FEM Simulation for Demolding Process in Thermal Imprint Lithography

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ABSTRACT

In thermal imprint lithography, most of the imprint failures occur during demolding, a process to separate the mold insert from the substrate after conformal molding. The success of demolding is determined by the stress generated in the resist layer on the substrate with respect to the yield stress of the resist. In this paper we have simulated the demolding process in thermal imprint lithography using the finite element method in order to study stress and deformation behavior in a poly(methyl methacrylate) (PMMA) resist layer. During demolding, the stress is concentrated both at the corner region of the PMMA resist and close to the corner of the moving stamp. The highest local stress value shows two maximums as demolding proceeds, indicating that a structural failure can occur both when demolding starts and immediately before demolding ends. Furthermore, we have investigated the influence of demolding angle and stamp geometry on the local stress and deformation.

Keywords: imprint lithography, demolding, finite element method.

1. INTRODUCTION

Imprint lithography is a technique with great potential to define micro- and nanoscale patterns with high throughput and at low cost [1]. The imprinting process consists of three sequential steps: molding (including preheating), cooling and demolding, which altogether determine the fidelity and stability of the replicated patterns. During the molding step, a stamp with desired structures is pressed into a substrate coated with a thin polymer resist. After conformal molding, the stamp/substrate assembly is cooled down, with pressure held constant, below the glass transition temperature of the resist. Finally, the pressure is released and the stamp is separated from the substrate. Extensive research has been performed both experimentally and numerically on polymer flow behavior during molding in order to improve the precision of pattern transformation and the yield of the process [2-6]. However, study of demolding is still lacking despite the fact that it is demolding that determines the success of the imprinting, because most of the structural damages occur at this step.

Demolding is a process to overcome all levels of chemical (adhesion) and mechanical interactions (residual stress) between stamp and substrate formed by the process histories during molding and cooling, which are strongly dependent on material properties. During demolding, resist at the interface experiences friction and adhesion forces (acting along and perpendicular to the interface, respectively), which result in a significant change in the stress distribution within the resist layer as demolding proceeds. Resist deformation is determined by the relative magnitude of the local stress to the yield stress of the resist and in the worst case a catastrophic imprint failure can occur. Recently, two research groups studied the demolding process in imprint lithography by finite element method (FEM) simulations [7-9]. They analyzed the stress in resist as a function of the location of the structure from the shrinkage center and concluded that building additional structures around the active pattern area will protect the active patterns from suffering high stress. The related experiments proved that the demolding force can be reduced up to 75% through this method [7, 9]. Guo et al also showed that a PTFE coating dramatically reduces the surface energy of nickel molds; facilitating demolding of high aspect ratio structures and prolonging the lifetime of the mold insert [9].

Despite some significant researches mentioned above, the mechanical response of polymer resist during demolding, which determines the success of demolding and stability of replicated patterns, has not been systematically investigated. Optimal process conditions, stamp geometries, and materials constraints that will allow for low stress during demolding are not known yet. Thus, a systematic study on the demolding process is imperative.

In this paper, we investigated stress and deformation behavior in a poly(methyl methacrylate) (PMMA) resist layer on Si substrate by performing FEM simulations for the demolding process under various demolding conditions. The aim of this work is to study details on the evolution of local stress in the resist layer with demolding time in order to understand the exact locations and time points when plastic deformation can occur in resist. In addition, we studied the influence of process and geometric parameters on the stress and deformation in the PMMA layer during molding.

2. SIMULATION METHODOLOGY

2.1. Mold Creation

A two-dimensional symmetric model, as shown in Figure 1, is created to represent a silicon stamp/PMMA resist/silicon substrate assembly. The plane stress assumption is made to simplify the simulation. The silicon stamp and substrate are described as isotropic elastic materials while the PMMA resist is modeled as thermo-viscoelastic material. The interface between the resist and the substrate is defined as glued interface; stress and displacement discontinuity is not allowed. The interface between the stamp and the PMMA resist is defined as a slip-allowed interface. This assumption can be justified because the adhesion at the stamp/PMMA interface is much lower than that at the PMMA/substrate interface due to an anti-adhesion coating that is applied on the stamp surface. A fixed boundary was applied to the bottom surface of the substrate and a symmetric boundary condition is applied on the central line to reduce calculation time. 4-node structural element PLANE42 is employed to mesh the PMMA resist, with controlled size of 0.2 μm.

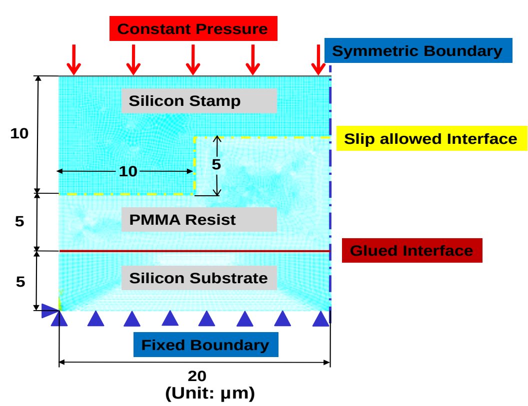

Figure 1 A 2-D model of stamp/resist/substrate assembly used in simulation.

