Simulation and optimization of roll to roll hot embossing based on viscoelastic material PMMA

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Abstract. The roll to roll hot embossing (R2RHM) is an innovative technique for rapid fabrication of polymer microcomponents. In this paper, ABAQUS simulation software is used to establish the roller model in R2RHM. Moreover, the polymer material model PMMA viscoelastic material model is given by Prony series and WLF equation. Based on these models, the influence of five factors, as pattern radius, velocity, interference, temperature and duty cycle, on the quality of R2RHM is studied by a control variable method, and the influence trend of each single factor on the quality of hot impression is obtained. It is resulted that the radius of the pattern has little effect on the quality of the hot impression, while the velocity, interference, temperature and duty cycle exhibited a significant effect on the quality of the hot impression.

1. Introduction

Nano-imprint includes two types of embossing as plane embossing and roll to roll (R2R) embossing. The plane emboss suffers from the drawbacks of low efficiency and high cost, while the continuous R2R embossing technique can provide a solution for high resolution, low cost and large scale throughput of reproducing microstructures\cite{1-3}. The R2RHM belongs to the R2R embossing, in which the polymer is set as a substrate for embossing materials, then a rolling mold with a micro-nano structure is used to heat and soften the substrate for continuous embossing\cite{4, 5}.

The main index to judge the rolling embossing is the copying accuracy, also known as the reproduction accuracy, which is a focus of the industry\cite{6}. The accuracy of the embossing pattern is related to many process parameters, but for rolling embossing, especially rolling hot embossing, there is still no complete process parameters to guide the production\cite{7}. To solve this problem, a viscoelastic material model of Polymethyl Methacrylate (PMMA) with R2RHM is established. Here, ABAQUS is adopted to simulate the demolding and cooling processes of PMMA R2RHM. In addition, the key technological parameters are studied to explore the influence of various factors on emboss pattern quality. Suitable technological parameters are obtained for R2RHM, so as to improve the complex precision of embossing pattern and provide theoretical guidance for practical industrial production.

1.1. Hot embossing theory

In plane hot embossing, the PMMA materials are heated to the transition temperature of glass\(T_g\), then the roller is pressed into the polymer material at a certain pressure as shown in
Finally, demolding is operated and the micro/nanostructures are obtained. The processes are shown in Fig.1.

![Plane hot embossing process][1]

For the plane hot embossing, the emboss materials has to be heated and cooled, which makes the efficiency greatly affected since it is a long heating period. Therefore, the thermal imprint lithography process must be improved for mass production, and the thermal R2RHM is introduced as a solution. In the R2RHM process, a resist sheet continuously passes through a small gap between the dual rollers. One of the rollers is usually wrapped or installed with a patterned stamp and the patterns on the stamp are directly transferred onto the resist surface. The continuous R2RHM process can improve the processing speed dramatically. Meanwhile, it is ensured that the resolution quality remains as good as that of other thermal imprint methods [9]. In addition, the R2RHM process can be done with relatively less imprinting force, because the mold makes line contact with the substrate, thus concentrating the imprint force on the imprinting area [10]. The R2RHM process is shown in Fig.2. In this paper, we simulate the process of figure 2(a).

![Two ways of R2RHM][2]

### 1.2. Three Finite element simulation models

Instead of solving for the 3D system which requires a considerable amount of computation time, a simplified model of feature filling process into a few units feature cavity is shown in Figure 3. The roller with a series of linear patterns on the outer edge does a pure roll relative to the embossed polymer, and at last the embossed patterns are obtained by heating, embossing, and demolding. The roller is assumed to be rigid-body in the simulation due to it's much harder than a liquid polymer.

![Finite element model of R2RHM][3]

PMMA is an imprinted substrate polymer material, and its material characteristics are shown in Table.1:

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[1]: Figure 1. Plane hot embossing process[8].
[2]: Figure 2. Two ways of R2RHM[11].
[3]: Figure 3. Finite element model of R2RHM.
Table 1. Three Scheme comparing.

| material parameter                  | value   |
|-------------------------------------|---------|
| density (g/cm³)                     | 1.19    |
| Poisson's ratio                     | 0.3     |
| young's modulus (GPa)               | 3.65    |
| specific heat capacity (J/Kg.K)     | 1470    |
| glass transition temperature (℃)    | 109     |

The viscoelastic properties of polymers are usually expressed by the FLW model equation of the Prony series in ABAQUS, and the glass transition temperature (Tg), reference temperature, C1 and C2 values of the given material are required for the description. In this paper, the Tg of PMMA material is 109℃, and the values for C1 and C2 are 16℃ and 56℃, respectively. The PMMA of Prony parameters are shown in table 2:

Table 2. Stress relaxation parameters of PMMA viscoelastic model [12].

| NO. | g/MPa | k/MPa | T_aui/MPa |
|-----|-------|-------|-----------|
| 1   | 0.2106| 0.2106| 7.92E-005 |
| 2   | 0.3385| 0.3385| 0.00612   |
| 3   | 0.2573| 0.2573| 0.179     |
| 4   | 0.1362| 0.1362| 2.67      |
| 5   | 0.0396| 0.0396| 27.5      |
| 6   | 0.0128| 0.0128| 216       |

2. The influence of various factors on the quality of embossing

In the initial simulation, the roller radius is set to be 5 mm, and the rotation speed is 0.1mm/s, the temperature is 112℃, the distance between mold and PMMA is -45 μm. In order to reduce the influence of the adjacent pattern of the imprinting, the duty cycle is 4 times of the pattern radius, the thermal conductivity coefficient is set 2.7e-5, and the semi-circle pattern radius is 100 μm. An initial result is presented in Figure 4. The area S1 denotes the reproduction area of the embossing pattern, and the area S1+S2 indicates the area of the original pattern, hence the area reproduction ratio is S1/(S1+S2).

