The IMPRINT software: quantitative prediction of process parameters for successful nanoimprint lithography

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ABSTRACT

The IMPRINT software is applied for simultaneous calculation of the resist viscous flow in thermal nanoimprint lithography (NIL) and the stamp/substrate deformation. From the presented comparison of calculated and experimental results, it can be concluded that the simulation allows predicting the residual layer thickness with accuracy better than 10%. The obtained results demonstrate the potential of the IMPRINT software as an efficient tool for choosing NIL process parameters and the optimization of the NIL stamp geometry.

Keywords: nanoimprint lithography, stamp and substrate deformation, computer simulation

1 INTRODUCTION

A homogeneous residual layer thickness in thermal nanoimprint can be achieved by optimizing the NIL stamp geometry (the distribution of cavities and protrusions, the stamp cavities depth and the stamp thickness) as well as by choosing NIL process parameters (the initial resist thickness, the imprint temperature and the duration of the imprint) (see [1] for example). This optimization produces the greatest benefit if its implementation is performed before expensive stamp manufacturing starts. To do this requires an effective tool for the simulation of NIL process.

Modeling of the resist viscous flow at the detail level (for a single cavity) is widely covered in the literature (see [2] and references therein). However, approaches for quantitative analysis of resist spreading in large areas are not described.

In this paper, the IMPRINT software for simulation of NIL at the structure-scale level is presented. The software is based on the mathematical model and the coarse-grain numerical algorithm from [3-5]. The IMPRINT software has been specially designed for use on standard Personal Computers, by using the GDS data of the stamp design (“Graphic Data System” is a database file format for integrated circuit layout data exchange). The software demonstrates a high computational performance. Typical simulation times for a test structure with 2×2 mm² area (see Section 3) are less than 20 min on an AMD Athlon 64, 2400 MHz processor.

2 MATHEMATICAL MODEL

In [4] the mathematical model for the simultaneous calculation of the resist viscous flow in NIL and the stamp/substrate deformation has been introduced. The model specifies the 2D temporal distributions of the pressure and the normal displacement of the stamp/substrate surface. The model has the following input parameters: the distribution of the stamp relief height \( h(x,y) \); the initial resist thickness \( d_0 \); the stamp velocity \( V_u \); the total force \( F \) acting on the stamp; the duration of the imprinting process \( T \); the dynamic viscosity of the resist \( \eta \).

In the model, at every point in time \( t \), the pressure distribution \( P(x,y,t) \) is calculated from the following problem:

\[
\nabla \left( \left[ D(x,y,t) + h(x,y) \right] \nabla P(x,y,t) \right) = 12 \eta \frac{\partial D(x,y,t)}{\partial t},
\]

\( (x,y) \in \Omega_\text{t}, \quad t \in (0,T], \quad P(x,y) = 0, \quad (x,y) \in \overline{\Omega}/\Omega_\text{t}, \)

\[
D(x,y,t) = d_0 - \int_0^t V_u(\xi)d\xi + \delta_\text{st}(x,y,t) + \delta_\text{sb}(x,y,t),
\]

where \( \Omega \) is the considered domain of the stamp; \( \Omega_\text{t} \) is the part of \( \Omega \), in which all cavities are filled with the resist, \( D(x,y,t) \) is the temporal distribution of the residual layer thickness. In (1) the zero value of the pressure on the boundary of the considered domain \( \Omega \) and in the unfilled cavities corresponds to the imprinting process performed in vacuum.

Note that equation (1) is derived from 3D Navier-Stokes equations with the understanding that the resist has very high viscosity and its motion is largely directed along the substrate surface.

For the calculation of the elastic normal displacement \( \delta_\text{st} \) and \( \delta_\text{sb} \) the stamp and the substrate are represented as semi-infinite regions (an elastic medium bounded by a plane). In this situation, the displacements are described by the following expression:

\[
\delta(x,y,t) = \frac{1 - \nu^2}{\pi\nu} \int_{\Omega} \frac{P(x',y',t)dx'dy'}{\sqrt{(x-x')^2 + (y-y')^2}}, \quad (x,y) \in \Omega
\]
where \( \sigma \) is Poisson's ratio and \( E \) is modulus of elasticity \([6]\).