2.2. Viscoelastic Model of PMMA

In the viscoelastic model, a deformation up to the yield point is governed by at least one, but usually more than one relaxation mechanisms. Each of these mechanisms has its origin at the molecule level and is activated by time and temperature [10].

The viscoelastic deformation is commonly described by a Boltzmann single integration representation in its relaxation form,

$$\sigma(t) = \int_{-\infty}^{t} E(t-t')\dot{\varepsilon}(t')dt'$$

The time-dependent modulus $E(t)$ can be captured by a mechanical model with a sufficient number of elastic and viscous elements. The elastic modulus of the spring-dashpot system (Maxwell model) can be expressed as follows.

$$E(t) = E_0 + \sum_{i=1}^{n_1} E_i \exp(-\frac{t}{\tau_i})$$

Here, τ_i = η_i/E_i refers to the relaxation time of the i^{th} Maxwell element. The strain rate dependence is neglected, thus relaxation time of each Maxwell element is input as constant.

Stress relaxation spectrum is shifted by the temperature change according to Williams–Landel–Ferry (WLF) Equation

$$\log a_T = -\frac{C_1(T-T_g)}{C_2+(T-T_g)}$$

where T_g refers to the glass transition temperature of PMMA; C_1 and C_2 are material constants. For our simulation, T_g is 110°C; C_1 and C_2 are 12.796 and 74.787, respectively, which were determined by dynamic mechanical analysis by Worgull et al. [8].

2.3. Process Assumptions

In order to simplify the simulation without losing generality, following assumptions were adopted:

1. The cavity in the stamp structure was completely filled by PMMA resist at the molding temperature of 170°C.
2. Flow stress generated in the molding step was neglected. This can be justified because the flow stress is smaller than the thermal stress generated due to the mismatch of thermal expansion coefficients during cooling.
3. The whole stamp/PMMA/substrate assembly was cooled down isochronously and heat transfer between different parts was ignored. Thus, the thermal-structural coupled analysis was simplified to the structural analysis. The demolding temperature was 70°C.

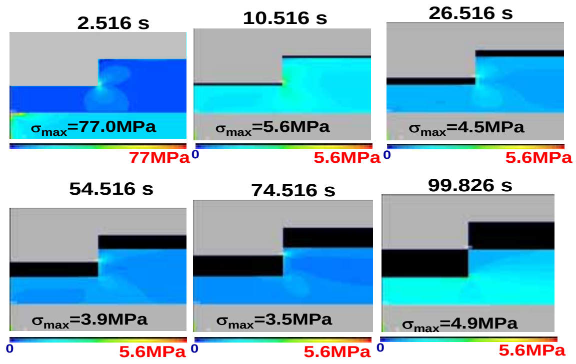

Figure 2. Von Mises stress distribution in PMMA as a function of demolding time. The maximum stress in the PMMA layer for each demolding time is also shown.

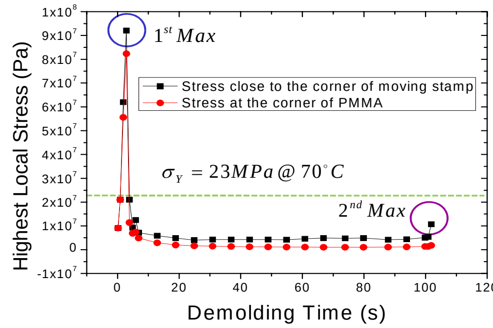

Figure 3. Highest local stress at the corner region of the PMMA resist and at the corner of moving stamp as a function of demolding time.

4. After cooling, a displacement of the stamp away from the substrate surface was applied to simulate the demolding process. The friction coefficient between PMMA and stamp surface was assumed to be 0.3. The demolding speed of 0.05μm/s was applied.

5. All the materials are assumed to be isotropic and material properties of silicon are assumed to be temperature and time independent.

