Molecular Simulation of Electron-Irradiation Damages in Resist Materials

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The electron irradiation damage is the serious problem in scanning electron microscope observation of resist materials. We have developed a molecular dynamics (MD) simulation including the interaction between an incident electron and a target material to study the structural changes of the materials under electron irradiation.[1,2] In the present work, electron-irradiation damages in resist materials are studied with the simulation.

Figure 1 shows the configuration of the present simulation. PMMA resin is selected as a resist material. The central part of PMMA resist on Si substrate is irradiated by electron beam. The interaction between an incident electron and an atom in the resist is modeled based on the binary collision theory using the screened Rutherford cross section. The inelastic collision is not considered. The motions of polymers under electron irradiation are calculated using the force field proposed by Okada et al.[3] in MD simulation. It consists of bond stretching, angular bending, torsion potentials, and nonbonding interaction including Lennard-Jones and Coulomb potentials. The temperature of the PMMA resist under electron irradiation is kept constant in the present simulation.

Figure 2 shows the number distributions of atoms in PMMA resist before and after electron irradiation. The irradiated areas are indicated by the colored rectangle and the width of the area is 1 nm. After electron irradiation at 1 kV, the number of the atoms in the resist around irradiated area decreases as shown in Fig. 2 (a). The width of the damaged area is about 4 nm. When the accelerating voltage becomes 10 kV, the decrease in the number of the atoms in the irradiated area becomes larger as shown in Fig. 2 (b). However, the width of the damaged region becomes narrower. The width is approximately 3 nm. With the increase in the accelerating voltage, more resist atoms are driven out from the irradiated area, but the damaged region becomes narrower.

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[2] Y. Chihara et al., J. Vac. Sci. Technol. B **29**, 06FG09-5 (2011).

[3]O. Okada et al., Comput. Theo. Polymer Sci. **10**, 371 (2000).

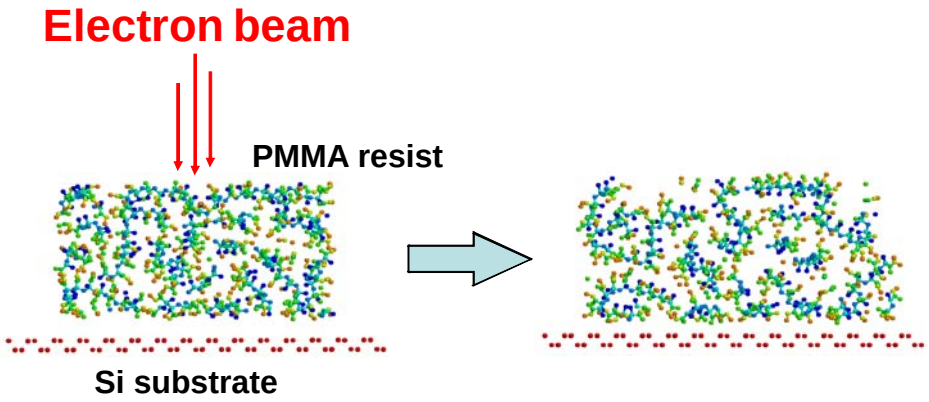

Fig. 1: Configuration of present simulation. The central part of PMMA resist on Si substrate is irradiated by electron beam. The motions of PMMA polymers under electron irradiation are traced by the MD simulation.

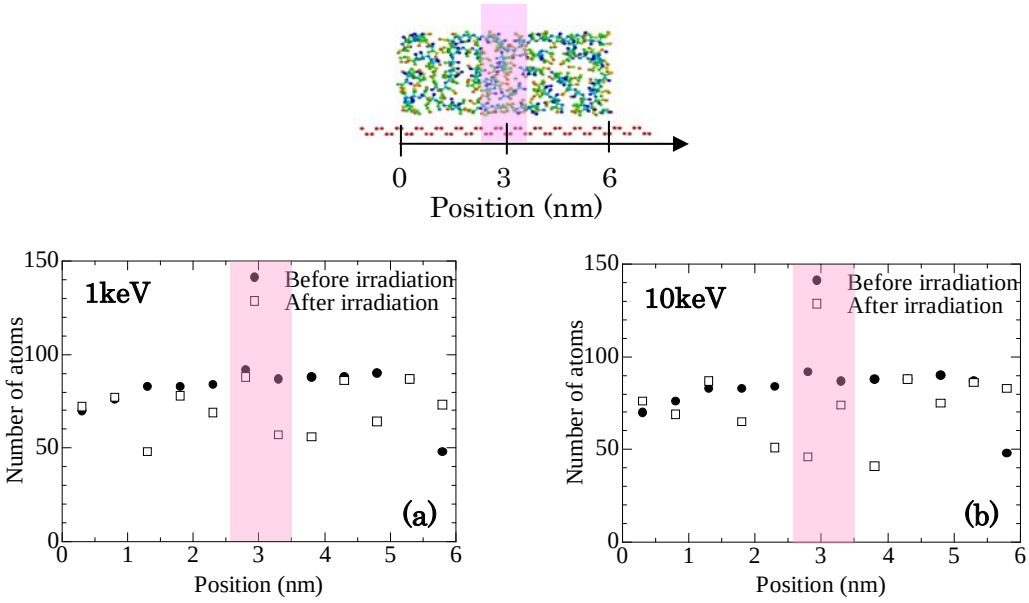

Fig. 2: Number distributions of atoms in PMMA resist before and after electron irradiation at (a) 1 and (b) 10 kV. The irradiated areas are indicated by the colored rectangular and the width of the area is 1 nm.