Stochastic simulation of pattern formation in electron beam lithography

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

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

Computational studies are indispensable to predict the pattern profiles and to correct the proximity effects in electron beam lithography (EBL). When the pattern size becomes smaller than several tens of nanometer, the behaviors of the polymer molecule in the resist become important to understand the pattern formation process. In the present work, we simulate the pattern formation in EBL using the stochastic method to understand the resist molecule behaviors.

First, we constructed the initial resist structure using the same method that we developed to simulate the UV-curing process in our previous study.[1] Monomers were randomly distributed in space. Then, the monomers were randomly connected to form the chained structure of the resist polymers.

The effect of electron exposure for negative resist was introduced by the crosslinking between the polymer chains as shown in Fig. 1. The crosslinking positions in the polymer chain were randomly selected. The selected unit reacted with another monomer unit within critical reaction radius and the monomers crosslinked with each other. The rate of the crosslinking was set proportional to the absorbed energy distribution in the resist calculated by the Monte Carlo simulation of electron scattering. By introducing chain scission in the randomly selected position, we can also simulate the electron exposure for positive type resist.

In the development simulation, the resist polymers with relatively small molecular weight were removed from the resist structure.

Figure 2 shows the molecular weight distributions of polymers in four initial resists prepared by the above-mentioned method. The number-average molecular weights for resist 1, 2, 3 and 4 are 7000, 4000, 2400 and 2200, respectively.

An example of the cross-sectional profile for 20-nm-wide line pattern obtained by the present simulation is shown in Fig. 3. The molecular chains of the polymers are observed as a typical roughness structures at the pattern surface.

The ratios of remaining polymers after development as a function of electron dose for negative type resist are shown in Fig. 4. With an increase in the resist molecular weight, the required dose to form the pattern decreases.

Then, the line edge roughness (LER) of 20-nm-wide line pattern was evaluated with the simulation. Figure 5 shows LER as a function of molecular weight of the resist. As a general rule, the LER increases with increasing molecular weight.

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

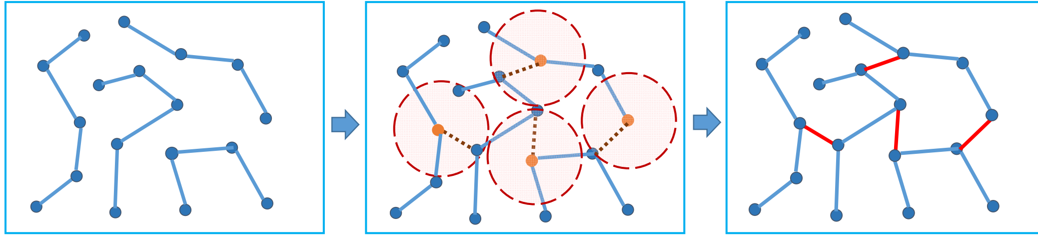

Fig. 1: Schematic illustration of the cross-linking model of the polymer chains in electron exposed negative type resist.

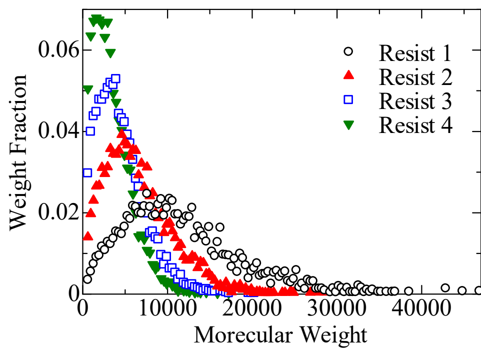

Fig. 2: Molecular weight distributions of the polymers in four initial (unexposed) resists.

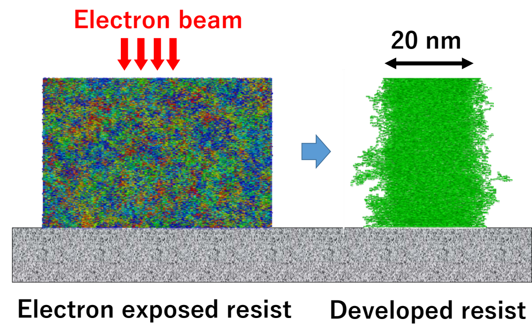

Fig. 3: Cross-sectional view of the developed pattern profile for negative type resist.

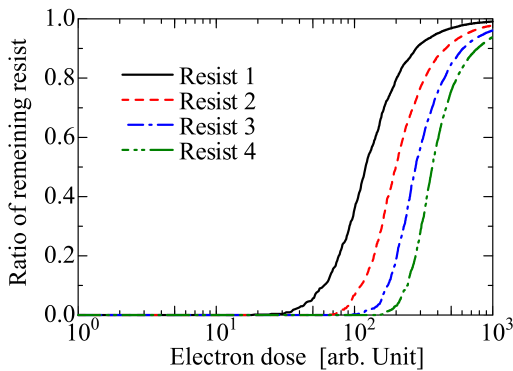

Fig. 4: Ratio of remaining resist polymers after development as a function of electron dose for negative type resists.

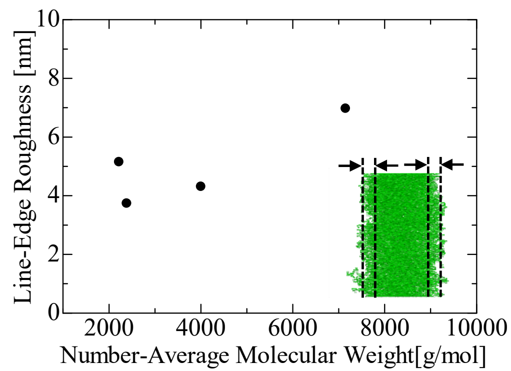

Fig. 5: Line edge roughness of 20-nm-wide line pattern as a function of molecular weight of the resist.