Molecular Dynamics Study of Line Edge Roughness in Nanoimprint Lithography

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When the pattern size becomes smaller than several tens of nanometers, the behavior of resist molecules plays an important role in nanoimprint lithography (NIL). Molecular dynamics (MD) simulation becomes powerful method to analyze the pattern formation process at such scale.[1,2] In the present work, we study the line edge roughness (LER) of the resist pattern formed by NIL with MD simulation.

The system of the present simulation consists of a Si mold, a PMMA resist and a Si substrate. Atoms in the mold and substrate are assumed as rigid body. The motions of polymers are calculated using the force field proposed by Okada et al.[3] in MD simulation. It consists of bond stretching, bending, torsion potentials, and nonbonding interaction including Lennard-Jones and Coulomb potentials. In order to introduce the effect from the antistick treatment on the mold surface, we multiply the intermolecular force between the Si mold and PMMA resist by the interaction coefficient (< 1). The mold is pressed and released from resist at a constant velocity of 200 m/s. The temperature of the resist is maintained at 400 K during the mold pressing using the velocity-scaling method. After filling the cavity of the mold with resist, the system is cooled to 300 K. Finally, the mold is released from the resist. An example of demolding process in the present simulation is shown in Fig. 1.

Figure 2 shows the LER of PMMA resist after demolding process as a function of interaction coefficient between Si mold and PMMA resist. The molecular weight (Mw) of the resist is 8000. The LER increases as the interaction between the mold and resist becomes large.

We also study the effect of Mw of the resist. Figure 3 shows LER for PMMA resist patterns with different Mw. The interaction coefficient is 0.1 in this case. The demolding forces are also calculated.[2] Tendencies of the effect of Mw on LER and the demolding force are almost same. The LER becomes the largest when Mw is 4000. The demolding force for Mw=4000 is also the largest.

In conclusion, the LER of the pattern is closely related to the demolding force even in the atomic-scale NIL.

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[1]A. Taga et al., J. Vac. Sci. Technol. B **28**, C6M68 (2010).

[2]R. Takai et al., J. Vac. Sci. Technol. B **32**, 06FG02 (2014).

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

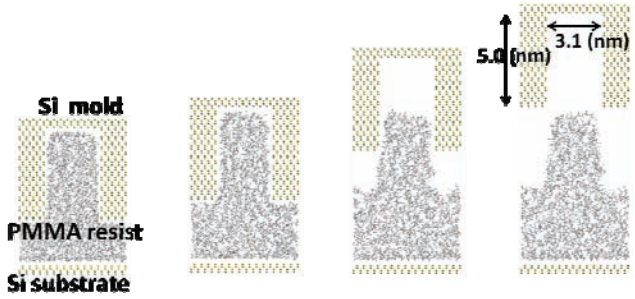

Fig. 1: An example of demolding process in the present simulation. The system consists of Si mold, 6-nm-thick PMMA resist and Si substrate.

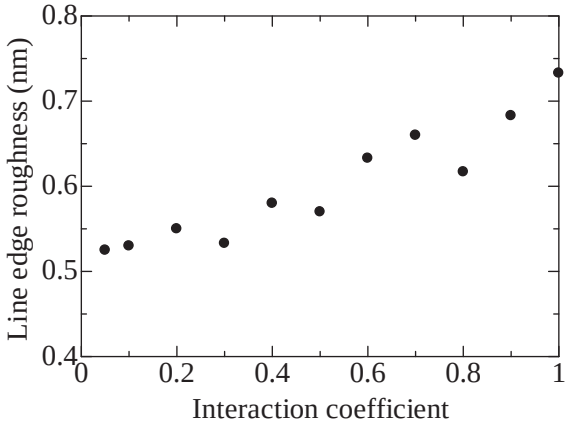

Fig. 2: The line edge roughness of PMMA resist after demolding process as a function of interaction coefficient between Si mold and PMMA resist. The molecular weight of PMMA resist is 8000.

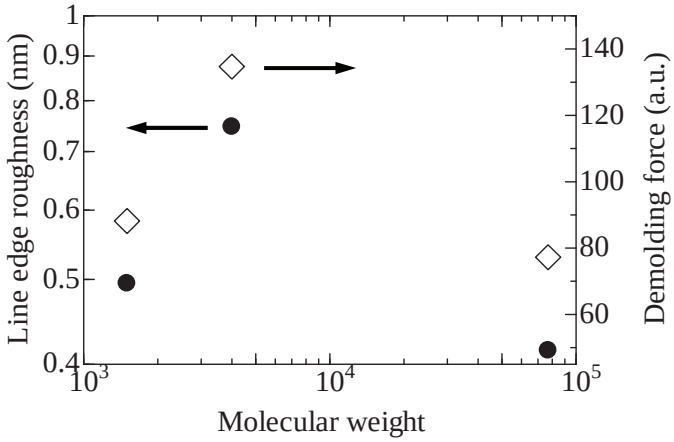

Fig. 3: The line edge roughness and demolding force for PMMA resists with three different molecular weights.