## Computational Study of Resist Pattern Shrinkage under CD-SEM Observation

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The resist pattern shrinkage is a serious problem in critical dimension scanning electron microscope (CD-SEM) observation. The shrinkage deteriorates the accuracy of the pattern size measurement using CD-SEM. In the present work, the resist pattern shrinkage by electron irradiation is studied with both molecular dynamics (MD) simulation and Monte Carlo simulation of electron scattering.

First, the shrinkage of the small resist pattern is studied with the MD simulation. Poly-(methlmethacrylate) (PMMA) resist on Si substrate is selected as sample material. The initial size of the PMMA resist is  $5 \times 5 \times 5 \text{ m}^3$ . During the chemical reaction caused by electron irradiation, decomposition gases (CO<sub>2</sub>, CH<sub>4</sub>, etc.) emit from the PMMA resist. This outgassing phenomenon is modeled by diminishing the component inside the resist in the MD simulation. The motions of resist polymers are calculated using the force field proposed by Okada et al.<sup>1</sup> It consists of bond stretching, bending, torsion potentials, and nonbonding interaction including Lennard-Jones and Coulomb potentials. Figure 1 shows the normalized pattern height as a function of resist component removal rate obtained by the MD simulation. The pattern height gradually decreases with increase in the component removal rate.

Because the size of the resist structure in the MD simulation is much smaller than the actual pattern due to the computational time, we use Monte Carlo simulation of electron scattering together with the MD simulation to analyze the shrinkage of the larger resist pattern. The absorbed energy distribution in the resist is calculated with the Monte Carlo simulation of electron scattering. Figure 2 shows the depth distributions of absorbed energy at 0.5 and 5 kV for 60-nm-high PMMA resist obtained by the Monte Carlo simulation.

Then, the pattern is divided into smaller cell whose size is same as that of MD simulation. If the emission of the decomposition gas is assumed to be proportional to the absorbed energy, the shrinkage ratio of each cell is obtained from the MD simulation result (Fig. 1). Figure 3 is the estimated pattern profiles for the 45-nm-wide, 60-nm-high resist pattern after electron exposure at 0.5 and 5 kV. The pattern shrinkage becomes serious at higher accelerating voltage.

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<sup>&</sup>lt;sup>1</sup>O. Okada et al., Comput. Theo. Polymer Sci. **10**, 371 (2000).



*Fig. 1:* Normalized pattern height as a function of resist component removal rate obtained by the MD simulation.



*Fig. 2:* Depth distributions of the absorbed energy in 60-nm-high PMMA resist exposed at 0.5 and 5 kV electron obtained by the Monte Carlo simulation. Electron trajectories are also shown.



*Fig. 3:* Estimated pattern profiles for the 45-nm-wide, 60-nm-high resist pattern after electron exposure at 0.5 and 5 kV.