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Deformation and viscouse flow in nano-imprinting

M. V. Chukalina, V. N. Matveev, V. V. Sirotkin, A. A. Svintsov and *S. I. Zaitsev*
Institute of Microelectronics Technology RAS, 142432 Chernogolovka, Russia

Abstract. The paper is concentrated on the theoretical consideration of imprinting process and of polymer flow during embossing of the master. Another activity was related to development of experimental techniques for performing imprinting.

Introduction

New technologies for mechanical pattern transfer in sub-100 nm regime with aim to replace conventional lithography in semiconductor mass production (on area 10 cm×10 cm) are now under extensive investigations. Mechanical imprint of a stamp (mold) in plastic polymer or printing with "inks" forming self-assembled monolayers (SAMs) are in the center of interest.

During imprinting resist changes its shape under a stamp, this leads to extraordinary situation when a part of material should be transferred on distances about 10 cm through narrow (less than 100 nm) canal. Due to polymer nature of the resist one could expect additional difficulties if molecular size becomes comparable with canal width.

1. Estimation of printing time and force

An order of magnitude of imprinting force was obtained considering simple situation (a round flat stamp of radius R moves with velocity u into resist layer of thickness h and viscosity η) solved firstly by Reynolds on the base of Navier–Stokes equations.

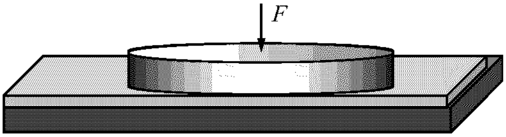

Fig. 1. A round flat stamp (of radius R) moves with velocity u into resist layer of thickness h and viscosity ν.

On the base of Reynolds solution estimations of force ($F_R = 3\pi\eta u R^4/2h^3$), time of imprinting T, pressure distribution, velocity distribution were obtained. Main conclusion from the analysis is that it is not possible to perform imprinting of 10 cm stamp for reasonable time (F_R is about 10^7 kg).

2. Optimization methods for design imprinting structures

One of the way to avoid enormous high force or time of imprinting is decreasing of polymer material transport. Practically it means design of structure with special cavities to gather extra material during imprinting. This means that some additional elements should be added to functional features of the structures during design to prevent flow on large distance. Some practical methods for the design and structure optimization are suggested and discussed.

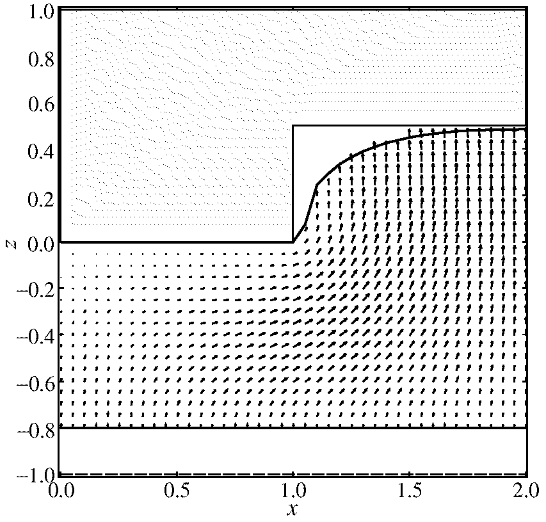

Fig. 2. Velocity field in nonstationary stage.

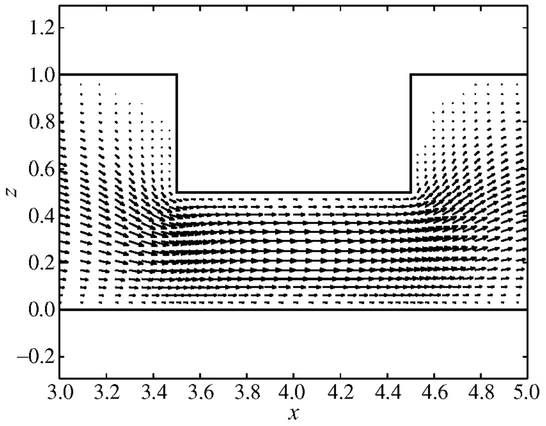

Fig. 3. Velocity field with filled stamp cavities.

3. Development of the numerical/analytical tool for approximate description (information capacity is 10^{12}–10^{14} pixels)

An information capacity of the structures is very high and could be estimate as ratio of a structure size (~ 10 cm) to minimal feature (10–100 nm). This gives 10^{12}–10^{14} pixels. It is clear that it is not possible to describe and simulate objects of such sizes. Some approximate methods should be developed for description/simulation.

One of ideas is to use natural hierarchy of microelectronics structures. On this way an equation of viscose flow for small units of the lowest level should be solved then considering the smallest units as structureless elements consider flow at higher spatial and temporal scale for the units of higher level and so on. This way could be combined with another idea to take into account relief of the stamp effectively considering viscosity dependent on coordinates.

Imprinting could be roughly divided into two stages, first (with short matter transfer distance) is filling of stamp space (cavities) by resist. After exhausting free stamp space further imprinting results to large distance of matter distance through narrow channels. Analyzing of the first stage is important to estimate duration of the stage. One more important reason is determination of resist shape near internal sharp edges when influence of surface tension and polymer coils size become essential.