Figure 4. duplicated pattern.

2.1. Influence of the semi-circle pattern radius for transfer quality

The semi-circle pattern radius is set to be 25 μm, 20 μm, 30 μm, 40 μm, respectively, and other simulation parameters remain invariant. The analysis results are shown in Figure 5, which shows that the area reproduction ratio varies between 89.53% and 92.36%, and the corresponding variation amplitude is only 2.83%. It can be concluded that the pattern radius has little effect on the quality of R2RHM.
2.2. Influence of the interference between mold and PMMA

Keeping other simulation parameters remain unchanged, in this section, the distance between mold and PMMA is set to be 0 μm, -15 μm, -30 μm, -35 μm, -40 μm, -45 μm, -50 μm, -55 μm, -60 μm, respectively. The analysis results are shown in Figure 6, which demonstrates that area reproduction ratio increases with the magnitude of interference. Hence we can get the conclusion of the influence of interference on the quality of R2RHM, which is the larger the interference, the better the quality.

Figure 5. Influence of the semi-circle pattern radius.

Figure 6. Influence of magnitude of interference.

2.3. Influence of the duty cycle

Figure 7 shows the results when the duty cycle is 0.5, 1, 1, 2, 2.5, 3, 4, and 6 respectively while keeping other factors constant. It can be seen that the area replication rate increases with the increase of duty cycle, and basically remains unchanged after duty cycle $\geq 3$. So it is concluded that the duty cycle has a great impact on the quality of hot stamping. To be more specifically, the better the quality is with the increase of duty cycle when duty cycle $< 3$, while the better the quality of hot stamping after the duty cycle $\geq 3$.

2.4. Influence of the temperature

When the temperature is lower than the polymer material glass temperature ($T_g=109^\circ C$), the material model is in the glass state, which is not easy to deform and cannot be used for hot embossing. Therefore, the R2RHM temperature in this topic is above 109°C. Figure 8 shows the results when the temperatures are 109°C, 112°C, 114°C, 116°C, 118°C, 120°C, 124°C, 128°C, and 132°C respectively while keeping other factors invariant. The result shows that the area replication rate increased firstly and then decreased with the increase of temperature, and reached the maximum near 116°C. When the embossing temperature is too high, PMMA material is in a viscous flow state, which is characterized by fluid property and high fluidity, resulting in a low area replication rate. When the temperature is between 109°C and 116°C, the PMMA state is in the transition interval from glass state to high elastic state, which cannot fully show the property of the high elastic state and easy deformation, thus resulting in the best quality of embossing near the temperature of 116°C.
2.5. Influence of the rotation speed for transfer quality

Figure 9 shows the results when the specific heat capacity ($K$) and rotation speed as shown in table 3.

| Speed (mm/s) | 0.01 | 0.1 | 0.3 | 0.5 | 1   | 10  | 50  | 100 | 200 |
|-------------|------|-----|-----|-----|-----|-----|-----|-----|-----|
| $K$ (e^{-4})| 0.034| 0.27| 1.0 | 1.85| 3.8 | 38  | 200 | 380 | 950 |

It can be seen from the graph that the area replication rate decreases rapidly with the increase in velocity. According to these data, we can draw the conclusion that speed has a great impact on the quality of R2RHM, and the smaller the speed, the better the quality of R2RHM. By checking the stress in the process of hot stamping, it is found that the maximum stress at the release time is 52050.4 N/mm$^2$ when the speed is 0.01 mm/s. When the velocity is 200 mm/s, the maximum stress at the release time is 445964 N/mm$^2$. When the speed is slow, the contact time between the mold and the polymer model is longer, and the stress relaxation reduces the internal stress of the material, leading to the smaller recovery deformation after demolding with a higher area reproduction rate. However, when the speed is accelerated, the contact time between the mold and the polymer model is shorter, and the stress relaxation phenomenon is not obvious, resulting in the internal stress of the material is larger when the mold is released, which is easy to recover the deformation. Therefore, the quality of hot stamping decreases with the increase in speed.
3. Conclusion

In the simulation, the forming polymer material PMMA is assumed to be a viscoelastic model. In summary, R2RHM process is investigated by numerical analysis, and the area reproduction rate of the pattern is taken as the main index to judge the accuracy of the embossing. The influences of several factors such as 1, 2, 3, 4, 5 are studied with a control variable method. Simulation results show that a smaller size pattern affects the accuracy of embossing patterns, in R2RHM permissible range, the greater the magnitude of interference, the higher the accuracy of embossing pattern and pattern duty ratio is 3, embossed graphic print effect best, with the increase of embossing temperature, the complex precision of graphics is presented to improve the phenomenon of lower, after the stamping the temperature about $116\,^\circ\text{C}$, the rolling precision of pattern is best, and with the increase of rolling speed, patterns fidelity showed a sharp decline in the trend. Therefore, in order to ensure the emboss accuracy of the rolling patterns, the interference value of the rolling mold and the embossing object should be larger, the duty cycle of the pattern should be greater than 3, the rolling temperature should be selected to be about $116\,^\circ\text{C}$, and the embossing speed should be selected to be as small as possible to meet the productivity requirements. The simulation results are helpful to optimize the R2RHM mold, polymer parameters and technological parameters of R2RHM process.

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