Molecular Dynamics Study of Line Edge Roughness in Electron Beam Lithography

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When the pattern size becomes smaller than several tens of nanometers in the lithography, the behaviors of the polymer molecule in the resist become important to understand the pattern formation process. We have recently developed molecular dynamics (MD) simulation of pattern formation in electron beam lithography.[1,2] In the present work, we study the atomic-scale line edge roughness (LER) in electron beam lithography with the MD simulation.

Figure 1 shows a configuration of the present simulation. The sample of the simulation is PMMA resist on the Si substrate. The line patterns are exposed by electrons. The effect of electron exposure is introduced by the chain scission of PMMA polymer molecule in the MD simulation. The breaking positions in the polymer chain are randomly selected. The rate of chain scission in the resist is set proportional to the exposure intensity distribution preliminarily calculated by the Monte Carlo simulation of electron scattering. The chain scission and the structural relaxation processes are alternately repeated in the exposure simulation. In the development simulation, the PMMA molecules are removed from the structure in ascending order (from smaller molecules to larger ones). The molecule removal and the structural relaxation processes are also alternately repeated.

Figure 2 is an example of the resist pattern exposed at 100 kV. The molecular scale roughness is observed on the sidewalls of the pattern. The prominences of the molecular chain superimposed on the undulating molecular network are observed as a typical structure of the atomic-scale LER. The atomic-scale concaves are also observed due to the lack of the molecular chain.

Figure 3 shows the LER of 2-nm-wide line pattern exposed at 100 kV as a function of polymerization degree of removed resist segment in the development process. The sizes of the removed resist segment are also shown. The LER increases linearly with the polymerization degree of removed segment. The LER clearly correlates with the size of the removed resist segment. In the conditions where the electron scattering effect is suppressed such as high accelerating voltage, the LER becomes close to the size of the resist molecule segment for PMMA resist.

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[1]M. Yasuda et al., Microelectron. Eng. **112**, (2013) 287.

[2]K. Michishita et al., Jpn. J. Appl. Phys, in press.

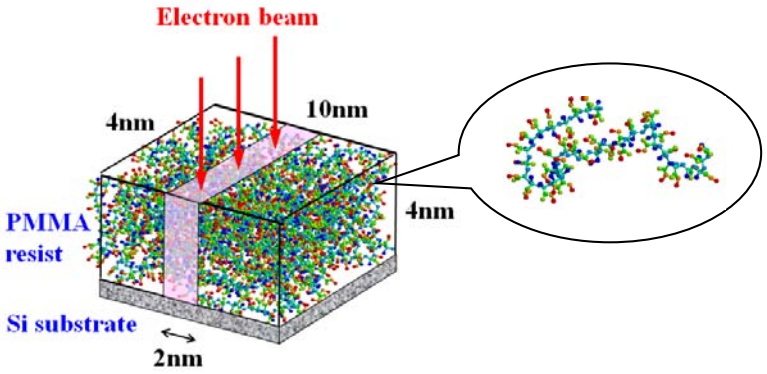

Fig. 1: Configuration of the present simulation. The sample of the simulation is PMMA resist on the Si substrate. The 2-nm-wide line pattern is exposed.

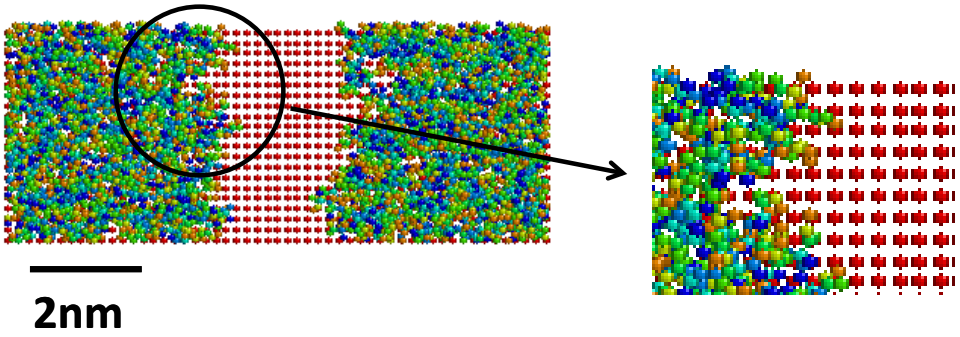

Fig. 2: An example of the molecular scale roughness structure observed in the present simulation.

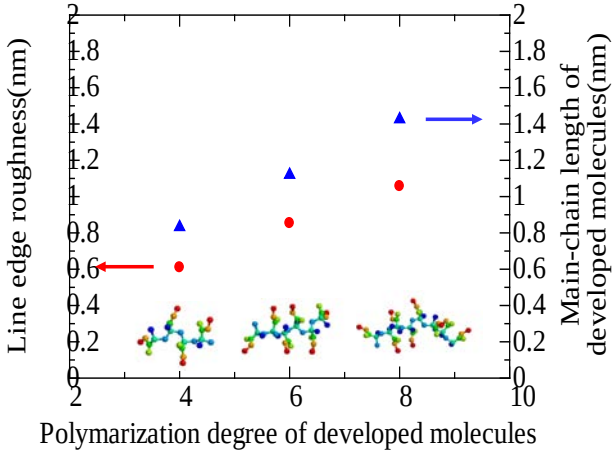

Fig. 3: The line edge roughness of 2-nm-wide line pattern of PMMA resist as a function of polymerization degree of removed resist segment. The sizes of the removed resist segment are also shown.