Prediction Model of Microlens Fabricated by Modified LIGA Process

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ABSTRACT

In this paper, we present a prediction model for microlens formation by means of a deep X-ray lithography followed by a thermal treatment of a PMMA (Polymethyl-methacrylate) sheet. According to this modeling, X-ray irradiation causes the decrease of molecular weight of PMMA, which in turn decreases the glass transition temperature and consequently causes a net volume increase during the thermal cycle resulting in a swollen microlens. Both a simple analysis and a Finite Element Analysis based on this model are found to be able to predict the variation pattern of the maximum heights of microlens which depends on the thermal treatment. The prediction model could be applied to optimization of microlens fabrication process.

Keywords: Microlens, Modified LIGA process, Prediction model, Glass transition temperature (T_g), Free volume theory.

1 INTRODUCTION

Recently, microlenses have emerged as essential components in optical communication, optical storage system, biomedical instruments, and so on. Ruther et al. [1] fabricated microlenses with deep X-ray exposed PMMA. And more recently our group (Lee et al.) [2] proposed a new fabrication method as explained below. A PMMA sheet gets exposed by deep X-ray with a certain dose and then is put into a furnace in which temperature is maintained to a preset temperature. (This temperature is called the "heating temperature" in this paper.) Then the PMMA sheet is cooled by air in room temperature. The detailed thermal treatment is described in [2]. Figure 1 shows the microlens fabricated by this new approach. To our best knowledge, a theoretical approach to describe the detailed physical process of microlens formation has not been reported yet. It would be of great importance to have an analysis tool, based on fundamental polymer physics, to predict the shape of microlens in view of optimizing microlens formation processing conditions to obtain microlens of a desired shape and designing a micro mold insert for micromolding processes. In this regard, we have developed a physical prediction modeling to predict the formation of microlens fabricated by the modified LIGA process.

(a) ϕ 500 μm microlenses (b) ϕ 300 μm microlens

Figure 1: Fabricated PMMA microlenses.

2 PHYSICAL MODELING

In a deep X-ray lithography, following experimental results of El-Kholi *et al.* [3], specific absorption dose is assumed to change only in the thickness direction of the PMMA sheet. Irradiated X-ray causes chain scission in PMMA sheet, which depends on X-ray dose. The chain scission results in the decrease of the molecular weight (M_w). We carried out optimal fittings of the experimental data of El-Kholi *et al.* [3] for M_w and X-ray absorption dose with respect to depth of PMMA sheet as follows:

$$M_w(h) = 0.6824h^{2.0255} \quad (1)$$

$$D(h) = 5.5346\times10^{6} h^{-1.7582} \quad (2)$$

where D is X-ray dose, h denoting the depth in thickness direction of a PMMA sheet with initial molecular weight of $M_{w0} = 2.05 \times 10^6$ g/mol. Figures 2 and 3 show the optimal fitting results based on Equations (1) and (2), for each case.

The molecular weight after the X-ray irradiation is often characterized by the polymer chain scission rate and cross-

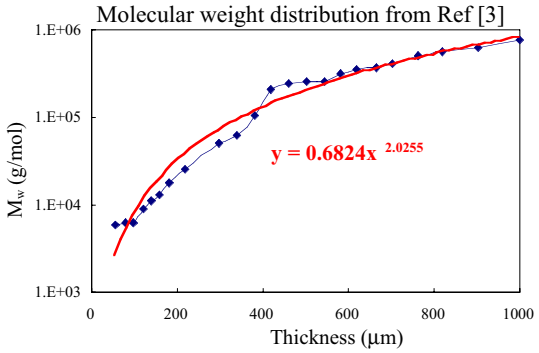


Figure 2: X-ray dose distribution in the thickness direction of PMMA sheet from the data of Ref [3].

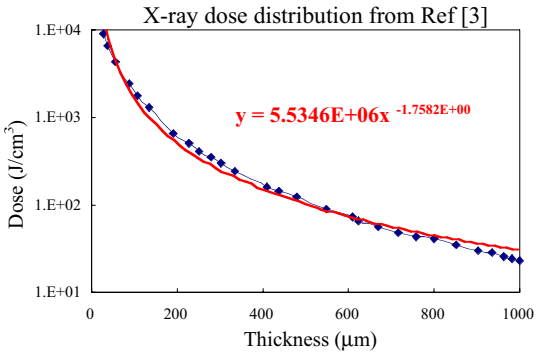


Figure 3: Molecular weight distribution in the thickness direction of PMMA from the data of Ref [3].

linking rate per energy absorbed together with the amount of dose [4]:

$$\frac{1}{M_w} = \frac{1}{M_{w0}} + \frac{(G_s - 4G_x)D}{200N_A}, \tag{3}$$

G_s and G_x denoting the amount of polymer chain scission and the number of cross-linking per 100eV of energy absorbed, respectively. N_A is Avogadro's number.