To meet the goals formulated a numerical methods were developed for the two stages analysis on base of non-stationary and stationary Navier–Stokes equations and first simulations were performed.

Figure 2 shows the velocity field near the "ridge" in non-stationary stage where as Fig. 3 shows velocity distribution in stationary stage. Other characteristics of the flow were calculated: the pressure P and the non-zero velocity components V_x and V_z. The calculation demonstrate the lengths of hydrodynamic stabilization for both velocity components are $\mathcal{O}(h)$, where h is the depth of the canal. Note that the stabilized flow is characterized by $V_x = 4(h/L)[1 - (z/h)](z/h)$ and $V_z = 0$ in total correspondence to Reynodls solution.

The calculation were performed for different sizes of ridge, similar characteristics were calculated for trench of different sizes. Special calculation were made for Re $= 10^{-2}$–10^{2}. It was shown that flow practically independent on Re for values below 10^{-1}. So one important consequence of calculations is conclusion that nonlinear term Navier–Stokes equations could be removed from equations.

4. Polymer chain size effects

Polymer matter has some specific features which become essential at scales considered in nano-imprinting. Roughly polymer could be considered as matter consisting of 'particles' with radius L related to polymer length N

$$L = L_0 N^{\frac{1}{2}}. \tag{1}$$

For molecular weight 950 K and 50 K this gives (at molecular weight of monomer equal 100 and effective length $L_0 = 1$ nm)

$$L = 20 - 100\,\text{nm}.$$

The particle size L is comparable with resist thickness and imprinting structure details. But at this scale Navier–Stokes equations should be used with some accuracy. Viscosity is now dependent on distance from the walls and is not further local characteristics.

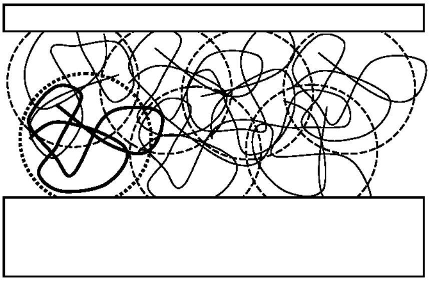

Fig. 4. Polymer resist comprises a melt of coils.

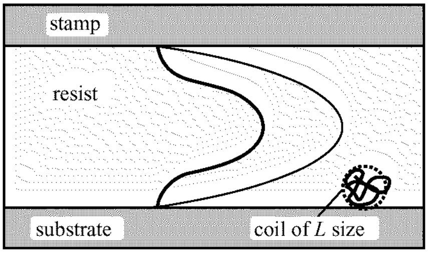

Fig. 5. Consideration of polymer coil size L results to remarkable change in velocity profile at resist thickness h comparable with L.

5. Viscosity near wall and Reynolds problem for polymer flow

To calculate nonlocal viscosity we supposed that any contact with the wall makes polymer chain immobile so only mobile part of polymer chains can contribute in flow. Effectively this means that viscosity becomes lower near the wall. Let $W(z)$ is a probability for a chain to avoid the wall for the chain starting at point z from the wall so only part $W(z)$ can take part in movement and viscosity $\eta(z)$ is reduced in comparison with bulk value η_b, $\eta(z) = \eta_b / W(z)$.

Function $W(z)$ was calculated considering polymer chain conformation (polymer coil) as a trace of random walk consisting of N steps. Mathematical model for $W(z)$ calculation is non-stationary diffusion equation with absorption on the boundary. It gives for small h/L

$$W(z) = \sin\left(\pi \frac{z}{h}\right) \exp\left[-\left(\pi \frac{L}{h}\right)^2\right].$$

Velocity, pressure distributions and force F_p were obtain for Reynolds problem, for example force

$$F_p = \frac{1}{2} \pi \eta u R^4 \exp\left[\left(\pi \frac{L}{h}\right)^2\right]$$

increases exponentially instead of power $(1/h^3)$ law in classical Reynolds solution.

As result one could expect impossibility to deform resist layer after reaching some thickness close to size L. It is seen immediately (due to (1)) that usage of resist with lower molecular weight could reduce the thickness of incompressible layer. Another way is to use monomer liquid with photo- (thermo-) polymerization after imprinting.

6. Development of technology components for imprinting

Technological steps developed for imprinting realization consist of several steps.

Electron lithography. Test structures were designed and fabricated with minimal features of 300 nm by electron beam lithography.

Etching/development. After thin Al deposition and lift off the samples were dry etched to depth about 1 μm.

Imprinting. The most important step was made in development of imprinting, a stage with controllable heating (up to 200°C) was fabricated.

First experiments with imprinting showed that transfer could be performed but it showed as well some resist pollution in trenches. Further optimization of regimes are desirable.

Diagnostics. For control of shape transfer optical and scanning electron microscopes were used. It is planned to use a specially developed device with diagnostic possibilities close to AFM mode is used for control as well.

Acknowledgments

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