# Numerical Study on Bubble Trapping in UV Nanoimprint Lithography

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## 1. Introduction

Bubble trapping into template grooves is one of the most significant issues in UV-NIL process<sup>1</sup>, however few investigations have been reported on the resist flow dynamics into grooves of the template<sup>2</sup>.

In this work, we numerically simulate the resist flow into the template groove and investigate the mechanism of the bubble trapping.

#### 2. Numerical model

Figure 1 shows schematic diagram of the resist flow. The resist droplet flows laterally in the squeezed space between template and substrate. In this work, the template and the substrate are set at the fixed position and resist flows into the cavity of the template from the left side in constant velocity v as illustrated in Fig.2. The resist is assumed to be in-compressive fluid and the Navier-Stokes equation and the continuous equation are solved using commercial available software  $\alpha$ -Flow<sup>3</sup>.

$$\rho \frac{\partial \vec{v}}{\partial t} + \rho(\vec{v} \cdot grad)\vec{v} = -grad P + \rho \vec{g} + \eta(grad \, div \, \vec{v})$$

$$1)$$

$$div \, \vec{v} = 0.$$

$$2)$$

The contact angles between resist and template  $\theta_T$  also the resist and the substrate  $\theta_s$  are modulated.

In this study, we handle relatively high viscous liquid as a ressit where the viscosity is 10 mPas.

#### 3. Results and Discussion

Figure 3 shows typical results of the resist flow. When the resist crosses over the cavity and the flow branches off, a bubble is trapped at the end of the cavity pattern (Fig.3-a). On the other hand, when the contact angle of template  $\theta_T$  is low, the resist reaches to the top of the cavity before it crosses over the cavity. As a result, the branching of the flow does not occur and it flows out at the end of the cavity (Fig.3-b). As a result, no bubble remains in the cavity. The bubble trapping depends on the geometrical configurations and contact angle of template and substrate.

Figure 4 shows the dependency on the contact angle of the template surface and substrate. When the contact angle between the resist and the template  $\theta_T$  increases, the resist flow is suppressed into the cavity. As a result, the resist flow is branched off at the corner of the cavity and the bubble is trapped into the cavity as discussed above.

As demonstrated above, the basic mechanism of the bubble trapping comes from the resist flow branching at the cavity corner. To avoid the bubble trapping, lower contact angle between the resist and template and larger between substrate are generally demanded. Nevertheless, the requirements are completely opposite directions for successful releasing of the template.

### **References**:

- [1] H. Hiroshima and M. Komuro; Jpn. J. Appl. Phys. 46, (2007) 6391.
- [2] S. Reddy, P.R. Schunk, R.T. Bonnecaze; Phys. Fluids 17, 122104 (2005)



Fig.1. Schematic resist flow in UV-NIL.



Fig.2. Schematic diagram of the simulation system



Fig.3. Mechanism of bubble trapping. (L=100nm, h=100nm,  $\eta$ =0.01Pas, d=50nm)



Fig.4. Dependence on contact angle template  $\theta_T$  and substrate  $\theta_S$  (L=100nm, h=100nm,  $\eta$ =0.01 Pas, d=50nm)