Microelectronic Engineering 123 (2014) 171–174

Contents lists available at ScienceDirect

Microelectronic Engineering

journal homepage: www.elsevier.com/locate/mee

Large scale three-dimensional simulations for thick SU-8 lithography process based on a full hash fast marching method

Zai-Fa Zhou *, Li-Li Shi, Heng Zhang, Qing-An Huang

Key Laboratory of MEMS of the Ministry of Education, Southeast University, Nanjing 210096, China

ARTICLE INFO

Article history:
Received 27 October 2013
Received in revised form 11 July 2014
Accepted 29 July 2014
Available online 7 August 2014

Keywords:
Thick photoresist
Lithography simulation
Diffraction
Light distribution
Fast marching method

ABSTRACT

Three-dimensional (3D) simulations are useful to optimize the lithography process of thick photoresists, however, less efficient models and etching surface advancement algorithms limits current application of various simulation tools. This paper presents a comprehensive aerial image model based on Fresnel diffraction to simulate the 3D inclined/vertical UV light intensity distribution into the SU-8 with the diffraction, refraction, absorbance and reflection during light transmission efficiently considered simultaneously. The aerial image model are solved by using adaptable element size in *x*, *y* and *z* direction to speed up the calculation. The improved two-dimensional (2D) Dill exposure model, the post exposure bake (PEB) model and the Enhanced Notch model are also extended to three dimensions. Furthermore, a 3D hash fast marching method is developed to calculate the final development profiles with less required memory elements. Thus various large scale 3D simulations of thick SU-8 lithography process can be well implemented, and the simulated development profiles have been verified by experimental results.

1. Introduction

Inclined and vertical ultraviolet (UV) lithography of thick photoresists plays an important role in manufacturing novel and complex high aspect-ratio MEMS elements with low cost and high resolution [1–6]. For many years, lithography simulation has been employed to optimize the design of micron and sub-micron devices and related devices in integrated circuits (IC) field. Although simulation software for the thin photoresist lithography processes in IC field has been commercialized [7], the lithography process of thick photoresists, such as thick SU-8, can not be accurately implemented by the software specified for the thin photoresists, since the thick SU-8 has properties different from the thin photoresists. Three-dimensional (3D) simulations are useful to optimize the lithography process and the design of some MEMS elements, however, some problems are expected to be solved for the efficient application of 3D lithography simulations, especially for large scale 3D simulations. For example, most current researches in UV lithography of thick photoresists are case to case study but not system modeling of the whole lithography process [8–15], focusing on various aspects such aerial image models and etching surface advancement algorithms for inclined and vertical UV lithography of thick photoresists. Furthermore, the accurate aerial image simulation to obtain the light intensity distribution into the resists is a time-consuming step, limiting the implementation of large scale 3D simulation. Finally, the surface advancement simulations using dynamic cellular automata methods are relatively slow [10,12,16]. For a relatively large 3D simulation array, the simulation using current fast marching method (algorithm) [17,18] is about 8 times faster than the dynamical cellular automata methods [16], but needs too many memory elements. For a simulation array with $500 \times 500 \times 500$ grids, the lithography simulations can not be implemented using current fast marching algorithms with a typical personal computer configuration: OS Windows XP SP3, CPU Intel Core2 @2 GHz, DRAM 2 GB, since the memory limit is exceeded.

In this paper, a comprehensive aerial image model based on Fresnel diffraction is specifically developed to simulate the 3D inclined/vertical UV light intensity distribution into the SU-8 with the diffraction, refraction, absorbance and reflection during light transmission efficiently considered simultaneously. The aerial image model is solved by using adaptable element size in each direction to speed up the calculation. The improved two-dimensional (2D) Dill exposure model, the post exposure bake (PEB) model and the Enhanced Notch model are also extended to three dimensions, similar to the 2D simulation cases [10]. In the photoresist etching simulation, the 3D hash fast marching method is

* Corresponding author. Tel.: +86 25 83792632 8817; fax: +86 25 83792939.
E-mail address: zfzhou@seu.edu.cn (Z.-F. Zhou).

http://dx.doi.org/10.1016/j.mee.2014.07.023
0167-9317/

developed to calculate the final development profiles with less required memory elements. Thus various large scale 3D simulation of thick SU-8 lithography process can be implemented. The comparisons of simulation and experimental results verify the approaches.

2. Methods

2.1. Models

The basic models for UV lithography simulations of thick photoresists include aerial image, exposure, PEB and development models [10]. Ideal contact exposure without any gap between the mask and the thick SU-8 is not practical for inevitable errors such as surface flatness, surface roughness, etc. To reduce the diffraction effects, different materials such as glycerol have been adopted as compensation materials to fill the air gap between the mask and the resist during conventional contact/proximity lithography [19]. Because of the large refractive index mismatch between air and SU-8, the application of inclined UV lithography is restrained to fabricate structures with inclined angles lower than 53.2° [13]. To overcome this limitation, glycerol and water have been employed in an exposure process for index matching materials [4,5]. For example, Glycerol is employed as an index matching material, extending the possible inclined angles from 54° (in air) down to 19° (in glycerol). As shown in Fig. 1, to model the 3D light intensity distributions during the thick SU-8 lithography for above cases, we define some parameters associated with the calculations of the UV light intensity distribution. δ and θ represent the incident angle in the air and the refraction angle of inclined UV light in SU-8, respectively, and δ_x is the angle between x-axis and the projection of incident direction on the xy-plane. n_1, n_2 and n_3 are defined as the refractive indices of air, compensation materials and SU-8 photoresists, respectively. λ_1, λ_2 and λ_3 stand for the UV light wavelength in air, compensation materials and SU-8 photoresists, respectively. R_1, R_2 and R_3 are the reflection coefficients at the interfaces of mask/compensation material, compensation material/SU-8 and SU-8/substrate interfaces, respectively.

