Stochastic simulation of UV-curing process in nanoimprint lithography: Pattern size and shape effects in sub-50 nm

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In UV nanoimprint lithograhpy (UV-NIL), chemical and physical behaviors could be modulated when the feature size becomes below several tens of nanometers. For example, the conversion slowly proceeds when the resist thickness decreases in UV-NIL.[1] Stochastic behavior of UV curing becomes remarkable in such scale region. In the present work, we study the pattern size and shape effects on UV-curing characteristics of the resist with stochastic simulation.

The present simulation model to trace the chain reaction is shown in Fig. 1. A monomer is expressed as a unit particle. Monomers are randomly distributed in space. Photoinitiators are also randomly distributed. The chain reaction starts when initiator is activated by UV exposure. Then, the activated unit reacts with monomer within critical reaction radius and the monomers are chained with each other. Then, the other monomer is activated and the chain reaction occurs within reaction radius. When a virgin monomer does not exist, the reaction radius is expanded step by step. When a virgin monomer does not exist within the maximum reaction radius, the reaction is halted. When the activated monomer react each other, the chain reaction is terminated. Although the simulation model is quite simple, the basic UV-curing characteristics can be well described with the simulation as previously reported.[2]

In the present work, we introduce the deactivation mechanism to restrict the chain reaction at the resist surface. The maximum reaction radius in the resist surface region is set smaller than that in the middle of the resist as shown in Fig. 2.

Cross-sectional view of the spatial distribution of unreacted monomers in the 40 nm cubic UV-cured resist is shown in Fig. 3. Unreacted monomers are remarkably observed in the resist surface region because of the introduced deactivation mechanism.

Figure 4 shows the conversion ratio of UV-cured resist as a function of pattern feature size for line and cubic patterns. The conversion ratio decreases with decrement of the feature size. The decrement of conversion ratio for the cubic pattern is more remarkable than that for the line pattern because the ratio of surface region to whole resist volume is larger in the case of the cubic pattern.

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[1] R. Suzuki et al., J. Photopolym. Sci. Techno., **25**, 211 (2012).

[2] M. Koyama et al., Digest of Papers of 2016 Int. Microprocesses and Nanotechnology Conf., 10D-6-3.

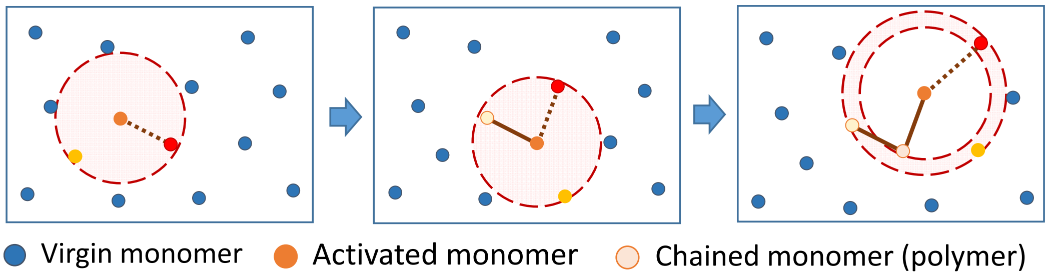

Fig. 1: Schematics of novel chain reaction model based on geometrical cross-linking of monomers.

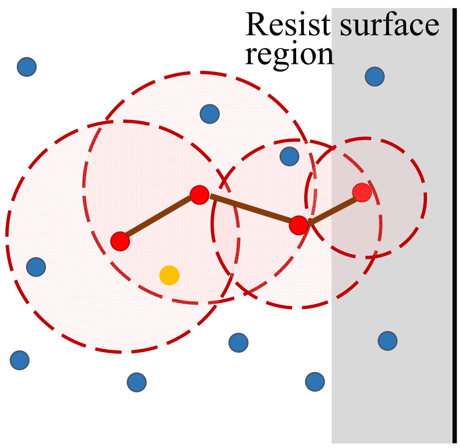

Fig. 2: Model of the deactivation mechanisms to restrict the chain reaction at the resist surface.

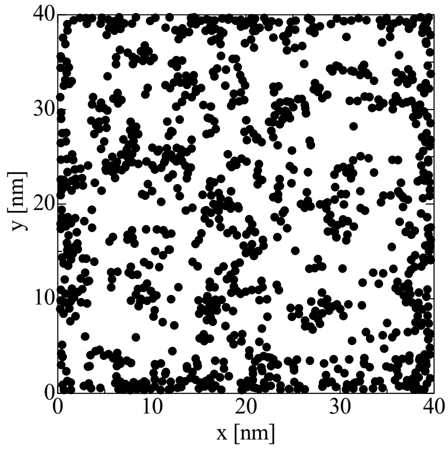

Fig. 3: Cross-sectional view of the spatial distribution of unreacted monomers in 40nm cubic.

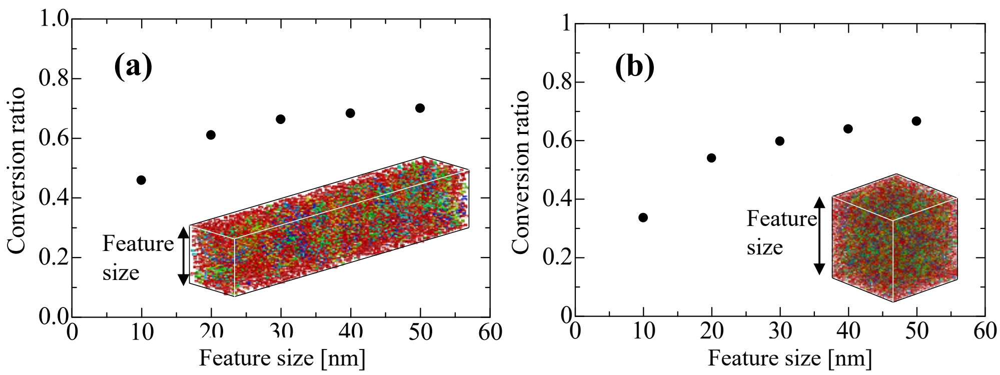

Fig. 4: Conversion ratio of UV-cured resist as a function of pattern feature size for (a) line and (b) cubic patterns.