Supporting information for:

Pattern Placement Accuracy in Block Copolymer Directed Self-Assembly Based on Chemical Epitaxy

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For the extension of the free energy model to account for interfacial tilt angle, the tilt angle is uniform throughout the film thickness. The domain cross sectional area was fixed as the film thickness (h) times one half the natural period (L_o), and no curvature of the interfaces between domains or complex domain deformation was allowed. The left and right PS-PMMA interfaces were allowed to tilt independently. Figure S1 depicts a schematic cross-sectional view of the deformations allowed in the "tilted" geometry.

The combination of displacement (Δ) and interfacial tilt angles (θ) that minimize system free energy were determined. The tilt angles are plotted as a function of pinning stripe width in Figure S2. In all cases, the maximum observed tilt is 7.1 degrees from vertical. This value arises from the competition between increased PMMA-HSQ contact (favorable), increased PS-PMMA interfacial area (unfavorable), and additional chain stretching/compression (unfavorable), all of which increase with increasing tilt angle.

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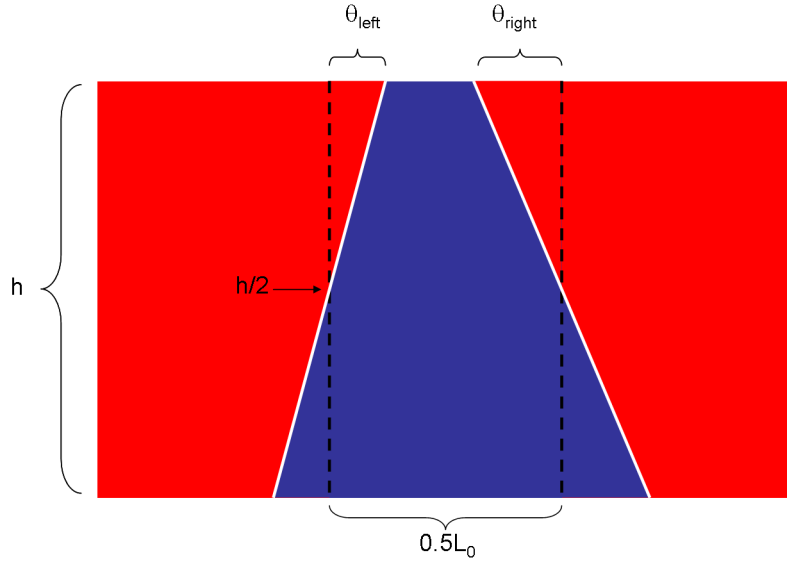
Figure S1: Schematic of the deformations allowed by the "tilted" geometry of a PMMA domain (blue) and its two flanking PS domains (red).
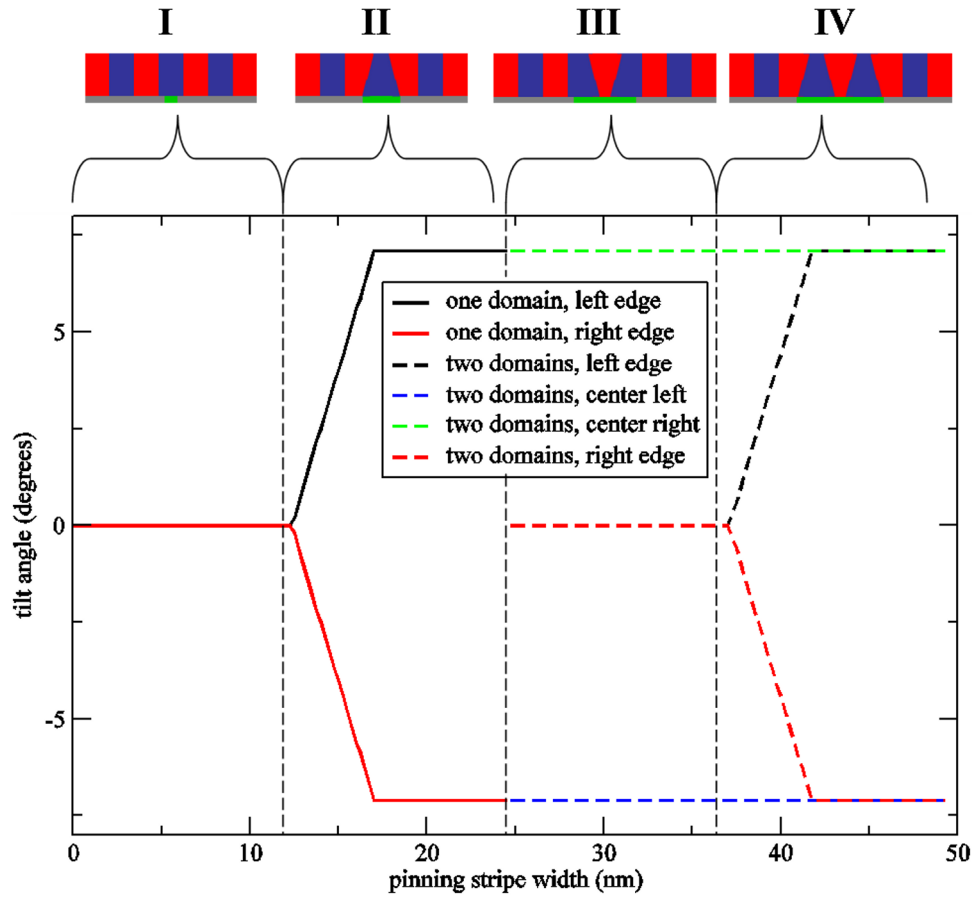

Figure S2: Interfacial tilt angle versus pinning stripe width.

In the application of the model, four different tilt geometry regimes were observed regarding the width of the pinning stripe (w) with respect to L_o:

I For $w \leq 0.5L_o$, a single PMMA domain sits above the pinning line and is not tilted.

II For $0.5L_o < w < L_o$, the two interfaces of the single PMMA domain tilt to increase the area of contact between the bottom of the PMMA domain and the pinning stripe.

III As the stripe width increases to $L_o < w \leq 1.5L_o$, there are now two PMMA domains above the pinning line. The outer interfaces of each domain remain perpendicular to the substrate, while the inner interfaces tilt to maximize PMMA and minimize PS area at the surface.

IV For widths $1.5L_o < w$, both the inner and outer interfaces of each domain tilt to maximize the PMMA surface area above the pinning line.

Schematic depictions of these tilt geometry regimes are included at the top of Figure S2.