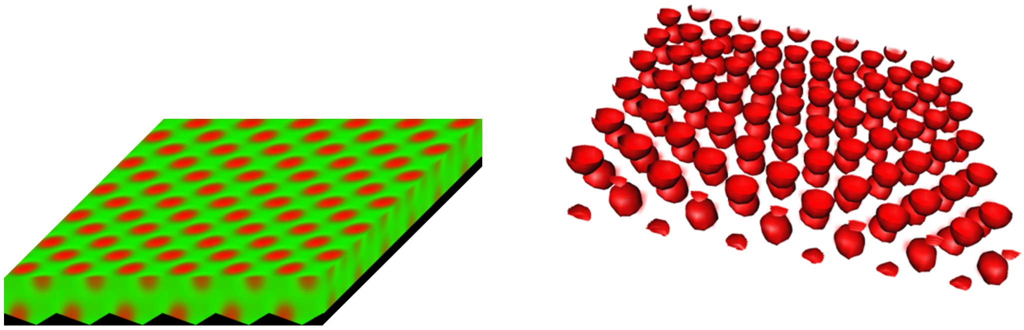
Figure S2. Plot of total free energy as a function of AB diblock copolymer thin film thickness with $f_A = 0.30$, $N = 60$, $\chi N = 15$, $\theta_1 = 17.6\,^{\circ}$, $\theta_2 = 32.4\,^{\circ}$, $H_{AS} = 0.0$, $H_{BS} = 0.0$, $L_0 = 3.80R_{g0} \sim 12.02R_{g0}$, $L_z = 2.85R_{g0} \sim 10.75R_{g0}$.



