Impact of Wafer Deformation on Pattern Fabrication for Thermal Nanoimprint Lithography

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The impacts of substrate deformation on the resist filling characteristics were investigated both by experiment and by simulation for thermal imprint process. A Si mold with line and space pattern of 2 μm half pitch was used. The pattern area was surrounded by the flat area and its surface is as high as the top of the line pattern, that is, the concave mold is used. The mold pattern was transferred to a poly(methyl methacrylate) (PMMA) film on various thick Si substrates by the thermal imprint process. When the thin substrate of 200 μm thickness was used, no filling defects could be found. On the other hand, when the thick substrate of 1000 μm thickness was used, a large amount of filling defects was observed. It was clear that the filling defect could be suppressed by the substrate deformation. The substrate deformation was simulated by use of a simplified model. The substrate position, $z_0$, which is the boundary between the substrate and the PMMA film, was calculated. The formation of the filling defects could be explained by the substrate position, $z_0$, quite well.

Keywords: Poly(methyl methacrylate), concave mold, deformation, filling defect

1. Introduction

Nanoimprint lithography (NIL) is a promising cost-effective nano-fabrication method [1,2]. The thermal nanoimprint process (T-NIL) is widely used because fine patterns can be replicated to various resin films [3] and its resolution is extremely high [4]. However, relatively high pressure (~ 10 MPa) is usually required for T-NIL. A substrate and/or a mold must be deformed during the press. Some problems are often induced by the substrate deformation, such as inhomogeneity of the residual layer thickness [5], demolding force [6]. Moreover, resist filling in cavity patterns becomes often incomplete by the substrate deformation [7]. When pattern areas are surrounded by large flat areas in a mold, the concave and the convex molds are usually defined as shown in Fig. 1. The height of the flat area is as high as the top of the mold pattern for the concave mold, and is as high as the bottom of the mold pattern for the convex mold. The filling defects are frequently observed for the concave mold because the resist resin has to flow into the cavities after both the large flat area and the top of the mold patterns are touched to the resist. One example of the filling defect is shown in Fig. 2 for the concave mold. The PMMA film is coated on the Si wafer of 675 μm thick. The sizes of the mold wafer and the pattern area is 10 mm, and 5 mm respectively. The edge of the pattern area is $x=2.5$ mm. The fabricated PMMA patterns at various lateral positions are shown in this figure. The lateral position is measured from the mold center. The filling defects are found at $x=2$ mm, because the height of the line pattern at $x=2$ mm is smaller than that at $x=0$ mm. The filling defects can be also observed at $x=2.4$ mm, because the pattern height is clearly decreased from the right edge (near the edge of the pattern area) to the left edge (near the center of the pattern area) of the picture.

In this paper, the effects of substrate deformation on the filling defect for the concave

![Fig. 1. Types of mold, (a) concave mold, (b) convex mold.](image-url)

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molds are studied. The used Si mold has line-and-space pattern (LS pattern) in the center. The pattern area is surrounded by a large flat area. The surface of the flat area is as high as the top of the LS pattern. The concave mold is pressed into PMMA film on various thick Si substrates. The substrate deformations are estimated by a simulation by use of simplified model. The experimental results are discussed based on the simulation results.

2. Experiment

Si mold is fabricated by using the anisotropic etching of KOH solution. Line pattern with vertical and extremely smooth side wall can be obtained by the anisotropic etching. A 2-µm half-pitch line-and-space pattern is fabricated in (110) Si wafer. The silicon wafer is etched by a mix solution of 5 mol/L KOH and isopropyl alcohol (IPA) with a volume ratio of 2:1 at 65 ºC for 15 min. The etching depth is about 3 µm. The detail of the fabrication process has been shown in the previous paper [6]. The mold wafer size is 10×10 mm. The line-and-space pattern is fabricated in the center of the Si wafer. The fabricated mold wafer is bonded on the graphite mold holder. Figure 3 show the fabricated molds.

