Molecular Dynamics Study on Polymer Filling Process in Nanoimprint Lithography for Multi-Layered Resist

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When the pattern size in nanoimprint lithography (NIL) becomes smaller than several tens of nanometers, the behavior of the polymer molecule plays an important role in the resist deformation process. We reported the molecular size effects on resist filling process in NIL with Molecular dynamics (MD) simulation [1]. In the present work, we study the resist filling process for multi-layered resist with MD simulation.

The configuration of the present simulation is as following. The system consists of a Si mold, a PMMA multi-layered resist and a Si substrate as shown in Fig. 1. The PMMA resists with molecular weight (Mw) of 500 and 5000 are stacked alternately in the multi-layered resist. We studied two types of multi-layered resists. One has a low Mw (500) top layer (Fig. 1(a)) and another has a high Mw (5000) top layer (Fig. 1(b)). Here, we refer to the resist shown in Fig. 1(a) and (b) as the low/high and high/low multi-layered resist, respectively. The motions of polymers are calculated using the force field proposed by Okada et al. [2] in MD simulation. A periodic boundary condition is adopted in the horizontal direction. Temperature is kept constant at 500K. Atoms in the mold and substrate are assumed as rigid body.

Figures 2 and 3 show the deformed polymer structures during filling process for the low/high and high/low resist, respectively. In the examples shown here, the mold has two cavities and the resist has four layers. The multi-layered resists are pressed by the forces required to fill the 3-nm-wide cavity. The required press forces for the low/high and high/low resists are 193 and 251 nN, respectively. The 60% volume of the 1-nm-wide cavity is filled in the case of the low/high resist as shown in Fig. 2 (b). On the other hand, only 24% is filled in the case of the high/low resist as shown in Fig. 3 (b). This indicates that the low/high resist is preferable to fabricate high aspect ratio pattern under low pressured condition.

As previously reported, the double-layered resist with low Mw top layer has an advantage in submicron high aspect patterning [3]. This advantage of the low Mw top layer is also shown in nanometer NIL process by the present MD simulation.

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

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

[3]T. Konishi et al., Microelectron. Eng. **83**, 869 (2006).

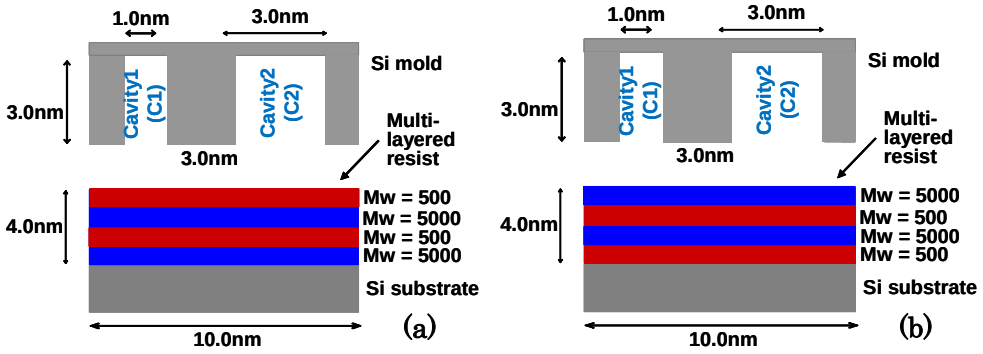

Fig.1: Examples of the configuration of the present simulation. The top layer consists of polymer molecules with (a) Mw = 500 and (b) Mw = 5000.

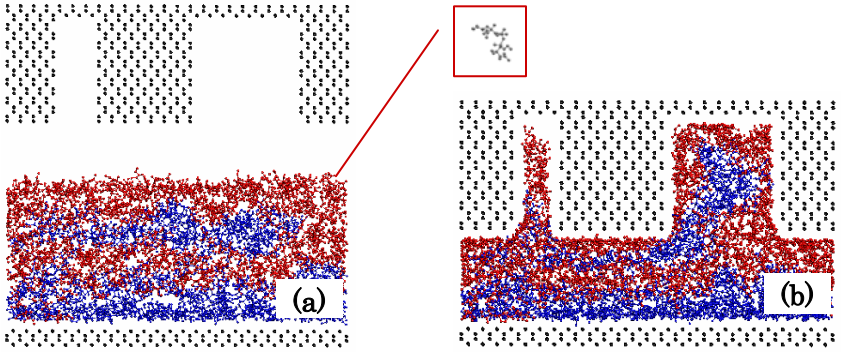

Fig.2: Polymer structures of the low/high multi-layered resist (a) before and (b) after pressing.

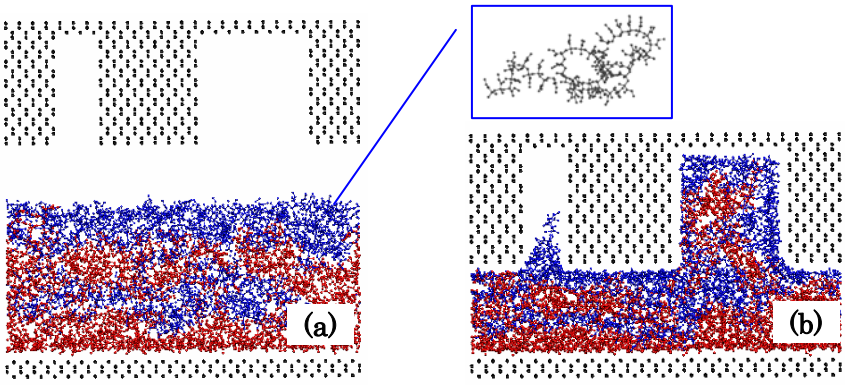

Fig.3: Polymer structures of the high/low multi-layered resist (a) before and (b) after pressing.