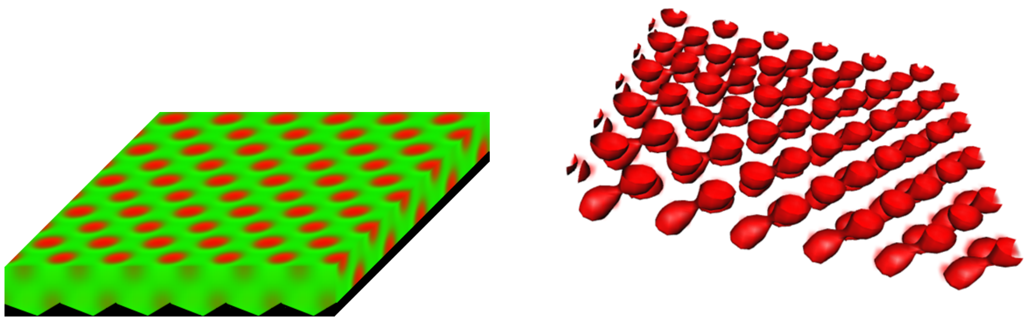
(a) CM_2



(b) CM_3



(c) CM_4



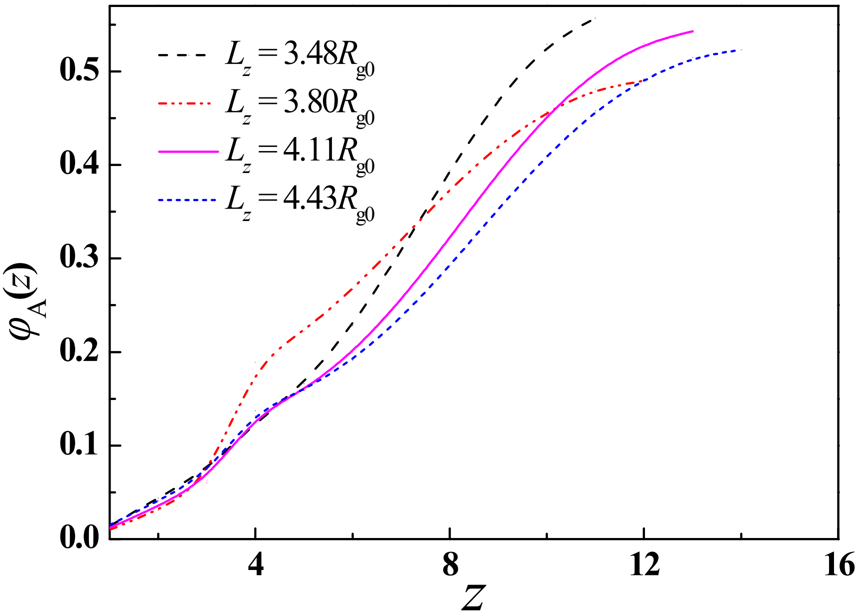
(d) CM_5

Figure S3. Some complicated structures formed by AB diblock copolymer thin films confined on the saw-toothed substrate. The isosurfaces of A-block (f_A = 0.30) are plotted in red color, and otherwise, the isofurfaces of B-block are plotted in green color (not shown here).

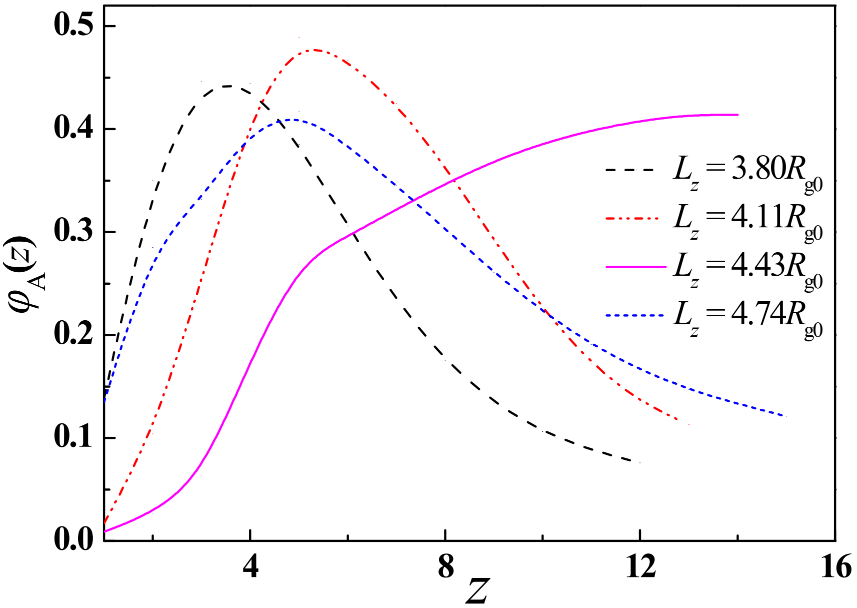
We can obtain the density profile of block copolymer along z-direction by Eq. (S1) as below:

$$\varphi_i(z) = \iint \phi_i(x, y, z)\mathrm{d}x\mathrm{d}y \,/ \iint \mathrm{d}x\mathrm{d}y \tag{S1}$$

where i belongs to A-block and B-block.