The pattern area sizes are 2.5 mm and 5 mm. These molds are named as the 2.5mm mold and the 5mm mold in this paper, respectively. The mold is pressed into PMMA (Mw=350 k) film on Si substrate. A thick PMMA film of about 8 µm is used except some experiments. The substrate size is 30 × 30 mm. The thicknesses of the used substrates, T_s, are 200, 675 and 1000 µm. An elastic film sheet of 200 µm in thickness is sandwiched between the silicon substrate and the stage of the press machine in order to obtain uniform pressing. The imprint conditions are 10 MPa at 180ºC for 15 min. The press pressure is released after cooling to 40ºC, and the mold is released from the substrate by the vertical pulling [7].

3. Simulation model

The conditions during the pressing process are simulated using the finite element method (FEM). In the experiment, a large number of cavities are contained in the mold. Since a long simulation time and a large number of cells are necessary for the simulation of the experimental system, the simplified simulation model is used in order to avoid heavy calculation task. Figure 4 shows a schematic diagram of the numerical simulation
model. A two-dimensional model is assumed, that is, the size in the y direction is infinite. The system has symmetric geometry at x=0 and the simulation is carried out in the right half (x>0). The cavity width used in the simulation is 125 µm, which is much larger than that in the experiment. Only 10 cavities are included in the pattern area of the 5mm mold. According to the cavity width enlargement, both the cavity depth and the PMMA thickness are also enlarged. Both the cavity depth and the initial PMMA thickness are 187.5 µm. The boundary condition between the PMMA film and the mold is touching without adhesion, and that between the substrate and the elastic film is also touching without adhesion. The substrate and mold are assumed to be a Si material (Young’s modulus =130 GPa). For the PMMA film, the modulus and Poisson ratio are assumed to be 3.0 GPa, 0.3, respectively [8,9]. These values correspond to those below the glass transition temperature of PMMA. Press pressure is applied to the system and the substrate position, z₀, which is the vertical coordinate of the boundary between the substrate and the PMMA film, is calculated. The FEM software used is MSC-Marc.

4. Results
Figures 5(a) and 5(b) show PMMA patterns at 0.25 mm inside from the edge of the pattern area for (a) 2.5mm mold and (b) 5mm mold. Only 10 cavities are included in the pattern area of the 5mm mold. According to the cavity width enlargement, both the cavity depth and the PMMA thickness are also enlarged. Both the cavity depth and the initial PMMA thickness are 187.5 µm. The boundary condition between the PMMA film and the mold is touching without adhesion, and that between the substrate and the elastic film is also touching without adhesion. The substrate and mold are assumed to be a Si material (Young’s modulus =130 GPa). For the PMMA film, the modulus and Poisson ratio are assumed to be 3.0 GPa, 0.3, respectively [8,9]. These values correspond to those below the glass transition temperature of PMMA. Press pressure is applied to the system and the substrate position, z₀, which is the vertical coordinate of the boundary between the substrate and the PMMA film, is calculated. The FEM software used is MSC-Marc.

4. Results
Figures 5(a) and 5(b) show PMMA patterns at 0.25 mm inside from the edge of the pattern area for the 2.5mm and the 5mm molds, respectively. The substrate thickness, Tₛ, is 1000 µm. Although the filling defects are observed for both patterns, the pattern shape for the 5mm mold is clearly better than that for the 2.5mm mold. The good pattern fabrication for the 2.5mm mold is more difficult than that for the 5mm mold. Therefore, the results for the 2.5mm mold is mainly shown in this paper. Figures 6(a) and 6(b) show the PMMA patterns at various lateral positions for Tₛ=1000 µm and Tₛ=200 µm, respectively. For Tₛ=200 µm, good PMMA patterns are obtained in the whole pattern area. For Tₛ=1000 µm the filling defects are clearly observed except the edge of the pattern area (x=1.25 mm). For typical case, good pattern can be obtained at the mold center as shown in Fig. 2, but no good pattern can be obtained even at the mold center for Tₛ=1000 µm.

