Computational Study on UV Curing Characteristics Based on Stochastic Model

M. Koyama, M. Shirai, H. Kawata, Y. Hirai and M. Yasuda

Department of Physics and Electronics, Osaka Prefecture University,
1-1 Gakuen-cho, Naka-ku, Sakai, Osaka 599-8531, Japan
hirai@pe.osakafu-u.ac.jp

In UV nanoimprint lithography (UV-NIL), when the pattern size becomes smaller below several tens nanometers, curing characteristics of UV resist could be affected by statistical fluctuation due to decrement of the total amount of molecules, which will affects the UV curing process. We proposed the stochastic simulation model for UV curing process and investigated the basic polymerization characteristics [1, 2]. In this work, we study the impact of initiator concentration. Also, we newly introduces volume shrinkage by curing to investigate resist profile modification.

A schematic illustration of the model is shown in Fig. 1 as follows: (a) Monomer and photo initiators of resist is expressed as a unit cluster molecule. Molecules are placed in space randomly and equilibrated by molecular mechanics (MM) method using Lennard-Jones potential. (b) The reaction begins when the initiator is activated by UV exposure. The activated molecule reacts with a randomly selected unreacted monomer within a reaction radius and a chemical bond forms between them. (c) The bonded monomer is then activated and the chain reaction occurs. (d) When no unreacted monomer is located within the reaction radius, the monomer diffuses and the reaction radius is extended up to the critical radius. (e) When the activated monomers react with each other, the chain reaction terminates. (f) Finally, the molecular positions are recalculated using the MM method and volumetric shrinkage due to polymerization was reproduced with the equilibrium particle distance according to the number of polymerizations.

Figure 2 shows the molecular weight distribution of a 50 nm cubic nonfunctional virtual resist with different initiator concentrations. With increment of the initiator, the average molecular weight decreases. In addition, the higher the concentration of the initiator, the higher the conversion rate. These results well qualitatively reproduces the UV curing characteristics reported by experiments in elsewhere.

Figure 3 shows the pattern profile modification due to shrinkage. The resist material is an acrylic-based virtual resist with the initiator concentration of 5%. We demonstrate the shrinkage of a thin film with a thickness of 20 nm (Fig. 3-a) and a line & space pattern with a residual film thickness of 20 nm, line width of 10 nm, and the height is 10nm (Fig. 3-b). The conversion of the thin film resist and the line & space pattern resist were 77% and 80%, respectively. The shrinkage of the thin film resist was about 6.2% from the change in film thickness.

As demonstrated above, the UV curing phenomena is successfully expressed using newly proposed stochastic model

[1] M. Koyama, et al., Jpn. J. Appl. Phys. **56**, 06GL03 (2017)

[2] M. Koyama, et al., J. Vac. Sci. Technol. B **35**, 06G307 (2017).

[3] R. Suzuki, et al., J. Photopolym. Sci. Technol. **25**, 2, (2012).

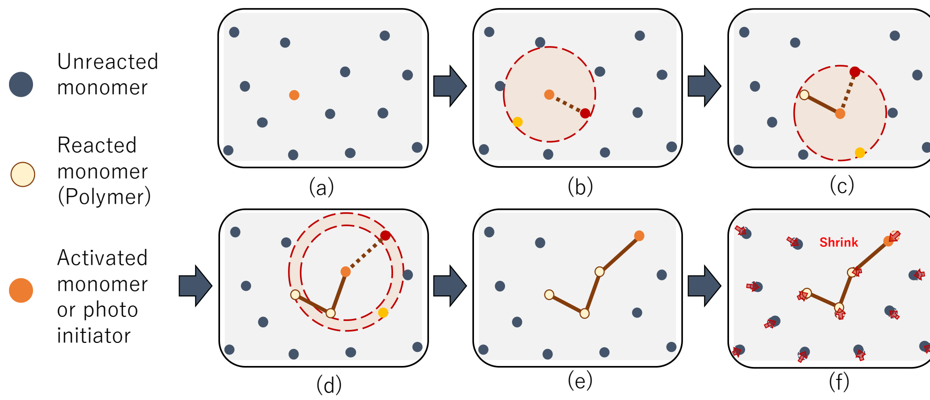

Fig. 1: Schematic illustration of the chain reaction model based on the stochastic approach.

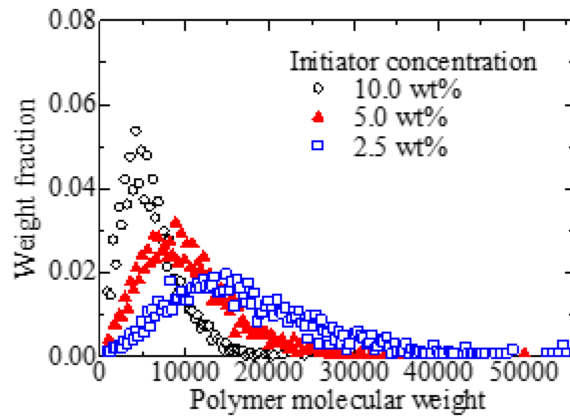

Fig. 2: The molecular weight distribution of the polymers generated for different initiator concentrations.

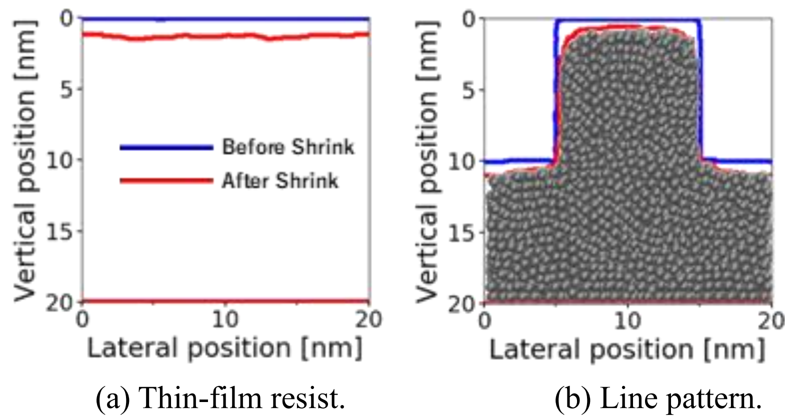

Fig. 3: Pattern shapes of before and after the resist curing shrinkage. (a) Thin-film resist. (b) Line pattern.