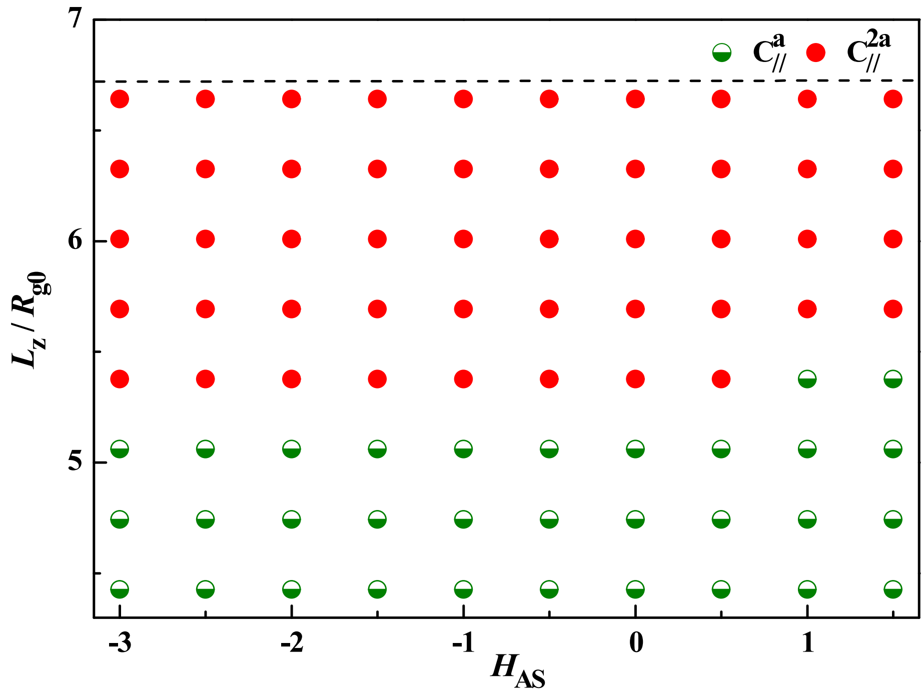


(a)

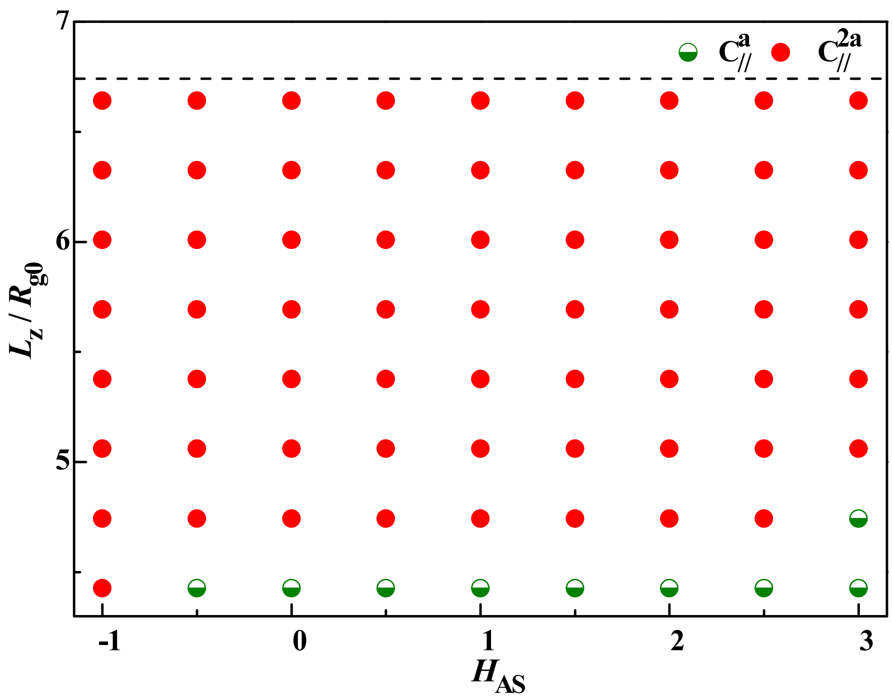


(b)

Figure S4. Density distribution of A-block along z-axis direction with $f_A = 0.30$, $N = 60$, $\chi N = 15$, $\theta_1 = 17.6\,^\circ$, $\theta_2 = 32.4\,^\circ$, $H_{AS} = 0.0$, $H_{BS} = 0.0$. (a) $L_0 = 5.69R_{g0}$, $L_z = 3.48R_{g0} \sim 4.43R_{g0}$, (b) $L_0 = 6.33R_{g0}$, $L_z = 3.80R_{g0} \sim 4.74R_{g0}$.