According to the theory behind the Equation (3), G_s and G_x might be just the function of temperature, independent of dose. However, experimental data of El-Kholi *et al.* [3] did indicate the dependence on dose. Therefore, in the present study, we assumed that G_s and G_x are nonlinear functions of dose. From the experimental data of El-Kholi *et al.* [3], one can indirectly find these functions collectively in terms of $G(D)$: making use of Equations (1) and (2), one can restate the Equation (3) as follows:

$$G(D) \equiv (G_s - 4G_x) = \frac{200N_A}{D(h)}\left(\frac{1}{0.6824}\left(\frac{D(h)}{5.5346\times10^6}\right)^{1.15203} - \frac{1}{M_{w0}}\right) \tag{4}$$

which is regarded as an intrinsic property of PMMA and thus will be used in our experiments and corresponding analyses.

In our experiments, we used X-ray from the LIGA beam line of Pohang Light Source (PLS) [2]. The dose of the X-ray of PLS indicated in Figure 4 is characterized by the following Equation:

$$D(h) = 2.5936\times10^{-10}h^4 - 1.4156\times10^{-6}h^3 + 3.0156\times10^{-3}h^2 - 3.3848 + 2397.6 \tag{5}$$

Therefore the molecular weight distribution of our experimental case can be calculated from Equation (3) with the help of G factor expressed by Equation (4) and the dose distribution Equation (5).

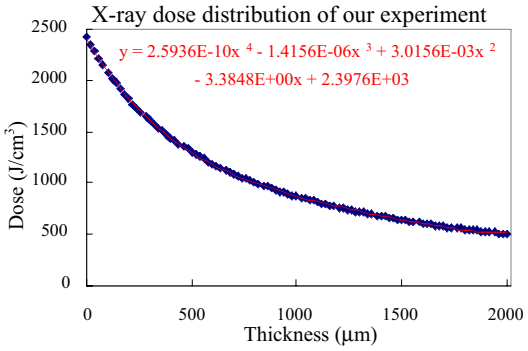


Figure 4: X-ray dose distribution in the thickness direction of PMMA sheet.

The decrease of M_w caused by X-ray exposure in turn causes the decrease of glass transition temperature (T_g). The most frequently used relation between T_g and chain-length of polymer is that of Flory and Fox, [5, 6]

$$T_g = T_{g,\infty} - \frac{K}{X_n} \tag{6}$$

where X_n is the number-averaged chain length (Note that $M_w = M_0 X_n$, where M_0 is a monomeric molecular weight, in particular, M_0 of PMMA = 100), K is a polymer-specific constant and $T_{g,\infty}$ is the asymptotic value toward which T_g tends as molecular weight increases. In this case, values of $T_{g,\infty}$ and K are 384±1(K) and 1607±170, respectively.

The change of T_g in the direction of thickness plays the key role of the lens formation due to the free volume increase during the heating and a subsequent cooling according to the free volume theory of polymeric materials. This mechanism of volume increase is, as schematically indicated in Figure 5, explained as follows:

The volume of PMMA follows curve 1 and 1' for different T_{g1} and T_{g2} during heating from T_0 to T_1. But it follows curve 2 and 2' during the subsequent rapid cooling

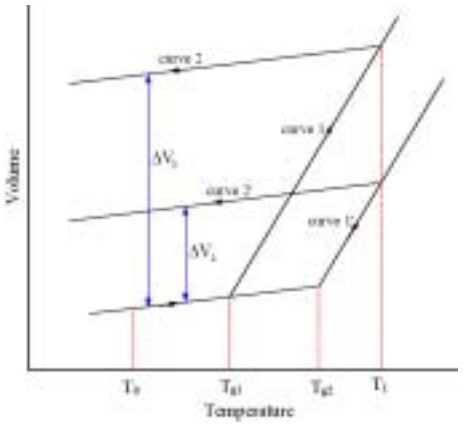


Figure 5: Free volume theory: relation between temperature and volume of polymer.

from T_1 to T_0. Therefore, heating followed by a rapid cooling result in net volume increases ΔV_1 and ΔV_2, respectively. The lower T_g is, the larger ΔV becomes. If, however, heating temperatures were less than T_g, there would be no net volume increase. The total net volume increase could be associated with the volume of the swollen lens shape. This lens formation mechanism results in the heating temperature dependence of maximum height of the final microlens shape.

