Refined Coarse-Grain Modeling of Stamp Deformation in Nanoimprint Lithography

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ABSTRACT

A refined version of the IMPRINT software is applied for simultaneous calculation of the resist viscous flow in thermal nanoimprint lithography and the stamp/substrate deformation. This version applies a modified coarse-grain method as well as takes into account the composition and elastic properties of the imprint setup (the stamp/substrate + "pressure buffer layers"). The presented comparison of calculated and experimental results confirms the potential of the IMPRINT software as an efficient tool for the reduction of the stamp bending.

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

1 INTRODUCTION

The inhomogeneous distribution of the residual layer thickness is a vital issue in thermal nanoimprint lithography (NIL). Using the simulation of NIL, this problem can be alleviated by optimizing the stamp geometry and by choosing process parameters.

In [1, 2] the IMPRINT software for modeling of NIL process has been presented. The software takes into account the stamp/substrate bending during squeeze flow and is able to predict the distribution of the residual resist thickness with an accuracy better than 10% [2, 3]. It should be noted that the above-mentioned results have been obtained using the deformation model in which the stamp/substrate are represented as semi-infinite regions (an elastic medium bounded by a plane).

In [3] a dramatic effect of the stamp thickness on the distribution of the residual resist thickness has been described. The experiments were performed for a typical R&D case where the grating is surrounded by a large unstructured area. For the simulation of these experiments the IMPRINT software has been modified. The software has been adapted for the calculation of the extensive deformation for the imprint setup (the stamp/substrate + "pressure buffer layers"). Consequently, the latest version of the IMPRINT software has been supplemented by: a multilayer model of the stamp/substrate deformation; and an adaptive multi-grid realization of the coarse-grain method for the simulation of structures having regard to surroundings.

Figs. 1-3 demonstrate the implementation of the modified IMPRINT software.

2 EXPERIMENTS

The experiments were performed for 4" silicon stamps with thickness of 400 and 1000 μm. On the stamps nine different arrays (gratings with 12 μm period) are placed. They are comprised of different areas (1×1 mm^2, 2×2 mm^2 and 4×4 mm^2) and different fill factors (0.25, 0.5 and 0.75). The stamps were imprinted on 300 nm thick of mr-I 7030 (Micro Resist Technology GmbH) coated on silicon substrates 500 μm in thickness. The stamp cavities depth was 170 nm. The imprint temperature was 140°C. The imprinting process lasted 1200 s.

In the simulation, the resist dynamic viscosity was taken to be 5×10^3 Pa·s. This value gave the best fit of calculated residual thickness distribution to the experimental one. For the calculation of the stamp and substrate deformation, elastic properties of single-crystalline silicon were used: modulus of elasticity – 10^{11} Pa, Poisson's ratio – 0.2.

By the coarse-grain simulation, two embedded grids were applied: the first (fine) grid was 128×128 pixel; the second (coarse) grid was 256×256 pixel.

In Fig. 4 experimental and simulated results are compared. It is evident that for the 1000 μm stamp the experimental and simulated results agree very closely. Slightly worse agreement is observed for the 400 μm stamp. The reason is the lack of information about the exact elastic properties of the "pressure buffer layer".

ACKNOWLEDGEMENT

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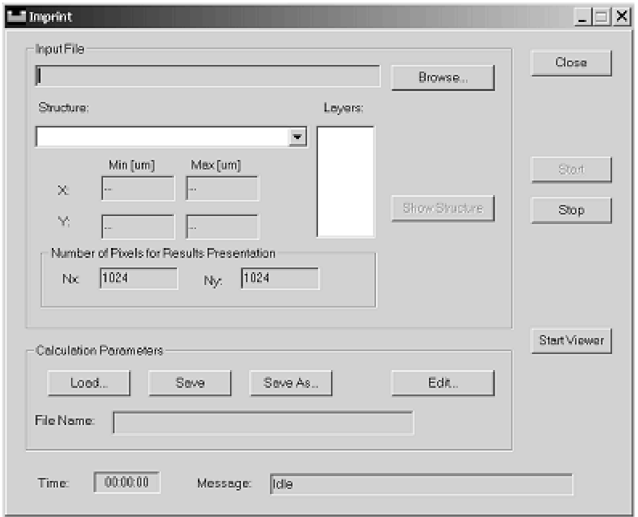


Figure 1: Main window of the IMPRINT software.

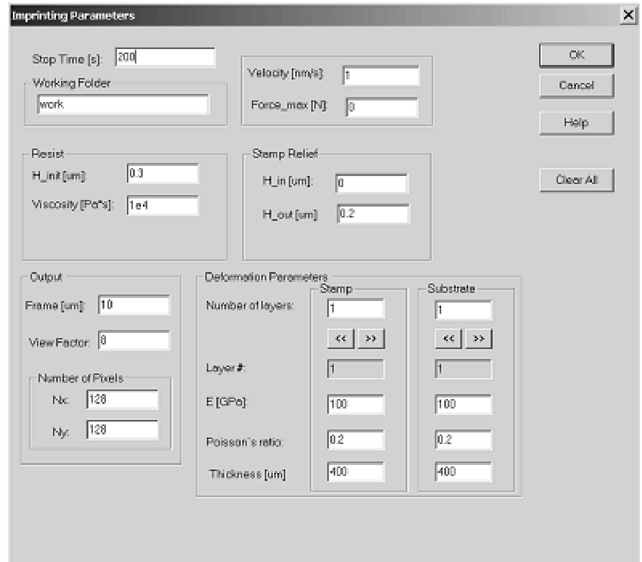


Figure 2: The IMPRINT software: list of simulating parameters (the default values).