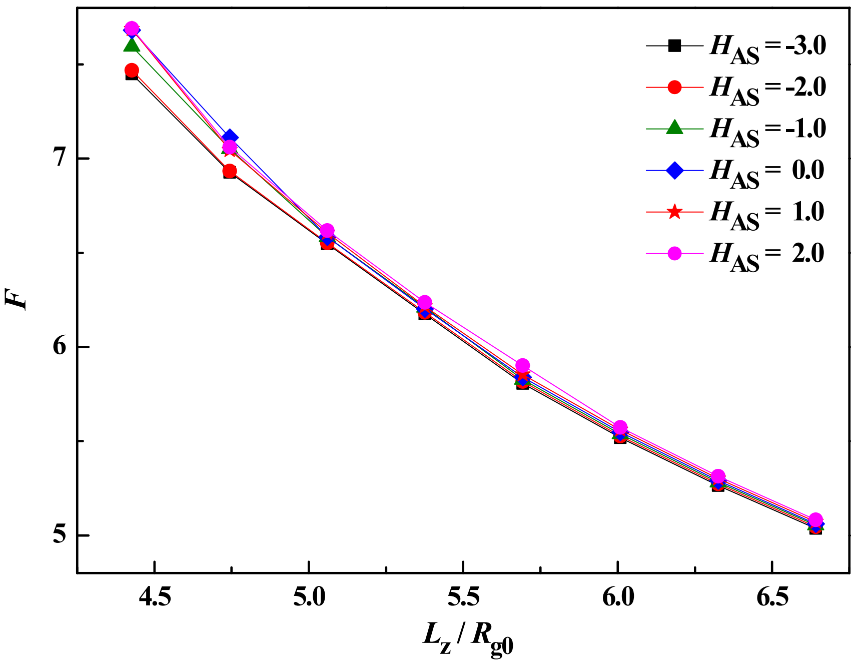


(a)

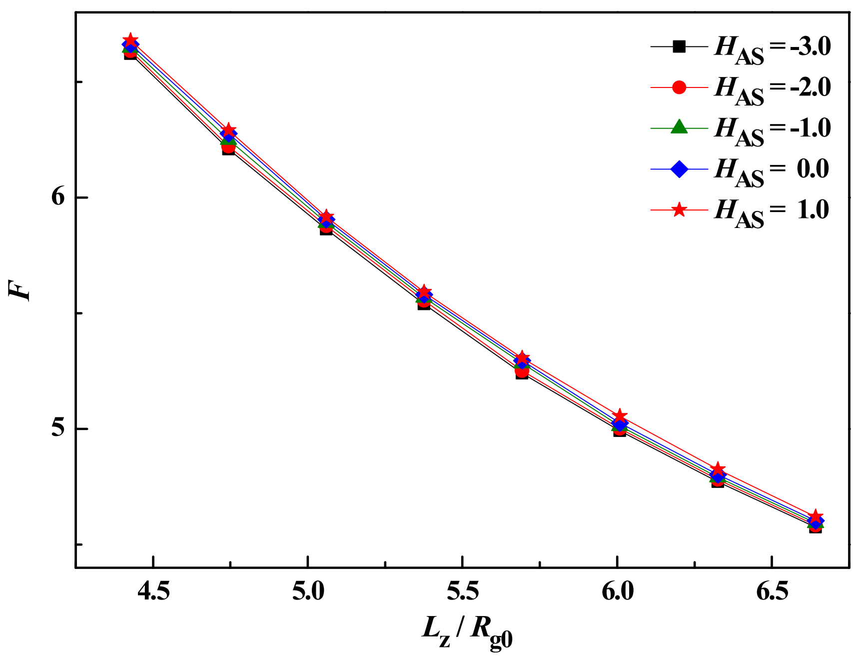


(b)

Figure S5. Morphological phase diagram in the plane L_z vs H_{AS} for AB diblock copolymer with f_A = 0.30, N = 60, χN = 15, θ_1 = 17.6 °, θ_2 = 32.4 °, H_{BS} = 0.0, L_z = 4.43R_{g0} ~ 6.64R_{g0}. The symbols indicated distinct structures in this study have been marked in the picture, respectively. (a) L_0 = 6.96R_{g0}, H_{AS} = -3.0 ~ 1.5, (b) L_0 = 10.12R_{g0}, H_{AS} = -1.0 ~ 3.0.



