Numerical Simulation of NIL Process Based on Continuum hypothesis

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ABSTRACT

Nano imprint lithography(NIL) is a cost-efficient, high-throughput processing technique to transfer nano-scale patterns onto thin polymer films. Polymers used as the resist include UV cured resins as well as thermoplastics such as polymethyl-methacrylate(PMMA). In this study, an analytic investigation was performed for the NIL process of transferring nano scale patterns onto polymeric films. Process optimization calls for a thorough understanding of resist flow during the process. We carried out 2D and 3D numerical analyses of resist flow during NIL process. The simulation incorporated continuum-hypothesis and the effects of surface tension were taken into account. For a more effective prediction of free surface, fixed grid scheme with the volume of fluid (VOF) method were used. The simulation results were verified with experimental results qualitatively. And the parametric study was performed for various process conditions.

Keywords: free surface flow, volume-of-fluid (VOF) method, surface tension, wall adhesion, nano imprint lithography

1 INTRODUCTION

There are different fabrication methods available for the production of nanostructures. Optical lithography technique, which is widely used in semiconductor industry, is limited by the light diffraction at nano length scale. Electron beam and scanning probe microscope (SPM) lithographies suffer from low productivity while the X-ray lithography requires a major capital investment. The nano imprint lithography (NIL) is known as a low cost alternative to these methods of fabricating nano scale patterns as small as 10nm [1].

The NIL process is classified into two categories, thermal type and UV-cured type. In the view of filling process, the most difference between two types is viscosity. Usually, the high viscous resist is used in thermal type and the low viscous resist is used in UV-cured type. Both types of NIL process consist of four stages in common. Those are coating, pressing, solidifying and removing stamp (Fig. 1).

As the structures become smaller and more complex, it is very important to understand the behavior of thin resist on the substrate. Due to the size of the pattern, experimental observation may be very difficult to avoid the several defects like incomplete filling and air bubble. Therefore, numerical simulation may serve as a useful tool to design and optimize the processing conditions [2].

There are two ways to simulate nano scale flows, namely top-down and bottom-up approaches. In the top-down approach, it is assumed that the resist flow is a continuum. On the contrary, the bottom-up approach employs the molecular dynamics (MD) technique.

Even though the bottom-up approach may provide more accurate details of the resist flow behavior, comprehensive modeling is not yet available. Moreover, calculation overhead is still prohibitively large. Therefore, as a practical consideration, the top down approach was used in this study. For the numerical analysis, 2D and 3D fixed grid system was chosen to obtain the effective prediction of the flow front. And the effects of surface tension in small scale were also considered.

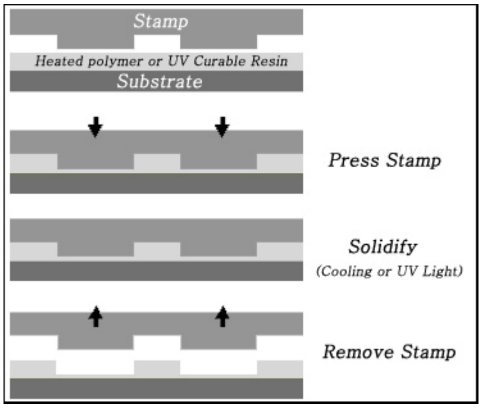

Figure 1: NIL Process

2 CONTINUUM MODEL

Behavior of thin resist during NIL process can be obtained by solving the following governing equations, continuity, navier-stokes equations [3]. We assumed the incompressible fluid and isothermal condition.

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \rho \frac{\partial u_i}{\partial x_i} = 0 \tag{1}$$

Navier-stokes equation:

$$\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = \frac{\partial}{\partial x_j} \sigma_{ji}(u) + \rho f_i \tag{2}$$

where $\sigma_{ij} = -p\delta_{ij} + 2\mu d_{ij}$, $d_{ij} = \frac{1}{2}(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i})$,

i=1,2 and j=1,2.

These equations are formulated with finite element method (FEM) using the penalty method. In the penalty method, equation (1) and (2) can be reformulated into a single equation by expressing pressure in terms of velocity as follows [4]

$$P = -\gamma_e \nabla \cdot u \tag{3}$$

where γ_e is a penalty parameter.

