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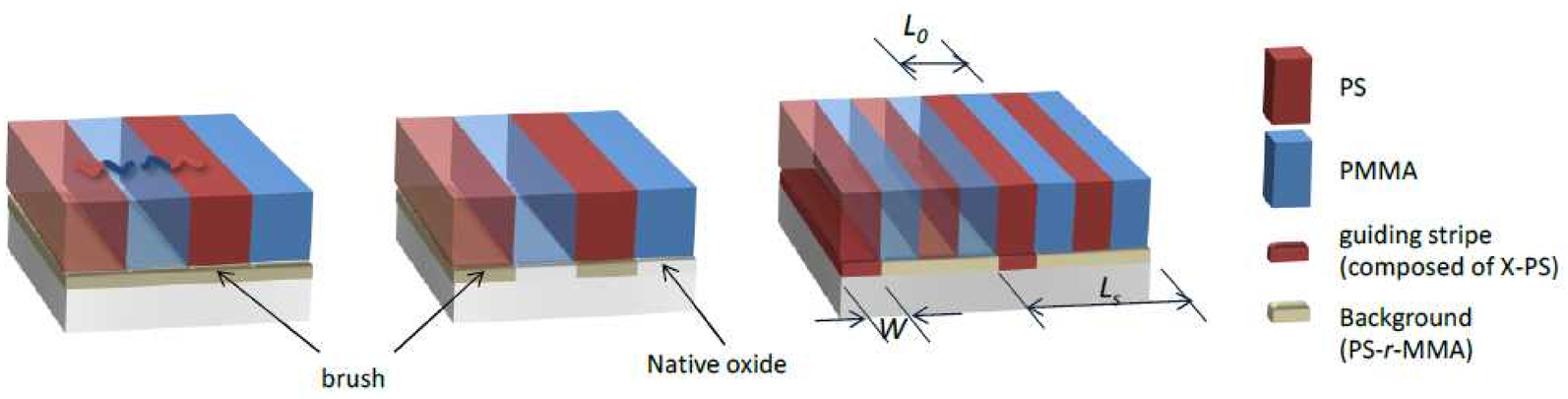
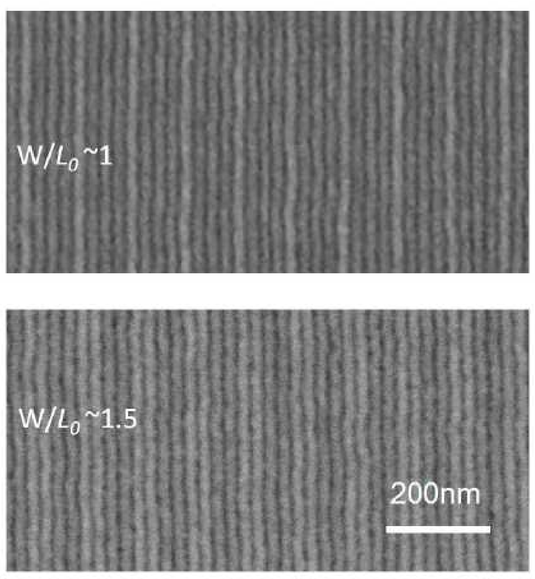
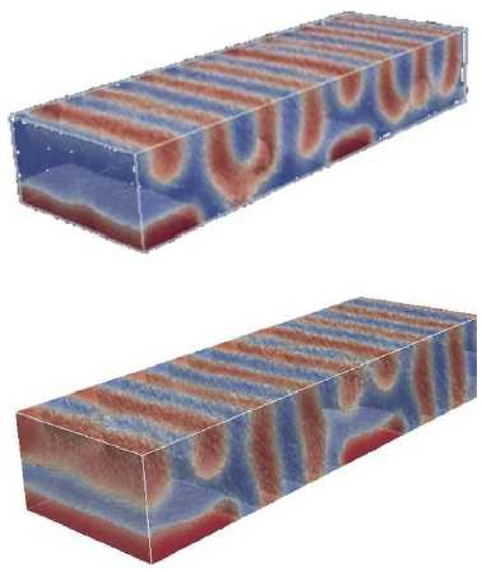
Directed self-assembly (DSA) of block copolymers (BCP) is a thermodynamic equilibration process of the entire BCP film system, including the top surface of the film and the interface of the BCP with the underlying, patterned substrate. In order to study the optimum patterned substrate conditions for DSA with density multiplication, we analyzed the effect of the chemistry of the chemical pattern and the density multiplication factor on assembly quality. Free energy calculations were also performed on jog defects.



