Effects of Contact States on Polymer Pattern Deformation during Demolding Process in Nanoimprint Lithography

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As a simple, inexpensive process used to fabricate micro- and nanometer-sized patterns with high throughput and resolution, hot embossing has become not only popular in laboratories but also applicable in mass production to produce large-scale parallel replication. 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. 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 mold/ poly (methyl methacrylate) resist was employed for the simulation, considering the adhesion and the friction forces as shown in Fig. 1.

According to the difference of the contact states between mold and polymer, demolding model is divided into three kinds of contact types. Through the analysis of necking displacement of nodes located different position in three kinds of contact types, it is easy to learn that the necking displacement at the middle of polymer embossment is the most obvious. Figure 2 shows the necking displacement of nodes located middle position in three kinds of contact type. About the initial stage of demolding process in three kinds of contact types, when demolding displacement is below 100nm, necking displacement aroused in incomplete contact type can be neglected and the necking displacement in sufficient contact type reach the maximum value. When demolding displacement is more than 100 nm, the demolding process of three kings of contact type enters a stage that friction of the vertical contact prevents demolding without exception. Therefore, necking displacement of three kinds of contact type has similar fluctuation trend in this stage and the gap of their maximum is smaller. Compared with complete contact type and sufficient contact type, demolding force in incomplete contact type corresponds to the same demolding stage is greatly reduced, which greatly reduces the possibility that the polymer embossment is teared and broken. Compared with sufficient contact type, the adhesion force of the lateral contact at the top in complete contact type determines the second peak of the demolding force and has no effect on demolding force other stages. It is also further shown that the adhesion force of the lateral contact at the top directly determines the maximum necking displacement that polymer embossment can reach in the whole demolding process. The excessive adhesion force of the lateral contact at the top will make polymer embossment tear or break, which will lead to serious defects in the imprinted polymer pattern and the failure of imprint. Therefore, reducing the adhesion force of the lateral contact at the top has a very important significance for reducing imprinted polymer embossment defects.

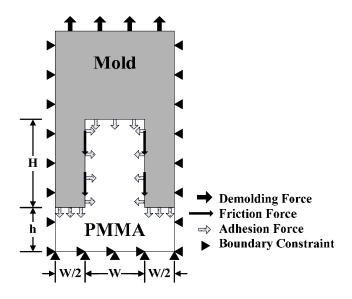


Fig.1. The geometric model and boundary conditions during demolding process.

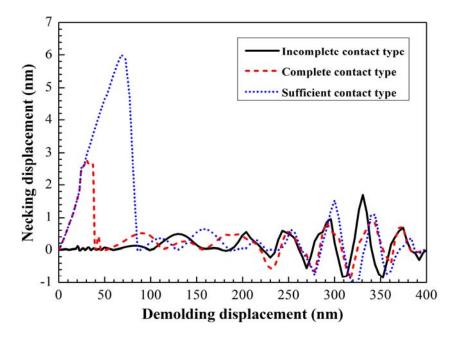


Fig. 2. Necking displacement of the nodes located middle position in three kinds of contact types.