A simulation study on defect annihilation dynamics in directed self-assembly lithography

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Although directed self-assembly (DSA) lithography has had a great progress for manufacturing line/space patterning in recent years[1,2], defect density still remains an issue of major concern. In wafer experiments, the observable defects constitute of not only stable "unexpected defective states" at thermal equilibrium but also "non-equilibrium defects". Non-equilibrium defects are kinetically "frozen" defects during the annealing or quenching processes. As for the equilibrium defects, defect density $\mathrm{n_d}$ can be evaluated using the energy gap $\Delta \mathrm{E_d}$ between the defective state and the perfect (defect-free) state. Large $\Delta \mathrm{E_d}$ destabilizes defective state and accordingly results in small $\mathrm{n_d}$. In our previous study[3], we investigated the free energy of "grid defect" which can be extensively observed in our EIDEC flow by use of self-consistent field theory (SCFT). In the report, we clarified that the energy gap of the observed defect $\Delta \mathrm{E_d}$ can be strongly influenced by the surface affinity of the neutral bottom layer. In this work, we report on the dynamics of annihilation of the non-equilibrium grid defects. Dissipative particle dynamics (DPD) simulation method was utilized to evaluate the dynamics. The chain configurations of block copolymers of defective states which is utilized as initial conditions of DPD simulations were prepared using SCFT and node density biased Monte Carlo method (NDBMC)[4]. One representative simulation result is shown in Figure 1. The annihilation dynamics of grid defects can be clearly observed. In the presentation, we will also discuss some comparison results with our wafer experimental results in more details. A part of this work was funded by the New Energy and Industrial Technology Development Organization (NEDO) under the EIDEC project.

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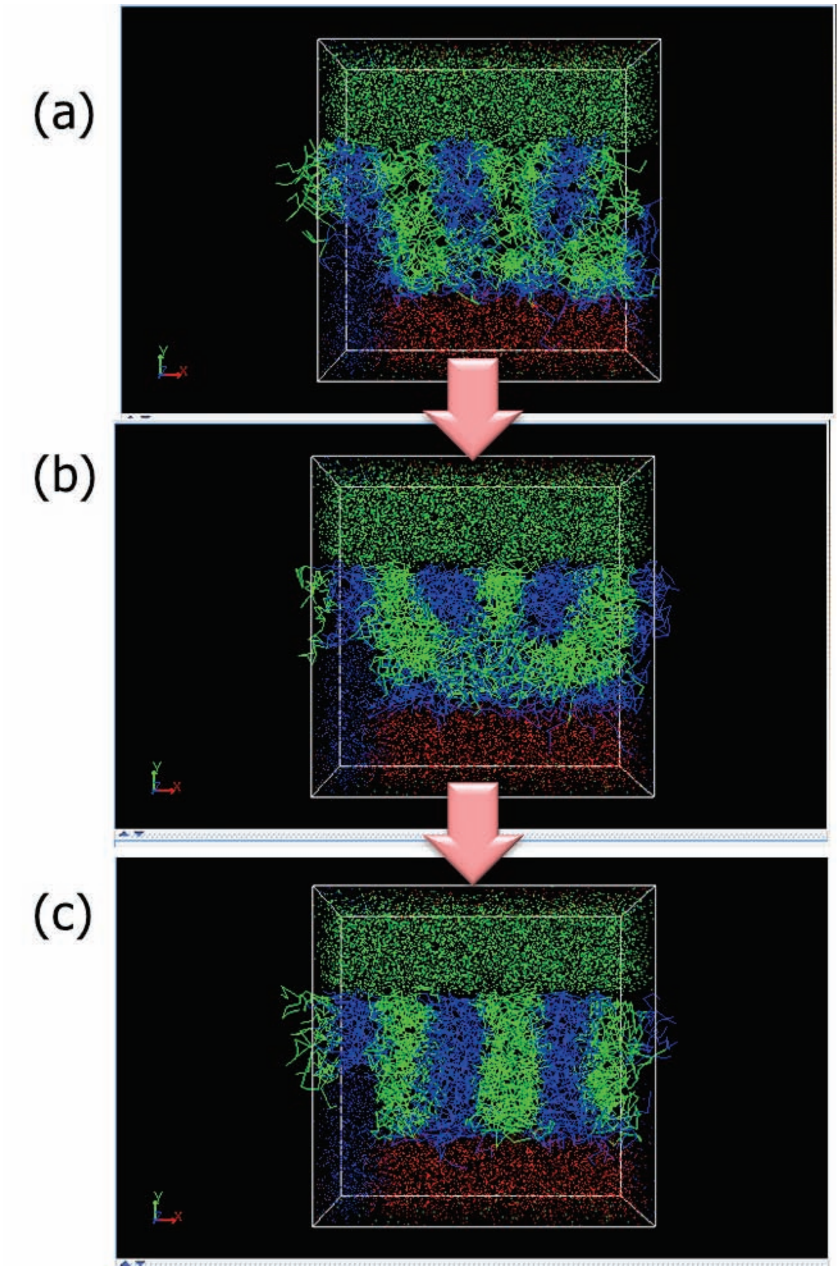

Figure 1: Simulation results on defect annihilation dynamics using DPD. (a) The initial condition (Grid defects can be seen.). (b) The intermediate state (Grid defects were partially destructed.). (c) The converged DPD results (Lamellar patterns without defects can be seen.)