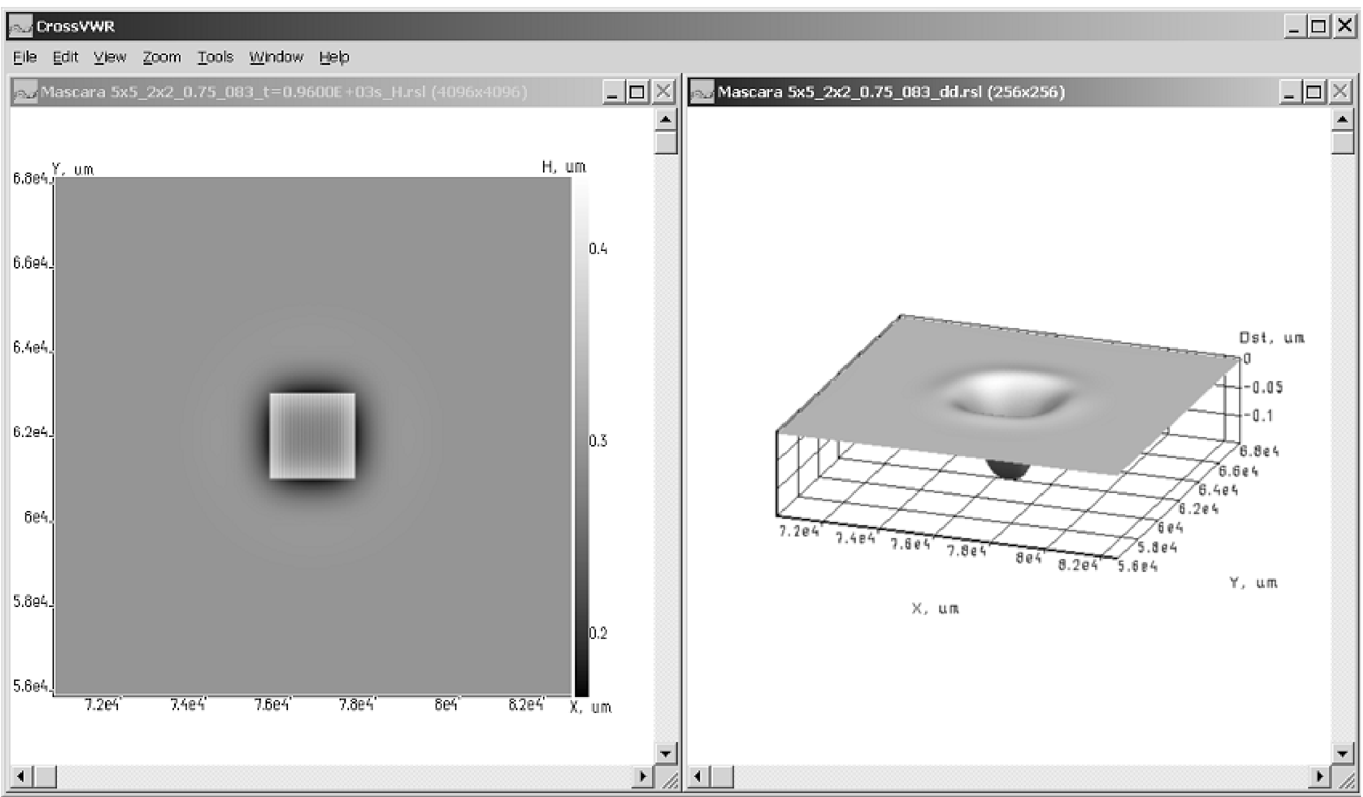
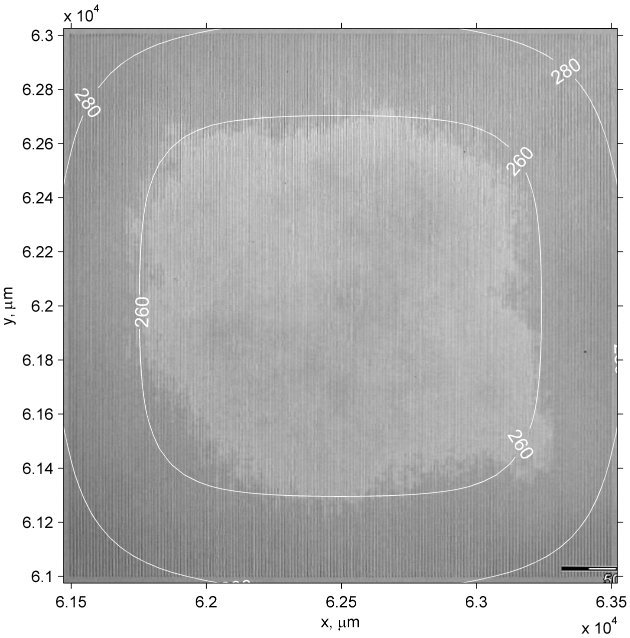
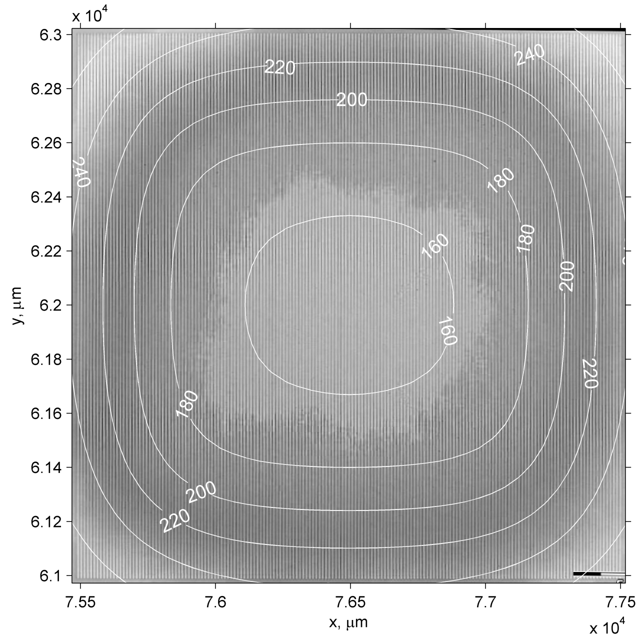