It might be mentioned that there exists a relaxation process during the cooling from T_1 to T_0 with a finite cooling rate. Therefore, the net volume increase is smaller than ΔV indicated in Figure 5. However, as the first simple analysis, we ignored the relaxation phenomena in the following analysis. For a more rigorous model, one should take into account the free volume relaxation phenomena [7].

The net volume increase induced during a thermal cycle, as shown in Figure 5, can be calculated according to

$$\Delta V = \int_V (\alpha_r - \alpha_g)(T - T_g(h))H(T - T_g(h))dV \qquad (7)$$

where α_r and α_g are volumetric thermal expansion coefficients in rubbery and glassy states, respectively. We assumed, in this study, α_r and α_g set to be constant values of 645×10^{-6}/K and 213×10^{-6}/K, respectively [8]. T is a heating temperature in each thermal treatment. A heaviside step function, $H(T\text{-}T_g(h))$, is introduced to consider the variation of glass transition temperature in thickness direction related to the heating temperature T.

3 ANAYSIS

Two types of analyses were carried out for microlens formation with various heating temperatures: one is a simple approximation based on the fourth order polynomial fitting for the shape of microlens and the other Finite Element Method (FEM) analysis based on the thermal stress equilibrium. Detailed approaches are as follows:

Simple Analysis: We assumed that the shape of microlens could be described by the fourth order polynomial since the fourth order polynomial was found to fit well the experimental shape of microlens. The fourth order polynomial assumed in this study is as follows:

$$y = \frac{y_{\max}}{R^4}\left(r^4 - 2R^2r^2 + R^4\right) \qquad (8)$$

where r is radial coordinate, $y_{\max}$ is a maximum value of the polynomial and R is the radius of microlens. With Equation (8) in mind, we replaced volume, V, in Equation (7) by the volume of solid of revolution generated by the fourth order polynomial obtaining the following Equation:

$$y_{\max} = 3\int_0^{h_{\max}} (\alpha_r - \alpha_g)(T - T_g(h))H(T - T_g(h))dh \qquad (9)$$

where $h_{\max}$ means the total thickness of PMMA sheet.

Finite Element Analysis: We conducted the FEM analysis based on thermal stress equilibrium to obtain the shape of microlens induced by the net volume increase. The cylindrical portion of the PMMA sheet having 2000μm radius and 2000μm thickness was defined as a domain of computation and the axisymmetric four node linear element is adopted. The domain was divided into 1,600 elements having 40 elements along each axis.

At $r = 0$, $r = R = 750\mu m$, and $r = r_{\max} = 2000\mu m$, the symmetric boundary condition ($u_r = 0$) was imposed and at two different points, essential boundary condition ($u_h = 0$) was applied to prevent the rigid body motion.

The increase of the net volume was introduced into the FE analysis as the initial strain which is converted to the load of each element.

$$\varepsilon_{rr}^i = \varepsilon_{hh}^i = \varepsilon_{\theta\theta}^i = (\alpha_r - \alpha_g)(T - T_g(h))H(T - T_g(h)) \qquad (10)$$

where $\varepsilon_{rr}^i, \varepsilon_{hh}^i$ and $\varepsilon_{\theta\theta}^i$ are initial radial, thickness and hoop strain, respectively.

With these conditions, thermal equilibrium state at the end of the thermal cycle ($T = T_0$) was obtained with the free surface being the part of FEM solution.

4 RESULTS AND DISCUSSION

The results of model prediction, introduced in this study, are presented below. The distribution of M_w calculated with the help of Equations (3)-(5) is shown in Figure 6. Then T_g distribution corresponding to molecular weight change is calculated based on Equation (6) as plotted in Figure 7. Figure 8 (a) and (b) show microlens shapes from the real experiments and corresponding ones predicted by the simple approximation (from Equation (8) and (9)) and FEM (from Equation (10)), respectively, for two heating temperature cases. Plotted in Figure 9 are variations of the maximum heights of microlens as a function of heating temperature obtained from the experiments, the simple prediction, and FEM.