Although the SEM observation is the powerful method in order to observe the filling defects, it is difficult to check the filling defect formation through a wide area. The area with the filling defects can be easily estimated by the height profile of the PMMA film surface. The height profile of the imprinted PMMA surface is measured by a surface profiler (KLA Tencor, Alpha step IQ). Figures 7(a) and 7(b) show the PMMA height profiles for Tₛ=1000 µm and Tₛ=200 µm, respectively. The PMMA surface positions are measured from the center (x=0 mm) to the mold edge (x=5 mm). In the following discussion, it is watched from the mold edge (x=5 mm) to the mold center (x=0 mm). In both figures, the PMMA surface positions are suddenly increased at the edge of the pattern area of x=1.25 mm, because the PMMA line patterns start. Since the step height is about 5 µm, the complete resist filling is obtained. However, for Tₛ=1000 µm, the
region with the high PMMA surface position is narrow, and the PMMA surface position is decreased rapidly. The filling defects appears and the PMMA pattern height decreases as shown in Fig. 6(a). The low PMMA surface position clearly shows the small pattern height induced by the filling defects. On the other hand, the PMMA surface position gradually decreases for $T_S=200 \, \mu m$. It is considered that the PMMA surface position gradually changes when no filling defects are generated.

The effect of the resist thickness on the filling defects is also checked. Figures 8(a) and 8(b) show the PMMA patterns at various lateral positions for the resist thickness of 10 μm and 3 μm, respectively. The substrate with 675 μm thickness ($T_S=675 \, \mu m$) is used. It is clear that the pattern shape for the thick resist of 10 μm is better than that for the thin resist of 3 μm.

5. Discussion

The variations of the substrate top, $z_0$, are simulated in order to estimate the substrate deformation. The results are also shown in Figs. 7. First, the result for $T_S=200 \, \mu m$ is considered by Fig. 7(b). Since the substrate is thin and easily deformed, the substrate position, $z_0$, is increased around the pattern area edge in the mold as shown in A’ in Fig. 7(b). The result can be explained in the following way. The mold surface during the press is considered. Since the mold cavities are filled by PMMA resist, half of the surface area is the PMMA resist in the pattern area, and whole area is Si in the flat area. Since the stiffness of the PMMA resist is much smaller than that of Si, the average stiffness in the pattern area must be smaller than that in the flat area. Then, the Si substrate is bended toward the low stiffness area around the boundary of the two different stiffness areas. Then, since the PMMA surface approaches to the mold surface, the production of the filling defects can be suppressed. In Fig. 7(b), the substrate position, $z_0$, gradually approaches to the mold and the PMMA surface position decreases.

![Fig. 7. PMMA height profile and the substrate position, $z_0$, for (a) $T_S=1000 \, \mu m$ and (b) $T_S=200 \, \mu m$.](image)

![Fig. 8. Impact of PMMA thickness on the resist filling for $T_S=675 \, \mu m$. The PMMA thicknesses are (a) 10 μm and (b) 3 μm.](image)
from x=1.25 mm to x=1.0 mm. If the mold surface is flat, the distance between the substrate and the mold surface decreases when the substrate position, $z_0$, increases. The resist thickness decreases as the substrate position, $z_0$, increases. Then, it is considered that both the residual layer thickness and the PMMA surface position decrease when the substrate position, $z_0$, increases. According to this discussion, since the $z_0$ value is almost constant within x=1.0 mm, the PMMA surface position is also constant. Around x=4.5 mm, the $z_0$ value has a valley as shown by B' and the PMMA surface position has a peak as shown by C'.

Next, the result for $T_S=1000$ μm is considered by Fig. 7(a). The substrate is thick and hardly deformed for $T_S=1000$ μm. The substrate position, $z_0$, is increased slowly as shown in A in Fig. 7(a). It is considered that the PMMA surface can hardly approach to the mold surface, and the filling defects must be induced. The mechanism of the filling defects can be qualitatively explained by the wafer deformation. However, since a very simplified model is used in this paper, the qualitative discussion is the future work.

6. Conclusions
The filling defect formation is investigated for thermal imprint of PMMA when the concave mold is used. The filling defect formation greatly depends on the substrate thickness where the PMMA film is coated. When the thin substrate of 200 μm thickness is used, no filling defects can be found. On the other hand, when the thick substrate of 1000 μm thickness is used, a large amount of filling defects is induced. It is clear that the filling defect can be suppressed by the substrate deformation. The substrate deformation is simulated by use of the simplified model, and the position of the boundary between the substrate and PMMA film, $z_0$, during the press is calculated. The filling defect formation can be explained by the substrate position, $z_0$, quite well. The qualitative discussion is insufficient in this paper and it will be a future work.

References