Coarse-grain simulation of viscous flow and stamp deformation in nanoimprint

V. Sirotkin, A. Svintsov, S. Zaitsev
Institute of Microelectronics Technology, RAS, Chernogolovka, Moscow district, 142432 Russia
H. Schift
Laboratory for Micro- and Nanotechnology, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland

The distribution of the residual layer thickness is a vital issue in nanoimprint lithography (NIL). In the case of "non-optimal" stamp geometry, i.e. a distribution of cavities and protrusions causing inhomogeneities in the ability of the resist to spread "in the immediate vicinity" for long imprint times, in some stamp areas the polymer has to flow laterally over large distances. These areas are characterized by increased values of pressure, which results in a deformation of stamp and substrate and consequently in a non-uniform residual layer thickness. Using resist flow simulation, this problem can be alleviated by optimizing the NIL stamp geometry and by choosing process parameters.

A coarse-grain method for simultaneous calculation of the resist viscous flow in NIL and the stamp and substrate deformation is presented. The method is based on an equation that specifies the 2D pressure distribution for a given resist thickness a stamp velocity. The equation is derived from 3D Navier-Stokes equations with the understanding that the resist motion is largely directed along the substrate surface. For the calculation of the deformation, the stamp and the substrate are represented as semi-infinite regions (an elastic medium bounded by a plane).

The coarse-grain method has been realized in software, which allows to analyze the temporal mapping of residual thickness and pressure on standard Personal Computers, by using the GDS data of the stamp design.

Figure 2 presents the implementation of the coarse-grain method for the simulation of an imprint process using two structures ("Sinus3" and "MEMS") from the experimental test stamps of the NaPa project. For the "Sinus3" structure the experimental and simulated results agree very closely. Slightly worse agreement is observed for the "MEMS" structure. The reason is that each structure is simulated separately without considering neighbor structures placed on the test stamp. The simulation performed for the whole stamp is able to provide reasonable results well suited for quantitative predictions of residual resist thickness.

“Sinus3” structure “MEMS” structure

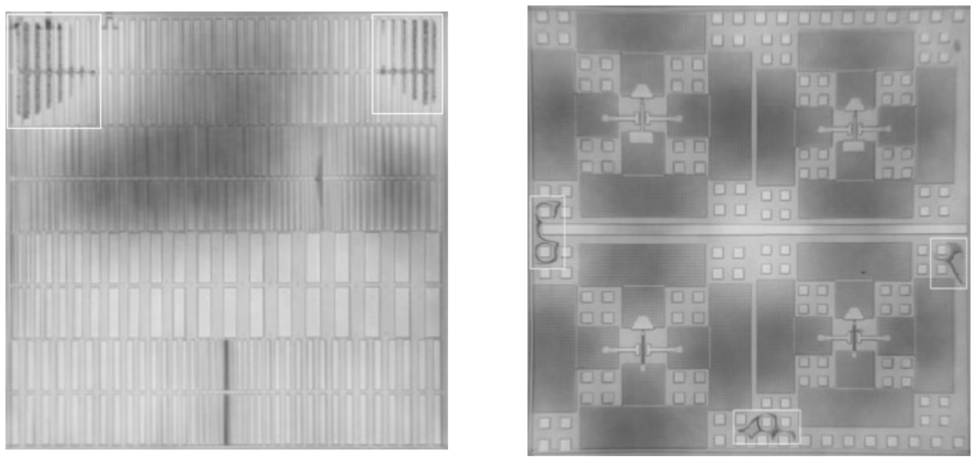

Fig 1: Photos of the imprinted structures. Dark spots correspond to areas with thicker residual layer. White boxes mark incomplete molding areas. The imprinted samples of the “Sinus3” and “MEMS” structures were made in PSI (Switzerland) and in Tekniker (Spain), respectively.

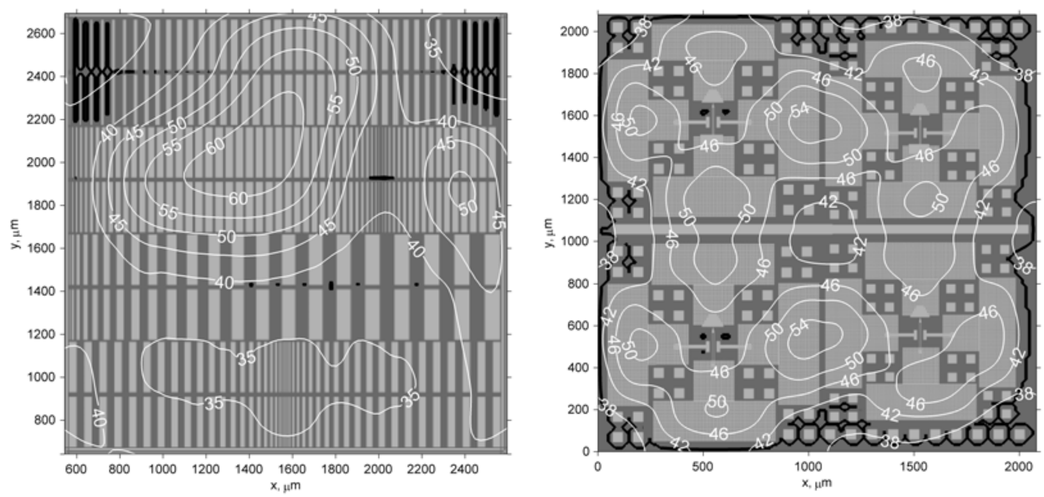

Fig 2: Simulation results: white isolines indicate the distribution of the stamp and substrate deformation (numbers signify the elastic displacement in nanometers); black lines bound incomplete moulding areas. As background, the original relief of the stamps is used (cavities and protrusions are painted dark and light grey, respectively).

Simulation parameters: the stamp cavities depth – 200 nm, the initial stamp-substrate gap – 300 nm, the final stamp-substrate gap – 100 nm, the resist dynamic viscosity – 10^3 kg/(m·s), the stamp velocity – 1 nm/s, modulus of elasticity – 5×10^{10} Pa, Poisson's ratio – 0.2.