In Figure 9, the prediction results seem to be generally in good agreement with experimental data. The sharp increase of the height seems to coincide with the glass transition temperature, and even the plateau was predicted in accordance with the experiments.

It may be mentioned that the analysis is based on the assumption that the X-ray dose is independent of radial direction so that there is no effect of microlens radius in the analysis. As far the radius effect of experimental data is

concerned, there is no clear trend in our data. One can also find that there is a systematic overestimation of prediction

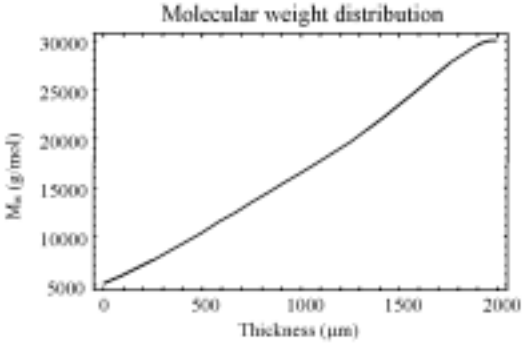


Figure 6: Molecular weight distribution in the thickness direction of PMMA.

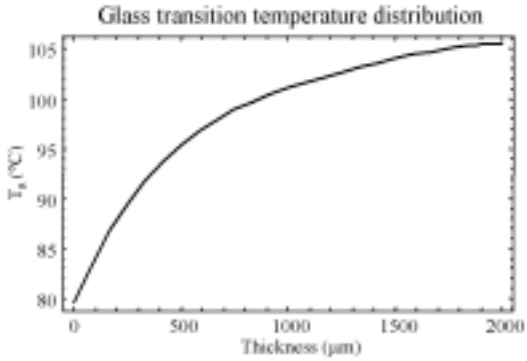
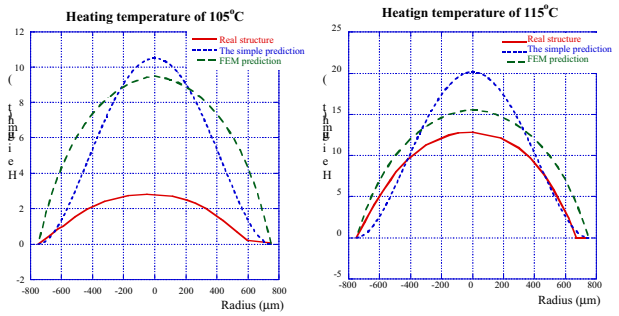


Figure 7: Glass transition temperature distribution in the thickness direction of PMMA sheet.



(a) 105°C case (b) 115°C case

Figure 8: Microlens shapes of real structure (solid line) and predictions by the simple (dotted line) and FEM (broken line) analyses at two different heating temperatures of: (a) 105°C (b) 115°C.

results in comparison with real experimental data. The overestimation could be due to the neglect of the relaxation process during cooling in thermal treatment. In this regard, it would be of great interest to incorporate the relaxation phenomena into the modeling for a more rigorous predictive numerical analysis tool.

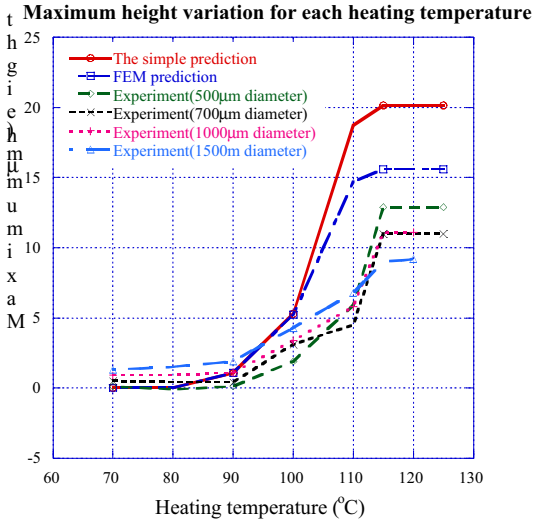


Figure 9: Comparison of the maximum heights of microlenses from experiments (dotted lines) and predictions by the simple (solid line) and FEM (broken line) analyses.

5 CONCLUDING REMARKS

The prediction model, suggested in this study, seems to successfully explain the physical process of microlens formation and to be capable of predicting the shape and the variation pattern of the maximum heights of microlens. The prediction model could be applied to optimization of microlens fabrication process and design of mold insert for microlens of micromolding.

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