Since the propagation of the incident UV light will be refracted on the compensation material/SU-8 interface, it is difficult to deal with the refraction in Fresnel–Kirchhoff diffraction integral equation. To solve this problem, the mask shifting approach is utilized to handle the diffraction and refraction effects simultaneously [13]. Based on our previous researches [10,13], the light intensity of any calculation point p in photoresist for inclined and vertical UV lithography can be derived as:

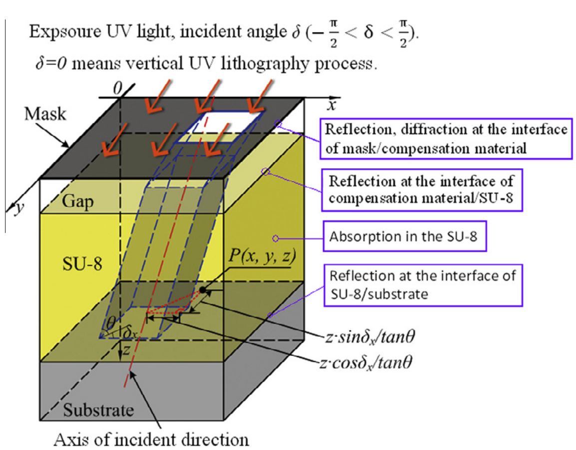

Fig. 1. Schematic modeling of the 3D inclined and vertical UV light intensity distribution into the SU-8 photoresist using the improved paraxial approximation.

$$I_p = \frac{(1-R_1)(1-R_2)\cdot I_{lamp}}{2}(\{[c(u_2)-c(u_1)]^2 + [s(u_2)-s(u_1)]^2\}\cdot\{[c(V_2)-c(v_1)]^2+[s(v_2)-s(v_3)]^2\} + R_3\{[c(u_4)-c(u_3)]^2+[s(u_4)-s(u_3)]^2\}\cdot\{[c(v_4)-c(v_3)]^2 + [s(v_4)-s(v_3)]^2\}) \quad (1)$$

where I_{lamp} is the original intensity of the incident UV light, $c(u)$ and $s(u)$ are the Fresnel integrals in x-direction while $c(v)$ and $s(v)$ are those in y-direction. u_i (i = 1,2,3,4) and v_i (i = 1,2,3,4) represent the Fresnel numbers in x-direction and y-direction, respectively, written as:

$$u_i^2 = \frac{2(n_3/n_2)}{\lambda_2(z-p_1+p_2)/\cos\theta}\cdot(x_i - x - (z-p_1+p_2)\cdot\tan\theta\cdot\cos\delta_x)^2,\quad i=1,2 \quad (2)$$

$$v_i^2 = \frac{2(n_3/n_2)}{\lambda_2(z-p_1+p_2)/\cos\theta}\cdot(x_i - x - (z-p_1+p_2)\cdot\tan\theta\cdot\cos\delta_x)^2,\quad i=1,2 \quad (3)$$

$$u_i^2 = \frac{2(n_3/n_2)}{\lambda_2(2d+p_1-z+p_2)/\cos\theta}\cdot(x_i - x - (2d+p_1-z+p_2)\cdot\tan\theta\cdot\cos\delta_x)^2,\quad i=3,4 \quad (4)$$

$$v_i^2 = \frac{2(n_3/n_2)}{\lambda_2(2d+p_1-z+p_2)/\cos\theta}\cdot(x_i - x - (2d+p_1-z+p_2)\cdot\tan\theta\cos\delta_x)^2,\quad i=3,4 \quad (5)$$

where x_i and y_i represent the latitudinal coordinates and longitudinal coordinates of the mask aperture, respectively. d represents the thickness of the SU-8 layer and z stands for the vertical distance from the mask plane to the calculation point in SU-8. p_1 is the primal gap thickness between the mask and SU-8, and p_2 represents the gap thickness after shifting the mask.

It should be noted that if no compensation material is employed to reduce the diffraction effects, our aerial image model is still corrected, by defining $n_2 = n_1$ and $\lambda_2 = \lambda_1$ in above equations. Furthermore, since the relationship between the incident and refractive angle always satisfies Snell's law for each medium, no matter whether compensation materials are utilized or not, θ in Eqs. ((2)–(5)) is obtained by,

$$\theta = \sin^{-1}(n_1\sin\delta/n_3) \quad (6)$$

For the case that index matching materials are employed during the lithography process, the presented aerial image model is also effective, only by defining n_1 equal to the refractive index of the specified index matching material.

For the 3D light intensity distribution calculation, the whole calculation domain in SU-8 is divided into a matrix of identical cubic elements (grids) with the same side length in our previous study. In this paper, adaptable element size of the cubic elements in x, y and z direction is adopted in the whole calculation domain, as shown in Fig. 2. Thus the total elements need to be calculated is obviously reduced. Generally, the total required simulation elements for the light intensity distribution calculation in [12] can be reduced by more than 7.5 times, so does the calculation time. After the light intensity distribution calculation, re-division of the whole calculation domain in SU-8 is carried out for the following simulation step.

With the light intensity distribution into the SU-8, an improved 3D Dill model directly extended from the improved 2D Dill model [16], is employed to calculate the exposure kinetics in thick SU-8 exposure processes. The improved 3D Dill exposure model accurately describes the nonlinear effects in thick photoresist