2.1 Volume of Fluid(VOF) Method

In the VOF method, the fractional volume is defined for element variable. The fractional volume is used to divide the total domain into two regions (occupied and empty). The values of the fractional volume (f) in fully filled cells, partially filled cells and empty cells are given by unity, between zero and unity and zero, respectively. The fractional volume is then computed and updated at each time step following the advection equation [5].

$$\frac{\partial f}{\partial t} + u_i \frac{\partial f}{\partial x_i} = 0 \tag{4}$$

where f is the fractional volume. The process of free surface construction consists of three steps: first, the flow field is solved at one time step. Then the fluid volume flux from one element to the neighboring element is calculated [14]. Finally, the fractional volume is updated. This process for each time step is repeated until the desired time is reached [6].

2.2 Surface Tension Modeling

Much attention needs to be paid to deal with surface tension because of its dominant influence on flow pattern in micro/nano scale. In order to consider the effect of surface tension in the Eulerian grid system, we used Brackbill's CSF model formulation [7], which converts the surface force to body force :

$$F = \frac{\sigma}{[f]} \kappa \nabla f, \quad \kappa = -(\nabla \cdot n), \quad n = \frac{\nabla f}{[\nabla f]} \tag{5}$$

where σ is the surface tension coefficient, κ is the curvature and $[f]$ denotes the jump of f across the interface.

2.3 Wall Adhesion

The boundary condition at the wall was imposed as the constant contact angle. This condition can be expressed using the unit free surface normal vector $\vec{n}_s$ along the wall as follows.

$$\vec{n}_s = \vec{n}_w \cos\theta + \vec{t}_w \sin\theta \tag{6}$$

where θ is the contact angle between the fluid and the wall, $\vec{n}_w$ is the unit normal vector directed into the wall and $\vec{t}_w$ is the unit tangential vector directed into the fluid.

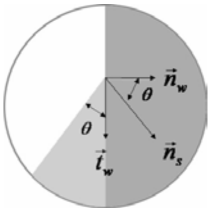

Figure 2: Illustration of wall adhesion

2.4 Rheological Behavior of Polymer Resist

The viscosity of resist shows various values according to the shear rate and the process temperature. Therefore, in thermal NIL, the viscosity of resist is calculated by the shear thinning viscosity model (Cross Williams-Lendal-Ferry model) [8].

3 VERIFICATION (THERMAL NIL)

The 2D computational domain is shown in Fig. 2. We consider the PMMA material property for simulation. The density is set to be constant (1.06×10^3 kg·m^{-3}), and the surface tension coefficient is also set to be constant (29.7mN/m).The shear-thinning effect in thermal NIL is considered with Cross-WLF model, where the viscosity is the function of shear rate and temperature.

The temperature of filling process is 170℃, the contact angle is 70º and the velocity of stamp is 10nm/s in simulation condition. To verify the simulation results, the experiment was performed in similar condition with simulation.

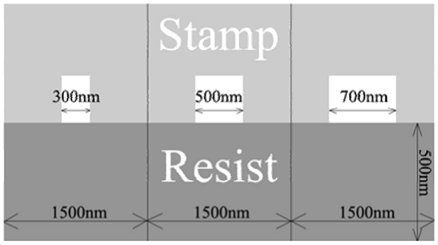

Figure 3: Geometry of 2D computational domain

When we perform the experiment to verify the simulation results, thermal NIL is more adequate than UV-cured NIL. Because the flow front is too fast phenomena to

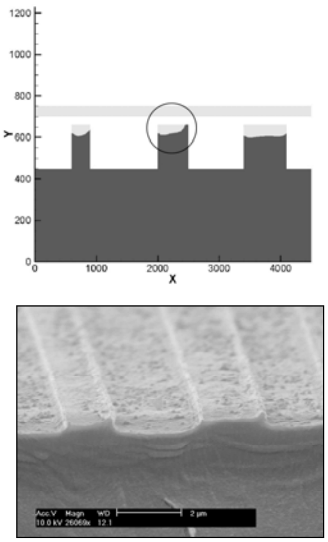

Figure 4: Verification of simulation module

observe in UV-cured NIL. So we compare the 'short-shot' experimental result of thermal NIL to the simulation result. In Fig. 4, both flow fronts show the slope of same direction which is toward the larger cavity direction. The simulation result shows the good agreement with experimental result qualitatively. Therefore, the simulation can be used to obtain the optimization of NIL process.

