Numerical Stress Analysis on Thermal Nano-Imprint Lithography

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ABSTRACT

In this paper, we investigate the stress distribution of polymer film in thermal nano-imprint lithography (NIL). In order to simulate this process, commercially available software was employed for NIL process simulation. The proposed model is imprinting a rigid SiO_2 stamp with a rectangular line pattern into a viscoelastic Polymethyl methacrylene (PMMA) film. The distribution of stress in the polymer film is calculated for the detail analysis of deformation behavior. These calculated results represent asymmetric von Mises stress distribution of the polymer around the external line caused by the squeezing flow under flat space.

Keywords: stress distribution, thermal nano-imprint lithography, viscoelastic, Polymethyl methacrylene film, von Mises stress

1 INTRODUCTION

Nano-imprint lithography (NIL) is one of the most promising techniques. Traditional photolithographic approaches make pattern transfer through the use of photons or electrons for modifying the chemical and physical properties of the resist. NIL relies on a direct mechanical deformation of the resist material and can therefore achieve resolutions beyond the limitations which are set by a light diffraction or a beam scattering. It enables both high resolution up to sub-25 nm which is not accomplishable in photolithography and fast throughput compared to serial processing methods such as electron beam or scanning probe microscopy (SPM) lithography, so it is expected as an alternative lithography method to conventional ones [1]. In addition, NIL is expected to realize a low cost and high-throughput production. In the thermal NIL process, a high speed imprinting was reported such as a role-to-role imprint [2]. In order to improve the NIL technology, it is essential to understand the deformation behavior of polymer during the imprinting process. Success of the pattern transfer in NIL depends on exact deformation of a polymer film according to stamp patterns and clear separation of a stamp from a polymer film [3]. Despite the prospective potential for nano-scale pattern transfer, there are few literature publications on the numerical modeling on NIL processes [4-6]. In this work, we modeled the NIL process and employed commercially available software, COMSOL Multiphysics, for the implementation of our model. In this paper, we report the stress distribution of the polymer deformation process on the imprinting pressure.

2 SIMULATION AND RESULTS

COMSOL Multiphysics bases its implementation of the structural mechanics application modes on the equilibrium

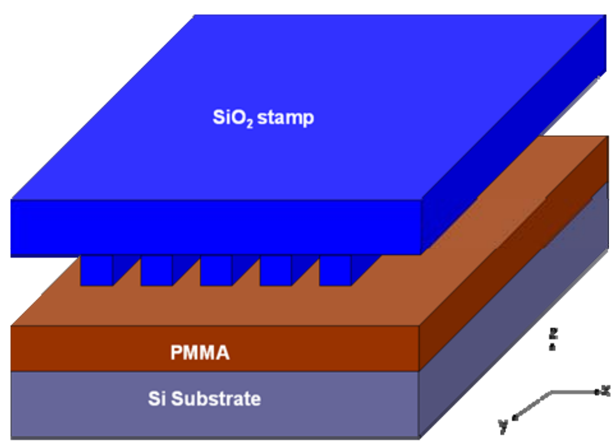


Figure 1: Schematic diagram illustrating the physical model.

equations expressed in the global stress components. For static analysis, substitution of the stress-strain relationship and the strain-displacement relationship into the static equilibrium equation produces Navier's equation of equilibrium expressed in the displacements. It is possible to completely describe the strain conditions at a point with the deformation components and their derivatives.

Figure 1 shows the schematic diagram of physical model about imprinting process. The mold has five line patterns with 1um whose width is 50nm and height is 50nm. Each line patterns are at intervals of 50nm. The polymer materials we used in our simulation were Polymethyl methacrylene (PMMA) and the imprint temperature was 140℃. The SiO_2 mold was modeled as a rigid body, and the PMMA resist was modeled as a viscoelastic material. Table 1 shows the material constants used for numerical analyses. $10N/m^2$ constant pressure was applied on the top of the mold and kept for various time periods during pressing process. After the pressing process, PMMA specimens were quickly cooled down so that the specimens almost kept the shape at the end of the pressing process.

Table 1: Material constants of PMMA resist.

Material constant	Value
Young's modulus	3 GPa
Poisson's ratio	0.4
Heat capacity	1420 J/K
Thermal expansion coefficient	$7.0*10^7$ K^{-1}
Thermal conductivity	0.19 W/(m*K)
Density	1190 kg/m^3

The stress distributions of the polymer are shown in Figure 2. The method is based on an equation that specifies the 2D pressure distribution for a given polymer thickness and a stamp velocity. The equation is derived from 3D Navier-Stokes equations with the understanding that the polymer motion is largely directed along the substrate surface. The contour of simulated results represents the residual von Mises stress. The major cause of the residual von Mises stress is that the thermal shrinkage arisen in cooling process uniformly. The nonuniformity of the residual von Mises stress is caused by the distribution of viscous strain at the end of the pressing process.

