Impact of Molecular Size on Resist Filling Process in Nanoimprint Lithography : Molecular Dynamics Study

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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]. In the present study, we analyze molecular size effects of the resist filling process in NIL with MD simulation.

We select PMMA resin as a polymer material. To save the calculation cost, a methyl and an ethyl groups 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. [2] in MD simulation. It consists of bond stretching, angular bending, torsion potentials, and nonbonding interaction including Lennard-Jones and Coulomb potentials.

The configuration of the present simulation is as following. 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. Temperature is kept constant at 500K. Atoms in the mold and substrate are assumed as rigid body.

Figure 1 shows the deformed polymer structures during filling process for 1nm line and space pattern. Fig. 1(a) shows a case that molecular weight of the polymer resist is 100. In this case, filling is completed by the press force of 220nN. Fig. 1(b) shows a case that molecular weight is 4000. In this case, filling is not completed by same press force. Larger press force is required to fill the polymer into the cavity of the mold as molecular weight becomes large.

Figure 2 shows mold size dependence of required press force to fill the mold cavity for various molecular weights. Press force increases with decrease in line width. It also increases with increase in molecular weight. For each molecular weight, a critical line width exists. Below the critical width, press force increases at a great rate. This critical width increases with increase in molecular weight.

In conclusion, the press force is closely related to the molecular size of the polymer, when the pattern width becomes single nanometer scale.

1. J. -H. Kang et al., Toribol. Lett. **25**, 93 (2007).
2. O. Okada et al., Comput. Theo. Polymer Sci. **10**, 371 (2000).

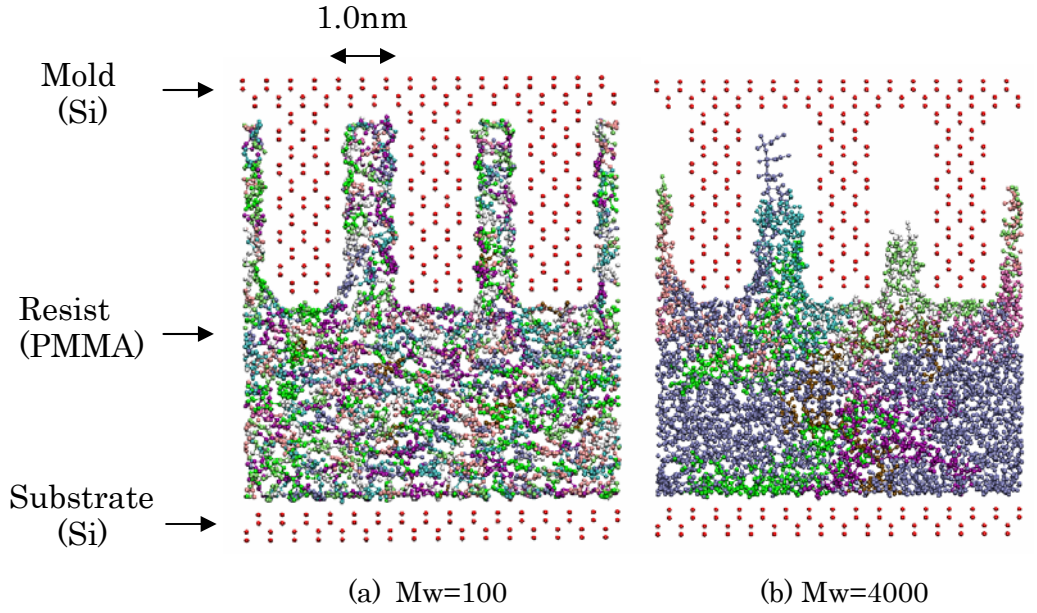

Fig.1 Deformed polymer structures. Molecular weights (Mw) are (a) 100 and (b) 4000.

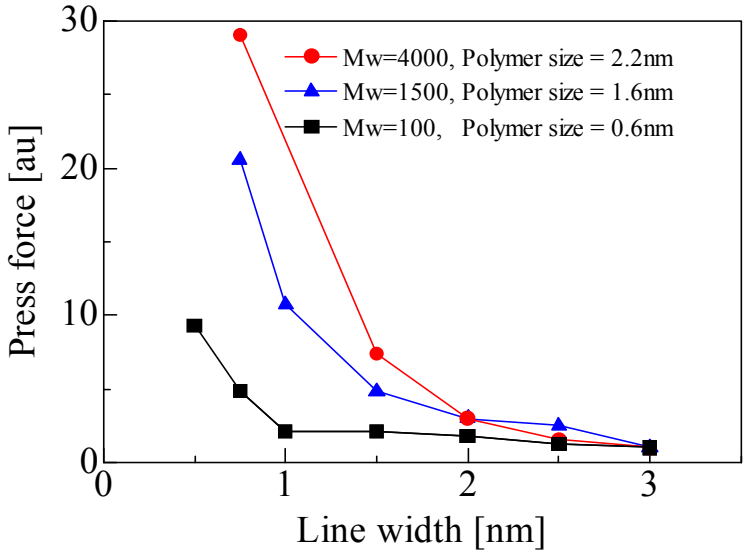

Fig.2 Press force as a function of line width for various molecular weights of PMMA (Line width = 1.0 nm).