Simulation Study on Bubble Trapping in UV Nanoimprint Lithography

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Bubble trapping in the template pattern during the resist filling process is one of the most serious issues in UV-nanoimprint lithography. The mechanism of bubble trapping is studied based on a numerical analysis of the resist flow in a simple model. Flow behavior of water-like low viscosity liquid as a resist is investigated for particular structures of the template and various contact angles for the template and the substrate. Time evolutions of the flow of the resist are simulated and the mechanism of bubble trapping is demonstrated. The results show that large contact angle between the resist and the template causes bubble trapping, also small contact angle between the resist and the substrate causes bubble.

Keywords: UV nanoimprint, resist, polymer, contact angle, bubble trap, template, viscos flow, surface tension

1. Introduction

Bubble trapping in the pattern cavity is one of the most significant issue in UV-nanoimprint lithography (UV-NIL), however a few investigation has been reported on the resist flow dynamics into grooves of the template [1-4]. Reddy et al., numerically simulates the bubble trapping in various structures of the pattern cavity. Hiroshima proposes novel bubble free process in UV-NIL. Understanding the mechanism of bubble trapping is essential for process and material design such as the surface tensions of the template (mold) or resists materials.

In this paper, a numerical simulation of the resist flow into the pattern cavity is carried out for typical UV-nanoimprint process in variation with contact angles of the resists with template and substrate. The basic mechanism of bubble trapping is investigated.

2. Numerical Simulation Model

Figure 1 shows a schematic diagram of the resist flow when the resist is filled into the pattern cavity. The resist droplet is put on the substrate and the template with fine cavity patterns is put on it. The resist spreads in laterally and flows into the space between template and substrate.

To simplify the analysis, the template and the substrate are put at a fixed position and the resist is injected into the space between template and substrate from the left side with a constant velocity \( v \) as illustrated in Fig.2. The resist is assumed to be an incompressible Newton fluid.

The Navier-Stokes equation and continuous equation are numerically solved using commercial available software using difference method [5].

\[
\rho \frac{\partial \vec{v}}{\partial t} + \rho (\vec{v} \cdot \text{grad}) \vec{v} = -\text{grad} P + \rho \vec{g} + \eta (\text{grad div } \vec{v}) \quad (1)
\]
\[
\text{div } \vec{v} = 0
\]

where \( \rho \), \( \eta \), and \( g \) are the density, the viscosity, and the gravitational acceleration, respectively.

Physical parameters are shown in Table 1. The characteristic of the resist is assumed to be low viscous liquid. The injection velocity \( v \) of the resist is set to be 0.01 m/s, which is determined in typical experimental condition.

3. Results and Discussions

3.1 Dependence on the contact angle between resist and template \( \theta_r \)

Figure 3 shows snap shots of time progress of the resist covertures with varying the contact angle between resist and template \( \theta_r \). When the \( \theta_r \) increases, the capillary force along the cavity wall decreases and the resist flow along the template surface is suppressed. As a result, the resist flows laterally along the substrate and the resist touches to the other side of the cavity edge. Then, the resist flow is divided into two branches at the cavity edge and a bubble is trapped at the end of the cavity (Fig.3-a).

On the other hand, when the contact angle \( \theta_r \) is small, the resist flows along the wall of the cavity and the flow comes out at the corner of the cavity without branching. As a result, no bubble remains in the cavity and the resist is successfully filled into the cavity as shown in Figures 3-b and 3-c.

To eliminate the bubble trapping, lower contact angle \( \theta_r \) is demanded. However, the demand is opposite to release the template in successfully because low contact angle leads adhesion between the resist and the template.

3.2 Dependence on the contact angle between resist and substrate \( \theta_s \)

Dependence on the contact angle between resist and substrate \( \theta_s \) is investigated as shown in Fig. 4. As the \( \theta_s \) increases, the flow along the substrate is suppressed and the resist flows into the cavity. As a result, the resist is successfully filled into the cavity as shown in Fig.4-b,c.

In the same way, higher contact angle \( \theta_s \) is demanded to eliminate the bubble trapping. However, the demand is opposite to release the template because higher contact angle leads poor adhesion to the substrate.

As discussed above, the mechanism of the bubble trapping is the branching of the resist flow at the cavity corner, which depends on the surface energy of the substrate and the template.
Figure 3. Dependence on the contact angle between resist and template.

\( \Delta t = 2.0 \times 10^{-11} \text{ s}, L=100\text{nm}, h=100\text{nm}, d=50\text{nm}, \theta_r = 40 \text{ degree}, \eta = 10\text{mPas}, v=0.01 \text{ m/s} \)

Figure 4. Dependence on the contact angle between resist and substrate.

\( \Delta t = 2.0 \times 10^{-11} \text{ s}, L=100\text{nm}, h=100\text{nm}, d=50\text{nm}, \theta_r = 45 \text{ degree}, \eta = 10\text{mPas}, v=0.01 \text{ m/s} \)

Figure 5. Schematics of the resist flow for various contact angles to the resist.
3.3 Dependence on the contact angles $\theta_r$ and $\theta_s$

Figure 5 illustrates the resist flow on the contact angles at the substrate and the template. When the $\theta_r$ is high and the $\theta_s$ is low, the resist touches to the cavity edge and the bubble is trapped. On the other hand, the resist is successfully filled into the cavity when the $\theta_r$ is low and the $\theta_s$ is high.

Figure 6 shows the simulation results of the bubble trapping in various $\theta_r$ and $\theta_s$. To avoid the bubble trapping, lower contact angle between the resist and template $\theta_r$ and higher contact angle between the resist and substrate $\theta_s$ are demanded.

In this particular case, the contact angle for the template is recommended to be less than 40 degrees and the influence by the substrate is not so significant. The quantitative values of the critical conditions depend on the physical parameters such as the resist viscosity, geometrical size and surface tensions of the resist, however the reynolds number gives suggestions because the flow behaviors are equivalent under the same reynolds numbers.

4. Conclusion

The bubble trapping behavior in a UV-nanoimprint lithography process is investigated by numerical simulation for typical resist material in various contact angles between the resist and the template, and between the resist and the substrate.

When the contact angle between the template and the resist is large, the bubble is trapped into the cavity, where the demand for surface treatment on the template is opposite for successful releasing of the template.

The results depend on the resist fluid characteristics, the geometry of the cavity and the injection speed of the resist.

Further investigations are demanded on various dimensions of patterns, pillar patterns, integrated patterns and high viscosity resists.

References