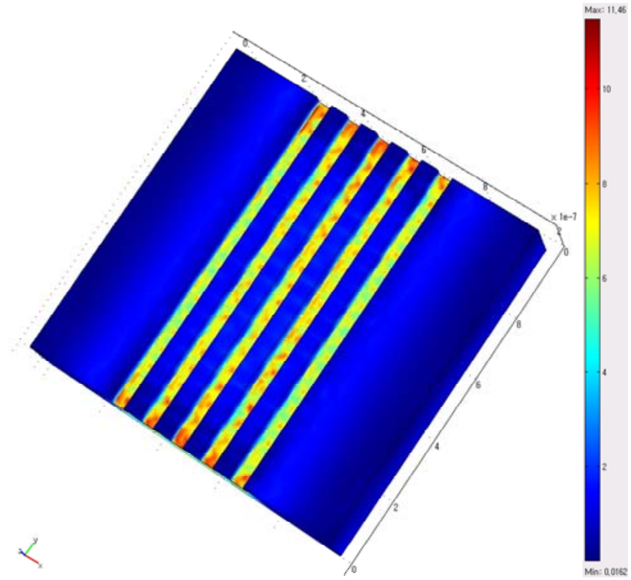
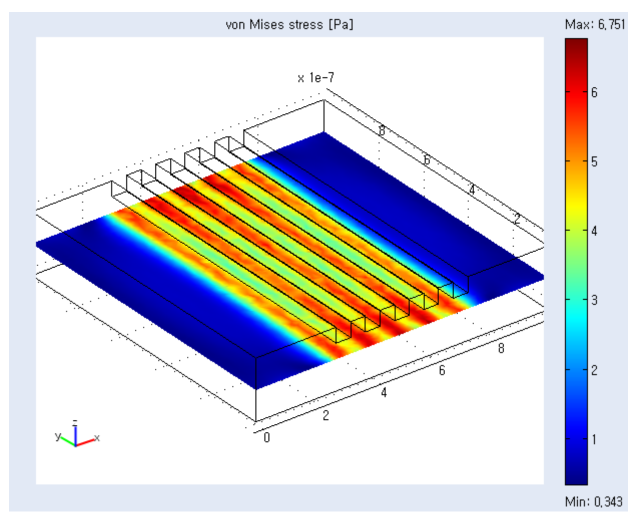


Figure 2: Stress distribution of the polymer.

Figure 3(a), 3(b) and 3(c) show cross-sectional profiles of von Mises stress distribution of the polymer by x-y, y-z and z-x plane, respectively. These calculated results represent asymmetric von Mises stress distribution of the polymer around the external line caused by the squeezing flow under flat space. Similarly, von Mises stress of the polymer around the outside of the line is higher than the inside of the line.



(a)

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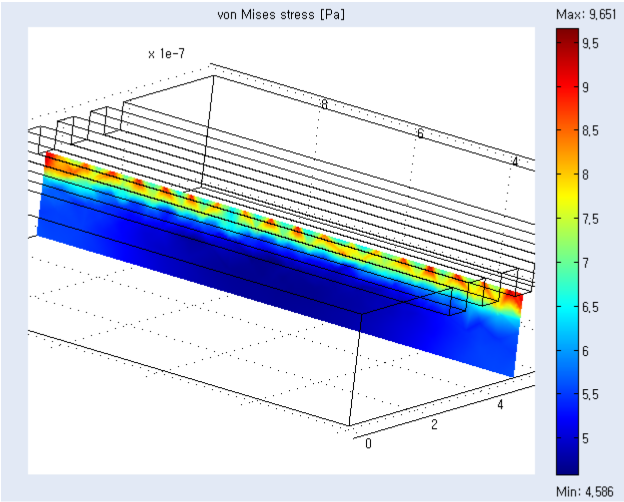

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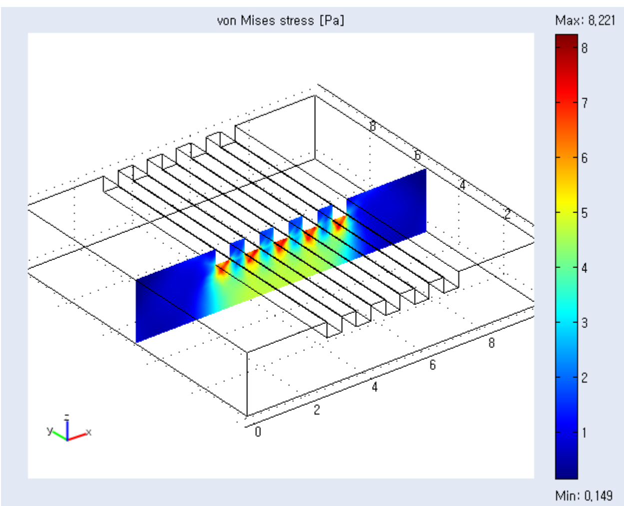

(c)

Figure 3: Cross-sectional profiles of von Mises stress distribution. (a) x-y plane, (b) y-z plane, (c) z-x plane.

CONCLUSION

A numerical simulation model imprinting a rigid SiO2 stamp into a viscoelastic polymer film is suggested in order to analyze the pattern transfer and its related phenomena in thermal NIL. The behavior of polymer deformation is investigated in detail by means of stress distribution analysis. In the imprint process, significant compressive stress is generated under the stamp pattern due to the compression of the polymer film, which causes the polymer to flow and to fill the cavity of the stamp for both patterns.

Numerical results explained characteristic phenomena which never appear in continuous line-and-space patterning cases. We believe that numerical simulations with more accurate material properties have possibilities to agree with experiments better enough for practical use. Our simulation approach could further be extended to accommodate deformation of the stamp and the sub-polymer platen.

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