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Polymer filling behaviors and imprinting velocities with pressure variation rates in nanoimprint lithography

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ABSTRACT

Polymer filling behaviors and imprinting velocities with pressure variation rate are investigated using numerical and experimental methods in nanoimprint lithography. In order to investigate the effects of pressure variation rate, a transient imprinting velocity is defined at each time step. Experiments are conducted in order to compare the polymer filling behaviors with the numerical results. A scanning electron microscope is used to capture the incomplete cavity filling phenomena. The results demonstrate that the imprinting velocities increased and the squeeze flow became dominant with the increases in the pressure variation rate at the pressure of 10 bar.

1. Introduction

Thermal nanoimprint lithography (T-NIL) [1] is a simple method for fabricating nano structures with a low cost and high throughput. However, imprinting failures can occur due to high pressure and temperature conditions. Therefore, a key issue in T-NIL is understanding the polymer filling characteristics in order to reduce these defects. Both experimental and numerical methods can be used to describe polymer shapes during NIL. However, because numerical analyses are used to explain the physical phenomenon in comparison with the experimental results, they must be performed.

In previous work, several researchers have investigated the polymer filling behaviors with factors such as polymer thickness, viscosity, pressure, and temperature [2–5]. Rowland et al. investigated three types of flow characteristics [2] and categorized them according to the ratio of the stamp geometry to the polymer thickness, e.g. pipe, squeeze, and stoke flows. The effects of temperature, pressure, and stamp geometry on the flow patterns were investigated by Lee et al. [3]. Furthermore, Scheer et al. explained the impact of the molecular weight and shear rate for NIL [4]. For the finite element method (FEM), Hirai et al. [5] proposed the Maxwell equation in order to demonstrate the polymer shrinkages during the demolding process. We demonstrated that the polymer filling ratios could be affected by the pressure variation rates, which must be considered as a parameter in NIL with low polymer viscosity. Moreover, the filling ratios at a constant pressure step (without considering the filling ratio at increasing pressure steps) increased with increases in the pressure variation rate even though the same pressure of 10 bar was maintained [6].

In this study, the polymer filling behaviors and the cause of the imprinting velocities are investigated when the same pressure is applied with various pressure variation rates. NIL experiments were conducted to compare the numerical results for verification. The polymer shapes were captured using a scanning electron microscope (SEM). It can be seen that both results agree well.

2. Numerical method

2.1. Overview

We performed NIL simulations using ANSYS FLUENT 14 to obtain the polymer filling behaviors and imprinting velocities, which were dominant for the filling ratio, according to the pressure variation with time (pressure variation rate). In conventional NIL simulations, the pressure variation regimes are not considered because a time step, at which pressure increased (increasing pressure step), is very short compared with a constant pressure step as depicted in Fig. 1. However, for high temperature processes, this stage could influence the overall polymer filling behaviors and the imprinting velocities due to the low viscosity. In this simulation, the pressure variation rates of 5.5, 10, 20, and 50 bar/s were defined as the parameter during NIL. The line

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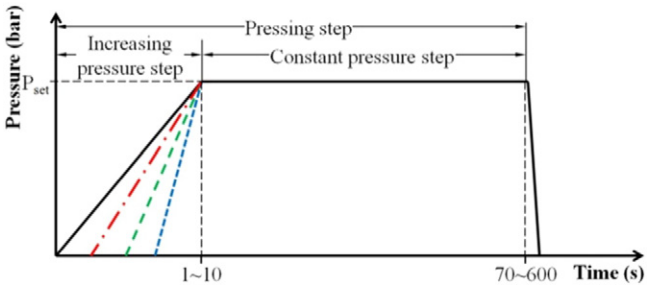

Fig. 1. NIL process and pressure variation rate.

patterns that were used were simply modeled using a two-dimensional domain as depicted in Fig. 2. Poly(methyl methacrylate) (PMMA; M_w = 75 k) was used and it was assumed to be a non-Newtonian fluid. The air was also assumed to be a compressible fluid.

2.2. Governing equations

Two governing equations [7], i.e. continuity, and momentum equations, are used in the simulation as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{v}\right) = 0, \tag{1}$$

$$\frac{\partial}{\partial t}\left(\rho \vec{v}\right) + \nabla \cdot \left(\rho \vec{v}\,\vec{v}\right) = -\nabla p + \nabla \cdot (\bar{\tau}) + \rho \vec{g}, \tag{2}$$

$$\bar{\tau} = \eta\left[\left(\nabla \vec{v} + \nabla \vec{v}^{T}\right) - \frac{2}{3}\nabla \cdot \vec{v}\right], \tag{3}$$

where ρ and ρg are the static pressure and gravitational body force, respectively. τ indicates the stress tensor; η is the molecular viscosity; and v is a velocity vector. Based on previous work, the surface tension and contact angle of the PMMA was 33 mN/m and 65° at 165 °C, respectively, calculated using the relationship of the surface energies [6].