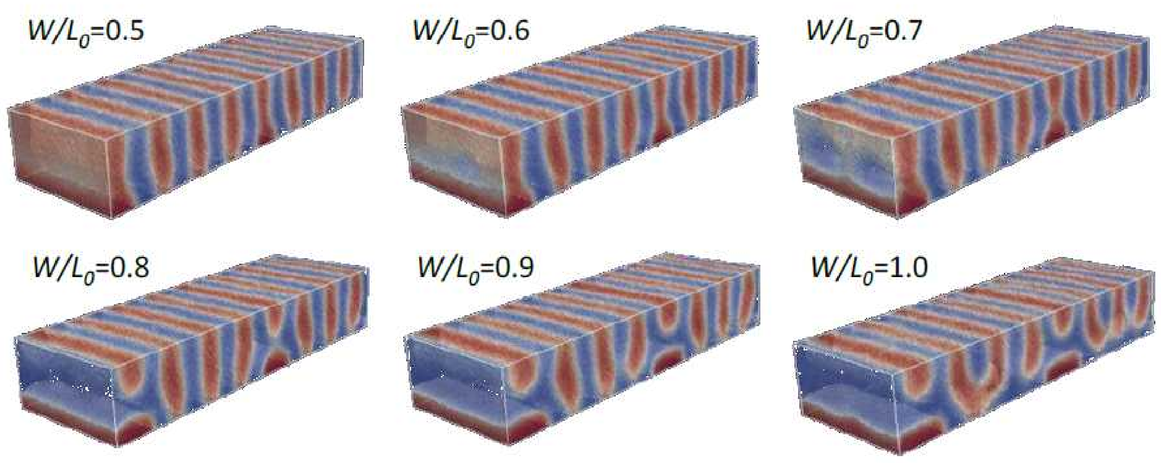
-An illustration of DSA on a homogeneous, chemically patterned surface, and density multiplication





-A side by side comparison of simulations and SEM images of poly(polystyrene-b-methyl methacrylate) for 4x density multiplication (L_s/L_0=4).

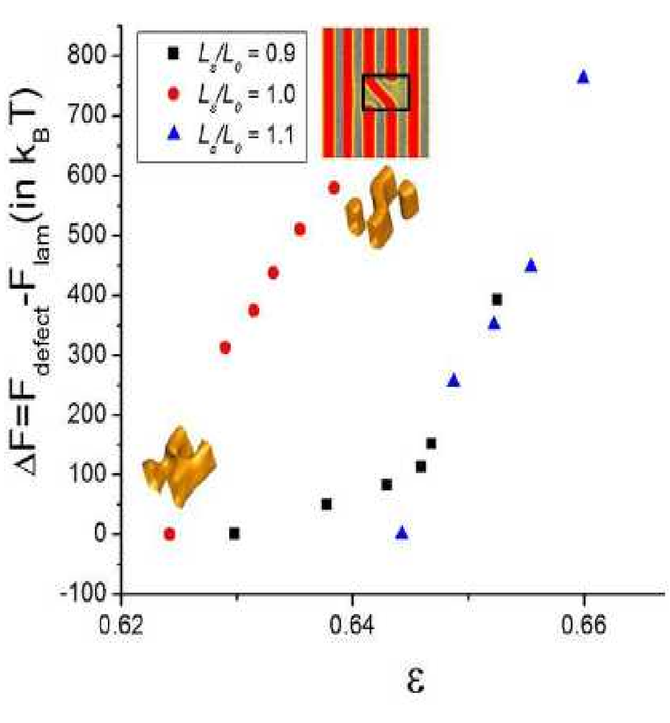
-The brighter lines show the “hovering” lines while the darker lines show lamella going through the entire thin film. Results are shown for two values of the width of the stripe(W).



-Simulations for 4x density multiplication when varying the value of W.

-As W increases “hovering” lines appear.

-The simulations have a constant value of the strength of chemical patterns ($\Lambda^A N$=2.0 and $\Lambda^B N$=0.15)



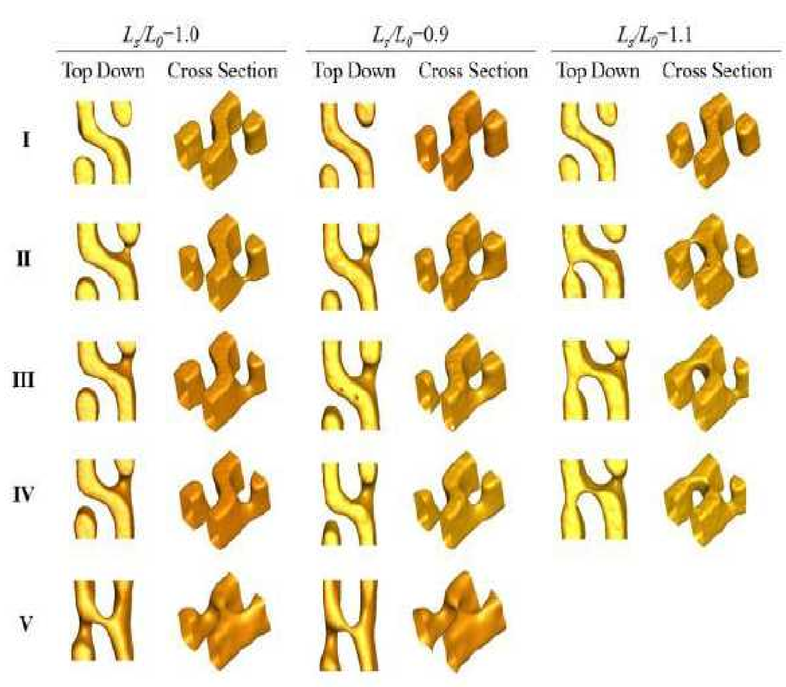
-An analysis of the partial defects at different annealing times. Stretched, regular, and compressed lamellae are also shown.

-Case I to Case IV for L_s/L_0 =1: the probability of increases from 10^{-237} to 10^{-120} , which shows that the likelihood of forming a defect is non-existent

-Case V for L_s/L_0 =0.9: The probability is 10^{-11}

-This shows that even a small preference of the stripe pattern renders defects unstable

$$\varepsilon = \frac{1}{V} \int_{defect} (\phi_A - \phi_B)^2 \, dV$$



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