Stress and Deformation Behaviors in Polymer Resist during Demolding Process of Hot Embossing via Finite Element Method

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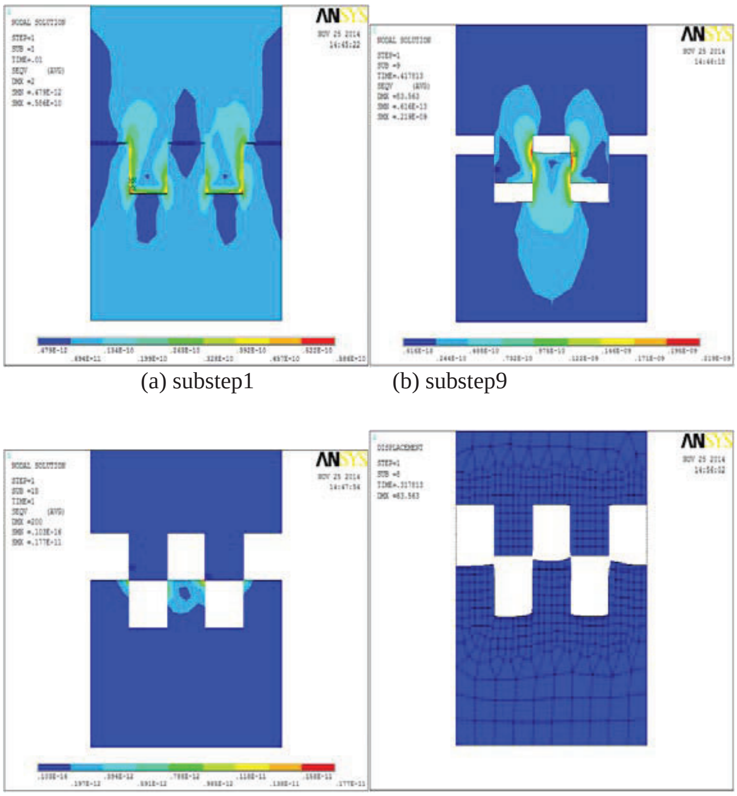
With the developments of large-scale parallel replication for hot embossing technologies, hot embossing has become not only popular in laboratories but also applicable in mass production. In hot embossing, a thermoplastic polymer is heated up over its glass transition temperature (Tg) , and a fine mold with desired structures is pressed into the polymer. [1] After cooling down below Tg, the mold is released and the fine patterns on the mold are transferred to the polymer. The process of demolding plays an important role to determine the success of imprinting fine patterns. In the demolding process, separating the mold from the patterned layer is easy to induce defects. Therefore, it's necessary to investigate the demolding behaviors in contact detaching process. In this report, the authors studied the stress and the deformation behaviors in polymer resist during demolding process of hot embossing via finite element method (FEM). A simple model structure of the nickel (Ni) mold/ poly (methyl methacrylate) (PMMA) resist was employed for the simulation, considering the adhesion and the friction forces.

Figure 1(a) ~ (d) show the evolution of the Von Mises stress and the deformation in PMMA resist for different substeps. From Figure 1(a) ~ (c) it can be seen that stress concentrates at two different key locations in PMMA. The first location is at root of the polymer microstructure, the transition corner zone between the replicated pattern and the residual polymer. The second location is the contact region with the releasing mold edge. Furthermore, as can be identified from Figure 1(d), necking deformation generated at the root and material transfer occurred at the top edge. Different from previous simulation work by Tang et al.[2], in which only stress distribution was observed, our simulation results clearly illustrate polymer deformations as well as Von Mises stress. And these deformations are in line with the pattern defects in actual demolding operation. This is attributed to the application of the Mooney-Revilin model parameters for PMMA in the simulation.

Figure 2 shows the single symmetric structure with one demolding centerline and a set of feature nodes, which located in the polymer microstructure. In order to obtain force regularities of the polymer resist, we simulated the contact forces of the top nodes and the root nodes in all stages of demolding process. In the initial demolding, the horizontal contact force on Node 3, H_3, changes little and remains negative value, which means that H_3 is in the opposite direction to the Horizontal, as can be seen in Figure 3. The vertical contact force on Node 3, V_3, is mainly positive value and reaches a peak value of 0.7 nN when the demolding displacement is 18 nm. At this moment, H_3 approximates to zero. Resultant force F_3 has an oblique direction. Simultaneously, the horizontal and vertical contact force on Node 4, H_4 and V_4, have peak values of 0.8 nN and 1.6 nN, respectively. These striking contact forces on polymer, F_3 and F_4, will trigger local high stress and obvious deformation

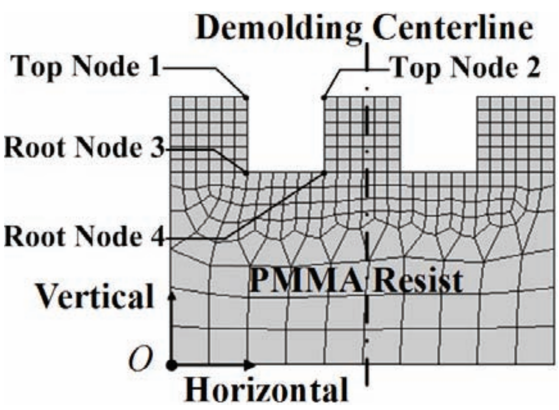
References:
1. Y. Hirai, S. Yoshida, and N. Takagi, J. Vac. Sci. Technol. B **21**, 598 (2008).
2. Q. S. Tang, J. Jin, X. Li, Z. L. Zheng, and X. D. Wang, Vacuum. **49**, 32 (2012).



(a) substep1 (b) substep9

(c) substep15 (d) deformation

Fig. 1. Equivalent stress contours of different substeps and deformation shape of polymer



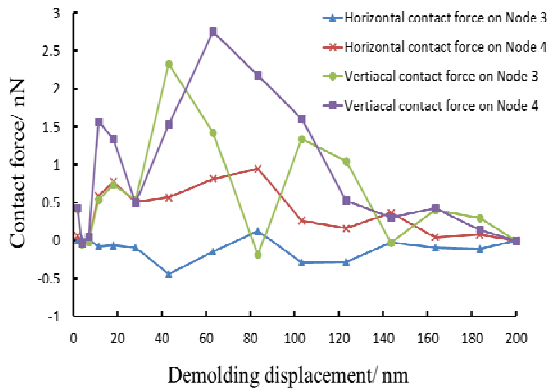


Fig. 2. The single symmetric structure with one demolding centerline and four feature nodes

Fig. 3. Contact force curves of root nodes