Study on resist profile estimation due to shrinkage and mold profile correction in nanoimprint lithography

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Introduction In nanoimprint lithography, resist shrinkage must occur due to thermal cooling or UV curing processes. The resist shrinkage causes critical dimension (CD) error and distortion of the resist profile. In nano scale pattern, quantitative value of the CD error is negligible but distortion of the resist profile becomes significant in micro scale structures such as micro optical elements. In our previous study, CD error for line pattern was estimated in various line width using specific filter functions for the periodical line pattern. Also, CD error correction by mold pattern modulation was demonstrated based on computational work [1].

In this work, we newly investigate distortions of the resist profile due to shrinkage and estimate resist profile by simple expression. Also, automatic mold profile correction to compensate distortions by shrinkage is proposed.

Estimation of pattern profiles using simple expressions Figure 1 shows schematics of the analysis systems for rectangular cross-sectional pattern. The resist is fixed on the substrate and the resist shrinks in isotopically. The initial resist height is unit length and the aspect ratio of the cross-section of the pattern is A. The mold is rigid body and the resist is elastic body. The resist is gulled on the substrate and touched on the mold. The resist profile is obtained by computational simulation using finite element method (FEM) based on continuum mechanics. To obtain simple expression of the resist profiles after shrinkage, we try to find estimation function for resist profiles in various aspect ratios and pattern shapes.

The resist profile after shrinkage is expressed by two profile functions. One is for the resist upper plane height profile $U_y(x)$ and the side wall width profile $S_x(y)$ as follows; For the upper plane, the both ends are supported and the resist is stretched in vertical direction. Then, the resist height $U_y(x)$ is expressed $U_y\,(x)=ax^2+c$, where a is fitting parameter and c is determined by the shrink ratio. The other is side wall profile function $S_x(y)$. The side wall of the resist is fixed on the substrate. As a result, and gradually shrink laterally in y direction. So, the lateral width $S_x(y)$at height y is expressed as $S_x(y)=\alpha(1\text{-}exp(\text{-}y/\beta))$,where α is determined by the shrink ratio and β is fitting parameter. The parameters are extracted from the resist profiles obtained by finite element method (FEM) for various aspect ratio of the mold patterns.

Figure 2 shows typical results for the fitting parameters in various aspect ratios of the patterns. The parameters are expressed by simple functions such as Gaussian, transfer function, and hyperbola like expressions for a, c, and β, respectively. The error between the estimation function and the FEM result is around less than 0.05% in standard deviation under 10% liner shrinkage. The profile after shrink is successfully expressed by these profile functions. This means that we can estimate resist profiles in any pattern features without computational simulations.

Automatic mold correction and pattern compensation Based on the profile estimation functions, the mold profile is automatically corrected to compensate the shrinkage. Figure 3 shows resist cross sectional profile simulations using conventional FEM with and without correction. The aspect ratio of the pattern is 1.0 and the liner shrinkage ratio is 10%. The resist shrinkage is successfully compensated. The error σ is compensated less than 0.03% in standard deviation. In the same way, triangular shaped pattern, spherical structures, and 3-D rectangular parallelepiped structures are estimated and the pattern profile distortions by shrinkages are successfully compensated.

[1] A. Horiba, et al., *Jpn. J. Appl. Phys.* **51** (2012) 06FJ06.

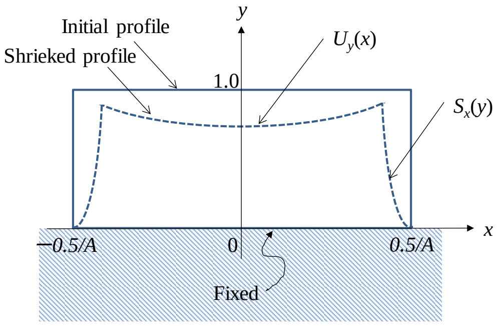
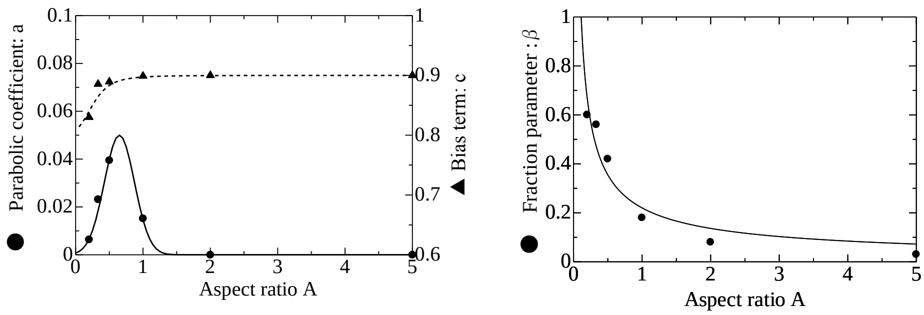
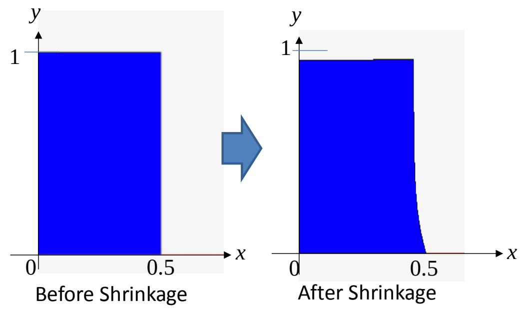


Fig.1. Schematics of the analysis system of the resist shrinkages. After shrinkage, the resist profile is shown in dashed line.

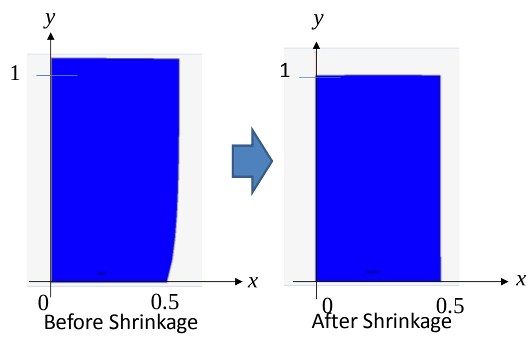


a) For upper plane hight $U_y(x)=ax^2+c$, b) For side wall width $S_x(y)=\alpha(1-exp(-y/\beta))$

Fig.2. Fitting parameters in various aspect ratio. The dots and triangles are extracted values, and solid and dashed lines are fitted curves using specific functions.



a) Without mold profile correction (σ=0.10)



b) With mold profile correction (σ=0.0029)

Fig.3. Computational study on the resist profile due to shrinkage with and without mold profile correction for rectangular cross-section pattern. The aspect ratio of the pattern is 1.0 and the liner shrinkage ratio of the resist is 10%. The scale is normalized unit length. By the correction, the standard deviation σ for the rectangular profile is reduced to 0.03%.