3. RESULTS AND DISCUSSION

3.1. Normal Demolding of Single Structure

To understand fundamentals of mechanical behavior in PMMA as well as at the stamp/PMMA interface during demolding, we first simulated a simple demolding process for a single symmetric structure, where the stamp is normally displaced from the interface. Figure 2 shows Von Mises stress distribution in the PMMA layer as a function of demolding time. Stress concentrates at two different locations during the whole demolding process. The first location is close to the corner of the stamp moving up and the second location is at the corner region of PMMA resist. The stress concentration in the PMMA layer resulted from its viscoelasticity. The stress in silicone is completely recovered from elastic deformation immediately after unloading. However, the stress in PMMA will not relax immediately, but follow multi-relaxation mechanisms, each of which is governed by a relaxation time. Thus, the residual stress will concentrate to the corner of PMMA, which is a geometric singularity. Stress concentration at the corner of the moving stamp is caused by the geometry confinement. Figure 3 presents the highest local stress values at both locations as a function of demolding time. The yield stress of PMMA is also shown. At the beginning of demolding, the highest local stress at both locations increases dramatically and reaches a maximum value (1^{st} maximum stress). The stress then decays rapidly and, just before the demolding process ends, slightly increases again (2^{nd} maximum stress). Under the simulation conditions used, a resist deformation is expected to occur only at the beginning of demolding, where the local stress exceeds the yield stress of PMMA. However, the appearance of the second maximum at the end of demolding indicates that structural failure can also occur at the end of the demolding process. This will be seen in the next section when non-normal demolding conditions are applied.

3.2. Influence of Demolding Angles

In practical operations, absolutely normal demolding is extremely difficult to achieve. For example, during the peeling-off process of the structure with dimensions shown in Figure 4, the angle for the microstructures in the center (O) and at the fixed edge (A) at a completion of the stamp/substrate separation is 0.22° and 0.88°, respectively.

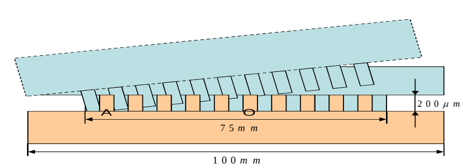

Figure 4. Schematics of a non-normal demolding situation (peel-off process).

We have simulated such non-normal demolding situations by applying a displacement of the stamp at different demolding angles. Figure 5 shows the highest local stress with demolding time for different demolding angles. With increasing demolding angles, there is a slight increase in the first maximum stress. However, the second maximum stress increases dramatically. At the beginning of demolding, lateral compression is small. Thus, the first maximum stress does not show a strong dependence on the demolding angle. However, at the end of demolding the cumulative effect of lateral compression becomes dominant, leading to a significant increase in the second maximum stress. Particularly, when demolding angle reaches 4.6°, second highest stress exceeds first highest stress and becomes the decisive factor in structural failures.

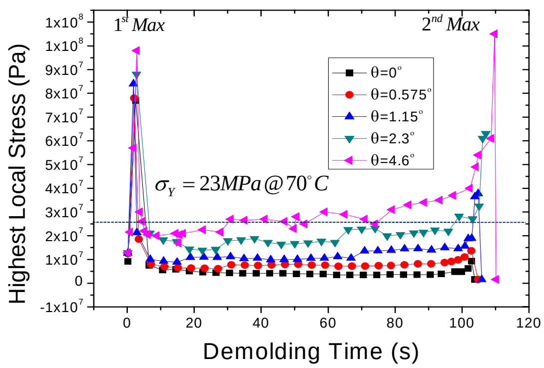

Figure 5. Highest local stress with demolding time for different demolding angles.

3.3. Influence of Structural Depths

Fabrication of high aspect ratio structures is a big challenge in imprint lithography because it is more probable for the structures to be damaged during demolding. Figure 6 shows the highest local stress for different depth ratios while the width of the structure and the thickness of the residual PMMA layer were identical. As expected, a significant increase in the highest local stress is observed as the depth/width ratio increases.

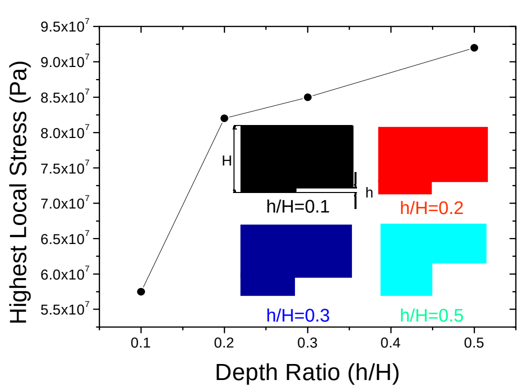

Figure 6. The highest local stress as a function of the depth ratio h/H.

4. CONCLUSIONS

The demolding process in thermal imprint lithography was studied by FEM simulation based on the viscoelastic model of PMMA. We found that there are two locations of stress concentration in PMMA: at the corner of PMMA resist and close to the corner of stamp moving up. During the whole demolding process, the highest local stress shows two maximums, indicating that demolding failure can occur both at the beginning and end of demolding. An accurate alignment in the demolding direction is critical to reduce stress in the resist layer. The results indicate that, with the increasing requirement of high aspect ratio and complex structures, the FEM simulation of the demolding process can be used as an economical and reliable tool to predict a range of process parameter values which will allow for successful demolding at the stage of a process design.

Acknowledgement

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