Ising model based simulation of block copolymer self-assembly in two-dimensional post lattice

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Directed self-assembly of block copolymers can generate complex and well-ordered nanoscale patterns for lithography. Previously, useful geometries such as bends and junctions have been self-assembled on a sparse array of chemically functionalized posts.[1,2] To model and predict the block copolymer morphology resulting from a given template, self-consistent field theory (SCFT) simulation has been commonly used. In SCFT simulation, a set of diffusion equations involving chemical potential fields must be numerically solved. In this work, we describe a new Ising model based simulation method for block copolymer self-assembly in two-dimensional post lattice template. This method is simple and fast, and can potentially be used to develop complex design rules for directed self-assembly.

To apply the Ising model to a post lattice template, we first defined a binary state (+1 or -1) between each adjacent pair of posts. We assigned +1 to a state when two adjacent posts were connected by a block copolymer structure, and -1 otherwise. Such assignment ensured a one-to-one mapping between a block copolymer pattern and the corresponding binary state array. Figure 1 shows a diagram of the Ising model setup in the post lattice template. The Hamiltonian of a state configuration σ was defined as

$$H(\sigma) = -J \sum_{\langle i\, j \rangle} \sigma_i \sigma_j - h \sum_j \sigma_j$$

where the first sum corresponds to energy due to nearest neighbor interactions, and the second sum corresponds to energy due to individual states. For simulation, we used the simulated annealing algorithm to approximate the minimum Hamiltonian configuration.

We compared the simulation results with the tile-based design rules reported by Chang et al. In these design rules, double posts were introduced to a square array of single posts to control the positions of bends and terminations. We performed simulated annealing with an initial binary state array where the states positioned between double posts were fixed to +1 while the other states were randomly chosen between +1 and -1 (figure 2a). As the number of iteration steps was increased, the minimum Hamiltonian configuration eventually reached the reported experimental result as well as the SCFT simulation result (figures 2b-2d).

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[1] J. K. W. Yang et al., *Nat. Nanotechnol.* **5**, 256 (2010)

[2] J. Chang et al., *Nat. Commun.* **5,** 3305 (2014)

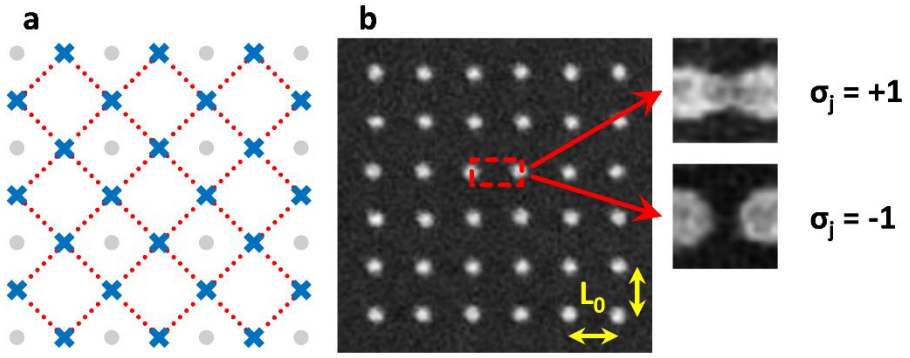

Figure 1: The Ising model setup in the post lattice template. (a) The post template (black dot), states defined between each adjacent pair of posts (blue cross), and nearest neighbor interactions (red line) are shown. (b) The post template fabricated by electron-beam lithography. Pitch was equal to the block copolymer equilibrium periodicity L_0. After the self-assembly, we assigned +1 or -1 to each state depending on whether two adjacent posts were connected or not.

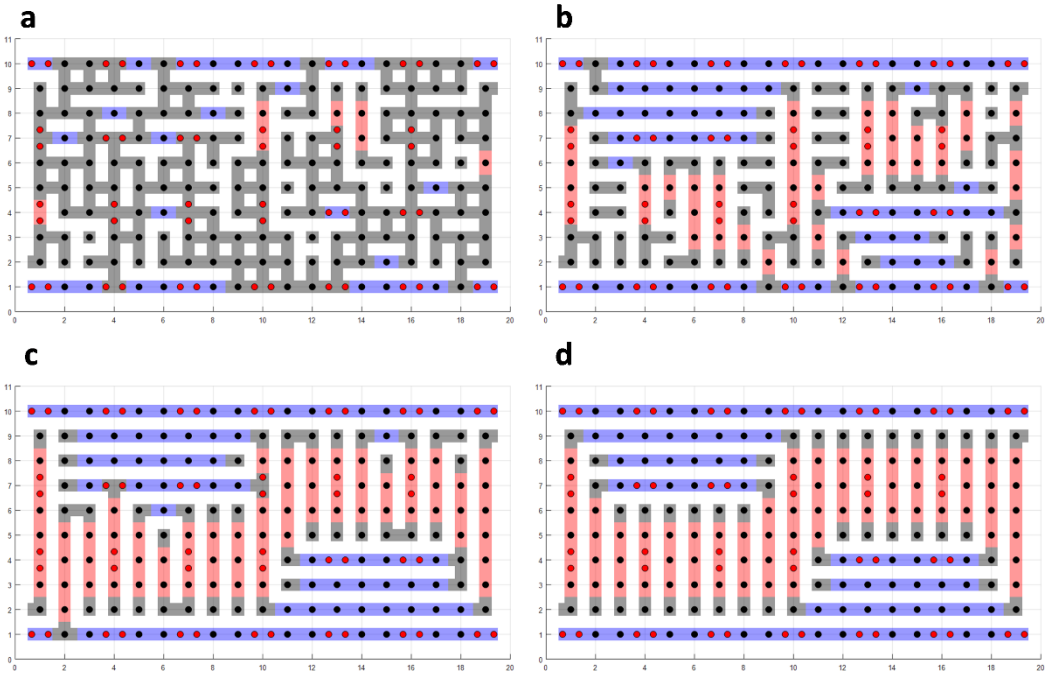

Figure 2: Simulation results. Black and red circles indicate single and double posts. For easier visualization, horizontal and vertical block copolymer structures are colored blue and red, while other morphologies (bends, terminations, and junctions) are colored black. (a) Random initial binary state array. States positioned between double posts were fixed to +1 since double posts force block copolymer structure connection by commensurability. (b) Resulting pattern after 500 iteration steps. (c) Resulting pattern after 5,000 iteration steps. (d) Resulting pattern after 229,500 iterations steps. The minimum Hamiltonian configuration shown in (d) agreed with the experimental result and the SCFT simulation result reported by Chang et al.