4 UV-CURED NIL

4.1 Parametric Study

The Parametric study according to several process variables (stamp velocity, vacuum degree and neighboring pattern effect) is performed. The 3D computational domain is shown in Fig. 5.

The velocity/pressure of the stamp is basic parameter which determines the filling time and the tolerance of resist thickness (too fast velocity makes the small filling time and the small filling mass flux, therefore the incomplete filling can be occurred). The simulation is performed in 20º (contact angle), 22.9 mN/m (surface tension coefficient). To compare the results of four 3D cases easily, the slice 2D results (flow front and velocity contour in each case) are displayed as follows.

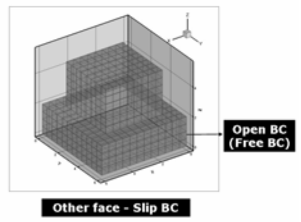

Figure 5: Geometry of 3D computational domain

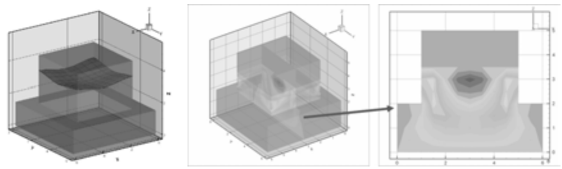
(a) (b)

Figure 6: 3D UV-cured NIL simulation result
(a) 3D Flow front in filling
(b) Sliced velocity 2D contour

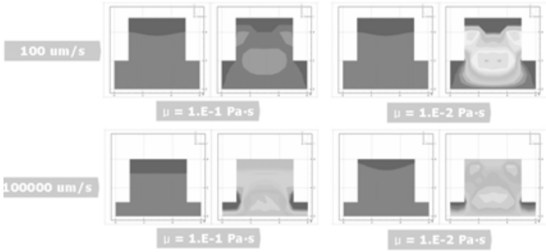

Figure 7: Slice result in 3D simulation

As can be seen from Fig. 7, we can observe that the small velocity is recommended to fill the cavity completely. As mentioned above, the requesting time to fully fill the cavity is related to the velocity/pressure of stamp. When the velocity is too high, there is not enough time to fill the cavity completely. Also, the viscosity effect can be observed from Fig. 7. As the viscosity become lower, the mobility of resist becomes higher and the filling time decreases due to the high mass flux through the resist thickness.

Next, the vacuum effect of process is simulated in range from O (~1 torr) to O (~100 torr). The simulation is performed in 20º (contact angle), 1×10^{-1} Pa·s (viscosity), 0 ㎛/s (velocity), 22.9mN/m (surface tension coefficient).

The vacuum effect in UV-cured NIL can be observed in Fig. 8 which shows the equilibrium state in process. We can see the fully filled cavity in case (a), the pulsating small bubble in case (b) and the big air bubble in case (c). Therefore, the process must be performed in vacuum degree under O (~10 torr) to fill the cavity without air bubbles.

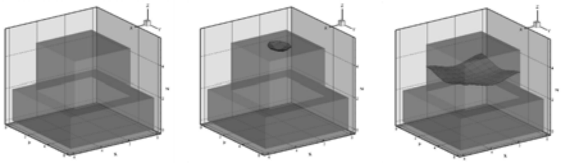
(a) (b) (c)

Figure 8: Vacuum Effect – UV cured NIL
(a) O (~1 torr)
(b) O (~10 torr)
(c) O (~100 torr)

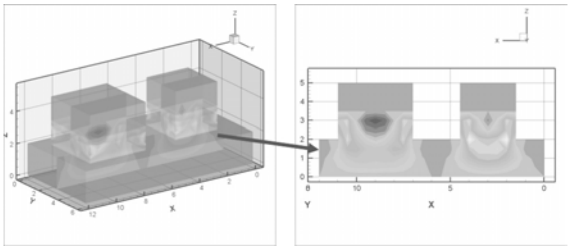

Figure 9: 3D computational domain & 2D slice results

Finally, the neighboring pattern effect is simulated in the following 3D two cavity domain and displayed with 2D slice results to compare the effects easily in Fig. 9.