It must be emphasized that a comparison of simulated and experimental results presented in Section 3 demonstrates the validity of the proposed deformation model. However, if required the displacement \( \delta_a \) and \( \delta_b \) can be specified using alternative models of the stamp and substrate deformation.

By the numerical approximation of the above-described mathematical model \((1)-(2)\), a special finite difference method is applied. The method provides a high precision of simulation results by using a reasonably coarse grid \([5]\).

3 EXPERIMENTS

Below it is given results for imprint processes using a structure from the experimental test stamp of the NaPa project \([7]\). The test structure measures \( 2 \times 2 \text{mm}^2 \) and contains arrays of circular protrusions (see Fig. 1). The average value of fill factor (i.e. relation between cavities area and the total area) for the structure is equal to 1/3. However, the local value of fill factor varies significantly from one array to another. Therefore, imprinted samples of the test structure demonstrate distinct inhomogeneities of the residual layer thickness related to the non-uniform deformation of stamp and substrate as well as to incompletely filled cavities.

![Figure 1: Simulated distribution of the residual layer thickness \( D \) for the test structure with cavities of depth \( h_c = 200 \text{ nm} \). The initial resist thickness is 200 nm. White contour lines are numbered in nanometers. Black lines bound areas with incompletely filled cavities. The duration of the imprinting process is 180 s. As background, the relief of the test structure is used (cavities and protrusions are painted light and dark grey, respectively).](image1)

![Figure 2: The simulated influence of the initial resist thickness on minimal (\( D_{\text{min}} \)) and maximal (\( D_{\text{max}} \)) values of the residual thickness as well as on cavities fillability for the test structure with different cavities depth \( h_c \).](image2)

In experiments, silicon stamps and silicon substrate are applied. The experiments were performed for different values of the stamp cavities depth \( h_c \): 100 nm, 200 nm and 300 nm. The stamps were imprinted into resist mr-I 8000 (Micro Resist Technology GmbH). The imprint temperature was 200\(^\circ\)C.

By the coarse-grain simulation, a 128x128 pixel grid is applied. For the calculation of the stamp and substrate deformation, elastic properties of single-crystalline silicon are used: modulus of elasticity \( 10^{11} \text{ Pa} \), Poisson's ratio \( 0.2 \). The stamp velocity is supposed to be \( V_{st} = 1 \text{ nm/s} \) (see in \([5]\) about loading regimes which are selected by modeling). In the simulation, the resist dynamic viscosity is taken to be \( 3 \times 10^3 \text{ Pa}\cdot\text{s} \). This value gave the best fit of calculated residual thickness distribution to the experimental one \([8]\).

Fig. 1 shows an example of simulated results for the test structure. In the figure the non-uniform distribution of the residual layer thickness and numerous areas with incompletely filled cavities are observed. The efect of the initial resist thickness \( d_0 \) on the homogeneity of the residual layer thickness and cavities fillability is presented graphically in Fig. 2. By the simulation, the duration of the imprinting process is chosen as \( T = (d_0 - 20 \text{ nm})/V_{st} \).

In Figures 3 and 4 the measured and calculated results are compared. The simulation confirms the high residual layer thickness variation ranging (the spacing between minimal and maximal values of the residual thickness is more than 45 nm for \( h_c = 100 \text{ nm} \), 75 nm for \( h_c = 200 \text{ nm} \), and 105 nm for \( h_c = 300 \text{ nm} \)) with a precision of 10%.

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Figure 3: (a) and (c) The optical microscopy images of the test structure imprinted into resist at two different values of the stamp cavities depth: 100 nm and 200 nm, respectively. The initial resist thickness is 230 nm. The imprint temperature is 200°C. The duration of the imprinting process is 200 s. Black horizontal lines indicate zones of profilometer measurements of resist thickness. Vertical scratches observed in the images have been applied for the determination of the residual layer thickness. White box marks an area with incompletely filled cavities. (b) and (d) Comparison of measured distributions of resist thickness H and simulated distributions of residual layer thickness D.
Figure 4: (a) and (c) The optical microscopy images of the test structure imprinted into resist at two different values of the stamp cavities depth: 100 nm and 300 nm, respectively. Other process parameters are listed in Fig. 3. Black horizontal lines indicate zones of profilometer measurements of resist thickness. White box marks an area with incompletely filled cavities. (b) and (d) Comparison of measured distributions of resist thickness $H$ and simulated distributions of residual layer thickness $D$.

REFERENCES