(a)



(b)

Figure S6. Plot of total free energy as a function of AB diblock copolymer thin film thickness with $f_A = 0.30$, $N = 60$, $\chi N = 15$, $\theta_1 = 17.6^\circ$, $\theta_2 = 32.4^\circ$, $H_{BS} = 0.0$, $L_z = 4.43R_{g0} \sim 6.64R_{g0}$. (a) $L_0 = 5.69R_{g0}$, $H_{AS} = -3.0 \sim 2.5$, (b) $L_0 = 4.43R_{g0}$, $H_{AS} = -3.0 \sim 1.5$.

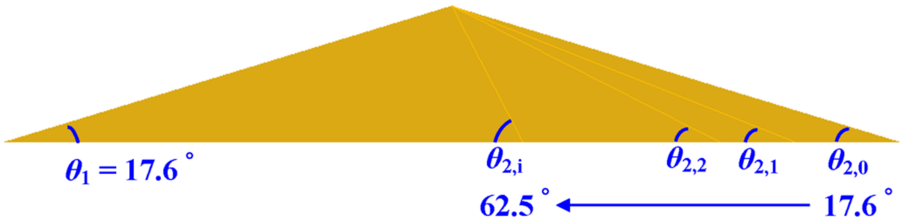


Figure S7. The schematic cross section of the saw-toothed substrate with only one lateral periodicity: one of the tilt angles $\theta_1 = 17.6\,^\circ$, and another θ_2 varies from $17.6\,^\circ$ to $62.5\,^\circ$.

Table S1. Summary the value of Δ corresponding diblock copolymer thin film thickness with varied substrate lateral periodicities L_0, fixed substrate tilt angles $\theta_1 = 17.6\,^\circ$, $\theta_2 = 32.4\,^\circ$.

$\boldsymbol{L_0}$ | L_0/R_{g0}	**Δ** | Δ/R_{g0}	$\boldsymbol{L_0}$ | L_0/R_{g0}	**Δ** | Δ/R_{g0}
12 | *3.80*	**2.538** | *0.80*	**26** | *8.22*	**5.499** | *1.74*
14 | *4.43*	**2.961** | *0.94*	**28** | *8.86*	**5.922** | *1.87*
16 | *5.06*	**3.384** | *1.07*	**30** | *9.49*	**6.345** | *2.01*
18 | *5.69*	**3.807** | *1.20*	**32** | *10.12*	**6.768** | *2.14*
20 | *6.33*	**4.230** | *1.34*	**34** | *10.75*	**7.191** | *2.27*
22 | *6.96*	**4.653** | *1.47*	**36** | *11.39*	**7.614** | *2.41*
24 | *7.59*	**5.076** | *1.61*	**38** | *12.02*	**8.037** | *2.54*

Table S2. Summary the value of Δ corresponding diblock copolymer thin film thickness with varied substrate tilt angle θ_2, fixed substrate lateral periodicity $L_0 = 18$ and tilt angle $\theta_1 = 17.6\,^\circ$.

$\boldsymbol{\theta_2}$ **(°)**	**Δ** | Δ/R_{g0}	$\boldsymbol{\theta_2}$ **(°)**	**Δ** | Δ/R_{g0}
17.6	**2.855** | *0.90*	**43.0**	**4.261** | *1.35*
21.8	**3.184** | *1.01*	**48.3**	**4.451** | *1.41*
27.1	**3.524** | *1.11*	**53.6**	**4.628** | *1.46*
32.4	**3.807** | *1.20*	**58.9**	**4.793** | *1.52*
37.7	**4.048** | *1.28*	**62.5**	**4.912** | *1.55*

The value of the Δ is calculated by $\Delta = \tan(\theta_1)\tan(\theta_2) / [\tan(\theta_1) + \tan(\theta_2)]\, L_0$.