The slope of flow front is similar with the verification case of thermal NIL as mentioned above. The global flow, which is affected by the several process conditions, determines the slope of the flow front. The slope of flow front according to stamp velocity is observed in Fig. 10. When the velocity is small, only capillary flow is dominant in the cavity. And the global flow goes towards the bigger cavity. And the flow front slants to that direction. On the other hand, when the velocity is too fast, the global flow goes towards out of cavity. And the flow front slants reversely. Using this slope of flow front, we can guess the location of incomplete filling and air bubble.

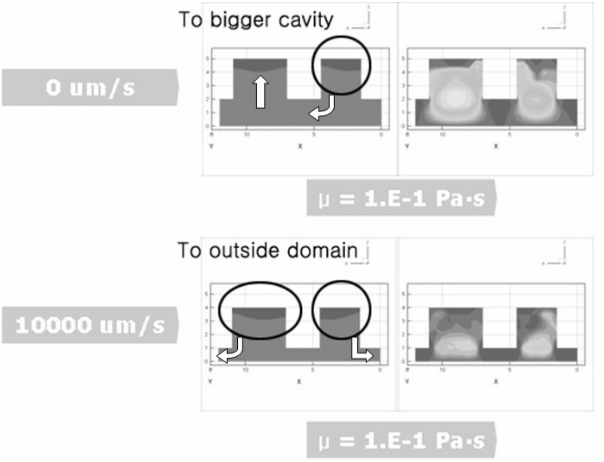

Figure 10: Slope toward the global flow

4.2 Flow Mechanism & Process Optimization

The flow mechanism in UV-cured NIL is related to three categories. The first one is material property (viscosity, surface tension coefficient and contact angle), the second one is process condition (stamp speed/pressure, vacuum degree and resist thickness), the third one is pattern shape and pattern location.

All variable of each category have relation with the filling behavior (flow mobility, wall adhesion, mass flux, etc). To optimize the NIL process, the setting of process variable must be based on this flow mechanism. We can observe the optimum of each process variable through this parametric study.

5 CONCLUSION

The flow behavior of NIL process was simulated using the simulation module based on continuum hypothesis. To simulate the nano scale free surface flow, the VOF method and the surface tension model was considered in simulation. The parametric studies such as stamp velocity, viscosity, vacuum degree and neighboring pattern effect were performed to understand the flow mechanism in NIL. Based on this flow mechanism, we can obtain the optimum parameters in NIL process.

REFERENCES

[1] S. Chou et al., 1996, "Imprint lithography with 25 nanometer resolution", *Science*, Vol. 272, pp.85-87.

[2] L.J. Heyderman et al., 2000, "Flow behaviour of thin polymer films used for hot embossing lithography", *Micro electronic Engineering*, Vol. 54, pp.229-245.

[3] L. D. Landau and E.M. Lifshitz, 1959, Fluid Mechanics, Pergamon, New York.

[4] J.N. Reddy and D.K. Gartling, 1994, “The Finite Element Method in Heat Transfer and Fluid Dynamics”, CRC Press.

[5] Hirt C W and Nichols B D, 1981, “Volume of fluid (VOF) method for the dynamics of free boundaries”, *Journal of computational Physics*, Vol. 39, pp. 201-225.

[6] Park J S, Kim S M, Kim M S and Lee W I, 2005, “Finite element analysis of flow and heat transfer with moving free surface using fixed grid system”, *International Journal of Computational Fluid Dynamics*, Vol. 19, pp. 263-276

[7] J. U. Brackbill et al., 1992, "A continuum method for modeling surface tension”, *Journal of Computational Physics*, Vol. 100, pp.334-354.

[8] Ferry J.D., 1989, Viscoelastic Properties of Polymers, John Wiley& Sons