2.3. Polymer model

It is known that when PMMA (M_w = 75 k) is above the glass transition temperature (T_g), it is a shear thinning fluid that can be well described using the Cross-WLF model [8], as follows:

$$\eta(\dot{\gamma}, T) = \frac{\eta_0(T)}{1 + \left(\eta_0(T)\,\dot{\gamma}/\tau\right)^{1-n}}, \tag{4}$$

$$\ln\left(\frac{\eta_0(T)}{\eta_0(T_0)}\right) = \frac{-C_1(T-T_0)}{C_2 + T - T_0}, \tag{5}$$

where $\eta_0(T)$, τ, and $\dot{\gamma}$ indicate the zero shear viscosity, critical shear stress at the transition to shear thinning, and shear rate, respectively. C_1 and C_2 are constant parameters obtained using the fitted Cross-WLF model. [3].

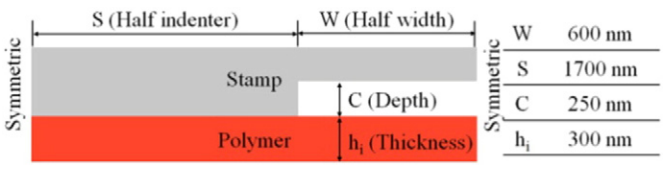

Fig. 2. Single cavity for NIL simulations.

The zero shear viscosity is dependent on the molecular weight (M_w), and it is represented using the critical molecular weight (M_c), as follows:

$$\eta_0 \propto \begin{cases} M_w & M_w < M_c \\ M_w^{3.4\pm0.2} & M_w > M_c \end{cases}, \tag{6}$$

where M_c is the critical molecular weight, which is 3 kg/mol for PMMA [9].

2.4. Imprinting velocity

The imprinting velocity was obtained from the squeeze model, as follows:

$$V = \frac{P(t)H^3(t)}{\eta(t)(S+W)^2}, \tag{7}$$

where H(t), η(t), and P(t) are the polymer thickness, viscosity, and pressure with time (pressure variation rate), respectively. S and W are the indenter and cavity widths, respectively.

3. Results and discussion

3.1. Imprinting velocity analysis

Fig. 3 demonstrates that the averaged imprinting and maximum velocities varied with the pressure variation rates in each pressure step, even though the same pressure of 10 bar was applied (Note that the results at increasing and constant pressure steps mean the averaged velocity at the step which the pressure increases until 10 bar and which maintained 10 bar for 1 s). The averaged imprinting velocity is defined as the reduced polymer thickness with time at the respective stages. In this simulation, the maximum imprinting velocity was calculated using Eq. (7) during the NIL. It demonstrated that the averaged and maximum imprinting velocities increased with the augmentation of the pressure variation rate. The imprinting velocity of 80 bar/s increased by 7%p and 11%p, respectively, compared with that of 5.5 bar/s at increasing and constant pressure steps. Furthermore, it had increased by more than 11%p when the two stages were compared.

In order to better understand this phenomenon, the variations of the pressure recorded by NIL equipment [6], polymer thickness, and viscosity according to time, where these factors strongly affect the imprinting velocity, were plotted in Fig. 4. The polymer viscosity slightly increased at the constant pressure step, in contrast to the polymer thickness

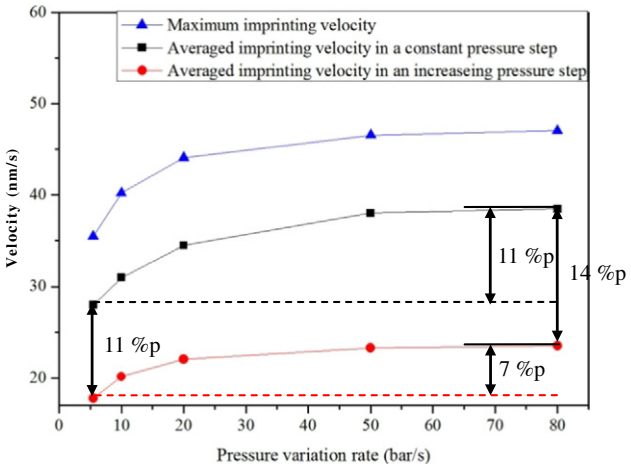

Fig. 3. Averaged and maximum imprinting velocities with the pressure variation rates in the increasing and constant pressure steps.