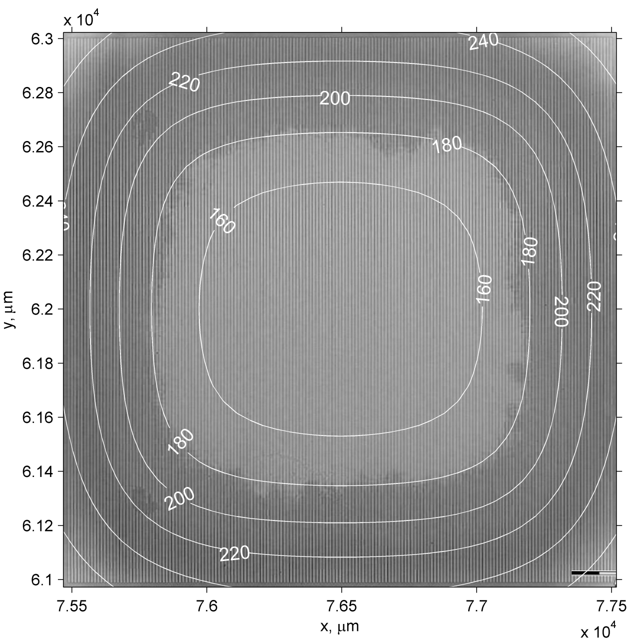
Figure 3: Presentation of simulated results using viewer built in the IMPRINT software. The calculated distribution of resist thickness (left window) and the calculated distribution of the stamp deformation (right window).



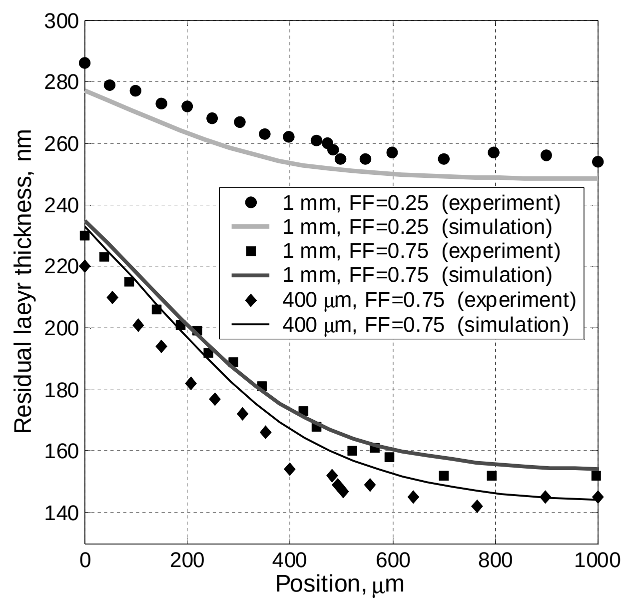
(a) 1 mm stamp thickness, fill factor = 0.25



(b) 1 mm stamp thickness, fill factor = 0.75



(c) 400 μm stamp thickness, fill factor = 0.75



(d)

Figure 4: **(a)-(c)** Optical microscopy images for a 2×2 mm^2 array size imprinted from different silicon stamp thickness and at different fill factors. White isolines indicate the calculated distribution of the residual layer thickness (numbers signify the thickness in nanometers). **(d)** Measured and simulated distributions of the residual layer thickness. Cross-sections are directed along the y-axis and through the centre of the grating. The position 0 shows the edge of the grating.

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