Molecular Dynamics Study on Demolding Process in Nanoimprint Lithography

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The analysis of the nanoimprint lithography (NIL) process in atomic level takes on a growing importance, when the pattern size becomes smaller than several tens of nanometers. Molecular dynamics (MD) simulation is one of the powerful methods to analyze this kind of phenomena.[1,2] In the present study, we analyze molecular size effects of the demolding process in NIL with MD simulation.

Figure 1 shows the configuration of the present simulation. The system consists of a Si mold, a PMMA resist and a Si substrate. A periodic boundary condition is adopted in the direction perpendicular to the line pattern. Atoms in the mold and substrate are assumed as rigid body. To save the calculation cost, a methyl and an ethyl groups in PMMA resist are assumed to be unit giant atoms. Then, a polymer chain structure which consists of the several monomers is assembled to form the resist structure. The motions of polymers are calculated using the force field proposed by Okada et al. in MD simulation. It consists of bond stretching, angular bending, torsion potentials, and nonbonding interaction including Lennard-Jones and Coulomb potentials. In order to introduce the demolding treatment of the mold, we calculate the interaction between the Si mold and PMMA resist with the intermolecular force diminished by 1 order of magnitude.

Figure 2 shows the snap shots of the resist structure at the early stage of demolding process obtained by the present simulation. The results for PMMA resist with two different molecular weights (Mws) are compared. In the case of Mw=1500, the mold is separated from the residual layer. On the other hand, the separation started from the bottom of the mold cavity in the case of Mw=70000. In the narrow mold cavity, the movement of the larger PMMA molecule is restrained. Therefore, the resist in the cavity does not follow the movement of the mold. As a result, the bottom of the cavity separates soon in the case of Mw=70000.

We also study the effects of the sidewall roughness of the mold. Figure 3 shows the demolding force as a function of the roughness pitch of the mold sidewall. The demolding force increases with increase in the roughness pitch. The sidewall roughness effect also depends on the Mw of the resist.

In conclusion, the demolding process is closely related to the molecular size of the polymer, when the pattern size becomes single nanometer scale.

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

[2]M. Yasuda et al., Microelectron. Eng. **88**, (2011) 2188.

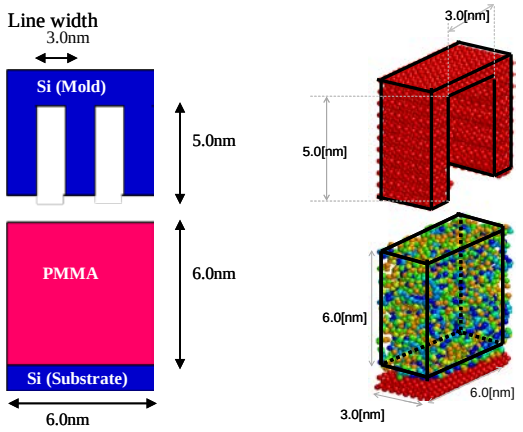

Fig. 1: Configuration of the present simulation. The system consists of a Si mold, a PMMA resist and a Si substrate.

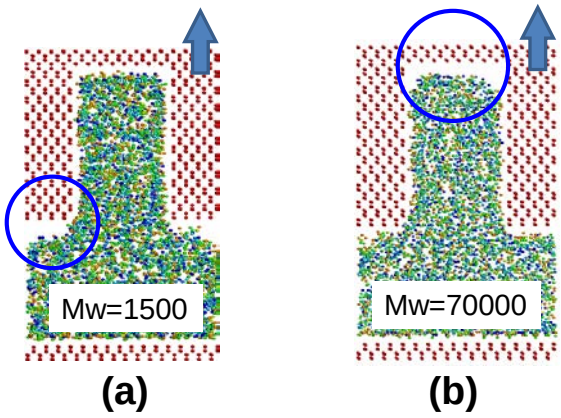

Fig. 2: Snap shots of the resist structure at the early stage of demolding process for PMMA resists with Mws of (a) 1500 and (b) 70000.

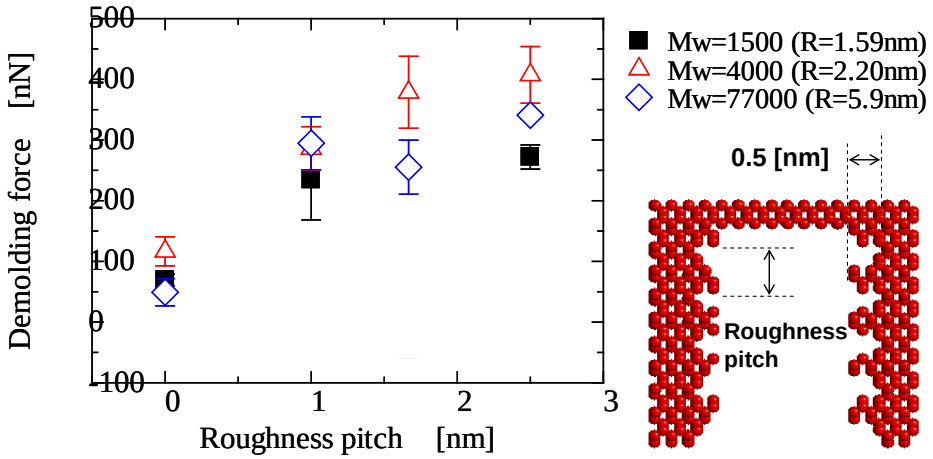

Fig. 3: The demolding force as a function of the roughness pitch of the mold sidewall. The results for resists with Mws of 1500, 4000 and 70000 are compared.