Impact of molecular size in sub 10nm nanoimprint lithography based on computational study

R. Sakata[1], M. Yasuda[1], K. Tada[2], Y. Miyashita[1], M. Shirai[1], H. Kawata[1], Y. Hirai[1]

[1]Physics and Electronics Engineering, Osaka Prefecture University, Sakai, 599-8537, Japan
[2]National Institute of Technology, Toyama College, Toyama, 939-8630, Japan
E-mail: hirai@pe.osakafu-u.ac.jp

Introduction

Progresses for industrial application of NIL have been reported in sub 20nm scale integrated systems [1]. Beside those technical progress, scientific issues comes out. Several experimental results have been reported about viscosity increment in squeezed liquid resin [2]. As the pattern width becomes narrow down to molecular size of the resist polymer, mechanical behaviors become important in nanoimprint process, however we could hardly investigate the molecule behaviors in experimentally. So, computational study is one of the effective approaches to investigate the dynamics in nano scale spaces.
In this work, the impacts of molecular size of polymer on required pressure for imprinting and evaluate line edge roughness of the pattern after de-molding using molecular dynamics simulations and investigate.

Molecular dynamics Simulation

To investigate polymer deformation and de-molding process, computational simulation based on the molecular dynamics study is carried using in-house software. We investigate impact of molecular diameter (ie. molecular weight) to pattern width on process conditions and imprinted results. Polymethylmethacrylate (PMMA) is used as an examined resist polymer in various molecular weights. Figure 1 shows schematics of the computational system. The Si mold is pressed to PMMA resist, where the molecular weights are varied. Table 1 shows molecule radius in various molecular weight Mn of PMMA. The required forces to fill the polymer into the pattern cavity are calculated for various molecular weight of the PMMA. Also, the line edge roughness of the imprinted pattern after de-molding are investigated.

Results and discussion

Impact of the relative cavity width w/Φ on the required pressure for imprinting and the line edge roughness of the pattern after de-molding are shown in Fig.2. , where w is pattern cavity width and Φ is molecular diameter of PMMA. The required pressure increases when the relative cavity width w/Φ is reduced below around 3 as shown in Fig.2 (a). Also, the line edge roughness (LER) increases when the relative cavity width is reduced as shown in Fig.2 (b). Those results are explained by the large deformation of the polymer chain related with the relative cavity width w/Φ.

Reference:

[1] T. Higashiki, Proc. of SPIE Advanced lithography (San Jose, 2019) [10958-9],
[2] S. Ito, ACS Appl. Mater. Interfaces, 9 (2017) 6591.

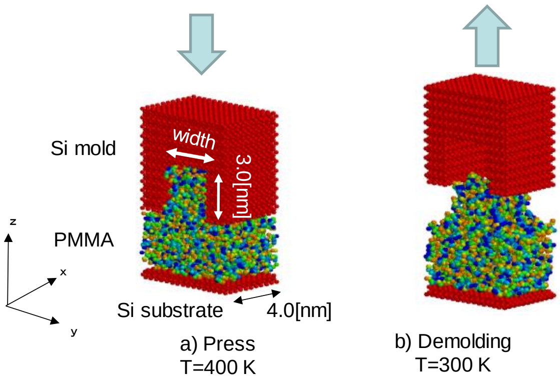

Fig. 1. Schematics of the systems.

Table. 1 Molecular diameter (PMMA)

Molecular weight[g/mol] Mw	Diameter of molecular chain [nm] *Φ*
500	1.1
1500	1.6
4000	2.2
8000	2.8

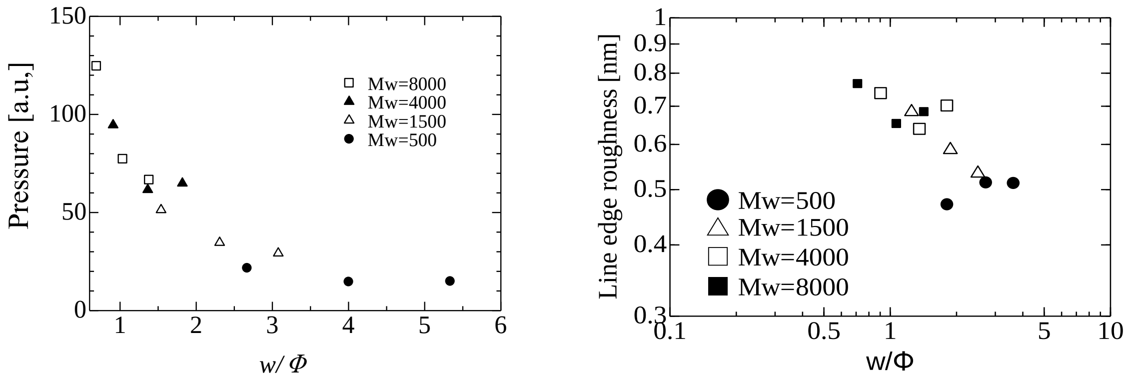

Figure 2. Impact of relative cavity width *w/Φ* on the required pressure (a) and line edge roughness of the pattern after de-molding (b), where *w* is pattern cavity width and *Φ* is molecular diameter of PMMA.