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Three-Dimensional Photoresist Exposure and Development Simulation

H. Kirchauer and S. Selberherr

Institute for Microelectronics, TU Vienna, Gusshausstrasse 27–29, A-1040 Vienna, Austria
Phone +43/1/58801-3750, FAX +43/1/5059224, e-mail kirchauer@iue.tuwien.ac.at

Among all technologies photolithography holds the leading position in pattern transfer in today's semiconductor industry. The reduction of the lithographic feature sizes towards or even beyond the used wavelength and the increasing nonplanarity of devices create complicated problems for the lithography process. A three-dimensional photolithography simulator including mask illumination, resist exposure and resist development is a cost effective tool for further improvements. We present a complete three-dimensional simulation model focusing on the resist exposure and resist development step.

Resist Exposure. Our three-dimensional simulation method is based on a spatial frequency domain solution of the Maxwell equations. In two dimensions a similar approach was proposed in [1]. According to Dill's 'ABC'-model the exposure state of the resist is described by the concentration of the photoactive compound (PAC) [2]. Part of the incident light is absorbed within the resist and destructs the PAC. Thereby the optical properties are changed. For that reason the resist is an optically nonlinear medium. However, the bleaching rate is small compared to the frequency of the EM field and a quasi-static approximation can be applied. By it the nonlinear time-dependent problem is transformed to a time-harmonic inhomogeneous problem for every time step and the EM field, e.g. $\mathcal{E}(\mathbf{x};t) = \mathrm{Re}\{\mathbf{E}(\mathbf{x})\,\exp(-j\omega t)\}$, obeys the Maxwell equations in the form of

$$\mathrm{curl}\,\mathbf{H}(\mathbf{x}) = -j\omega\varepsilon_o\,\varepsilon_r(\mathbf{x})\,\mathbf{E}(\mathbf{x}), \qquad \mathrm{curl}\,\mathbf{E}(\mathbf{x}) = j\omega\mu_o\,\mathbf{H}(\mathbf{x}). \tag{1}$$

We solve (1) under the following two assumptions: (i) the geometry is laterally periodical with periods a and b and the simulation domain is a rectangular prism ($a \times b \times h$) containing the resist and all nonplanar layers; (ii) the incident light is quasi-periodic with periods a and b. Then the EM field within the resist is quasi-periodic, too. Consequently, we expand the inhomogeneous permittivity $\varepsilon_r(\mathbf{x})$ and the complex amplitudes $\mathbf{U}(\mathbf{x}) = \mathbf{E}(\mathbf{x})$, $\mathbf{H}(\mathbf{x})$ in Fourier series

$$\varepsilon_r(\mathbf{x}) = \sum_n\sum_m \varepsilon_{r,nm}(z)\,e^{j2\pi(nx/a+my/b)}, \qquad \mathbf{U}(\mathbf{x}) = \sum_n\sum_m \mathbf{U}_{nm}(z)\,e^{j2\pi(f_{x,n}x+f_{y,m}y)}, \tag{2}$$

with $f_{x,n} = f_x^i + n/a$ and $f_{y,m} = f_y^i + m/b$. For off-axis illumination f_x^i and f_y^i are nonzero and determined by the angle of the incident light. Next, we insert the expansions of (2) into (1) and transform the partial differential equations to an infinite number of coupled ordinary differential equations (ODEs) for the Fourier coefficients $\mathbf{E}_{nm}(z)$ and $\mathbf{H}_{nm}(z)$. Above and below the resist an analytical expression for the EM field can be found [1]. Matching these expansions with the ODEs yields the boundary conditions on top and at the bottom of the resist. Now the sums in (2) are symmetrically truncated, i.e. only $(2N_x + 1) \times (2N_y + 1)$ Fourier modes are considered. Furthermore, the vertical field components can be expressed analytically by the transversal components. Hence, only the latter ones, i.e. $\{E_{x,nm}(z), E_{y,nm}(z), H_{x,nm}(z), H_{y,nm}(z)\}_{|n|\le N_x,|m|\le N_y}$ are related by the final $4 \times (2N_x + 1) \times (2N_y + 1)$-dimensional complex valued first order ODE system. This two-point boundary value problem is solved numerically with the shooting method [3], where an explicit integration scheme is used. Therefore, the numerical costs and memory usage of our algorithm are of the same order as of the recently proposed waveguide method [4]. An advantage of our method is, that we avoid to solve an eigenvalue problem and just have to do numerically less expensive matrix multiplications.

Resist Development. The development of the resist is as usually modeled as a surface-controlled etching reaction. We use Kim's 'R'-model to relate the final PAC distribution to a spatially inhomogeneous etch or development rate [5]. This development rate is stored on a tensorproductgrid, because the frequency domain solution of the Maxwell equations requires a laterally equal spaced grid to apply the numerically highly efficient two-dimensional Fast Fourier Transform algorithm. For the simulation of the time-evolution of the etching front we adapted the recently developed cell-based topography simulator of [6] to read the development rate from the tensorproductgrid. The basic idea behind this surface advancement algorithm is to apply a structuring element along the exposed surface which removes resist cells of the underlying cellular geometry representation. The shape of the structuring element depends in our case on the precalculated development rate.

Simulation Results. In Fig. 1 and Fig. 2 we demonstrate the capability of our approach. In both figures a contour plot of the PAC is shown in the right picture and the developed resist profile in the left picture. Contours are shown for PAC = 0.1, 0.2, . . . , 1.0. The $0.75\,\mu m \times 0.75\,\mu m$ wide mask-opening is in the center of the $1.5\,\mu m \times 1.5\,\mu m \times 1.0\,\mu m$ large simulation domain. The cut is along $y = 0.75\,\mu m$. The used wavelength is $0.365\,\mu m$, the exposure-dose is $120\,mJ/cm^2$ and the development time is $50\,sec$. The simulation parameters are for the Dill-model $n_o = 1.65$, $A = 0.55\,\mu m^{-1}$, $B = 0.045\,\mu m^{-1}$, $C = 0.013\,cm^2/mJ$ and for the Kim-model $R_1 = 0.25\,\mu m/sec$, $R_2 = 0.0005\,\mu m/sec$, $R_3 = 7.4$ (cf. Table IV in [5]).

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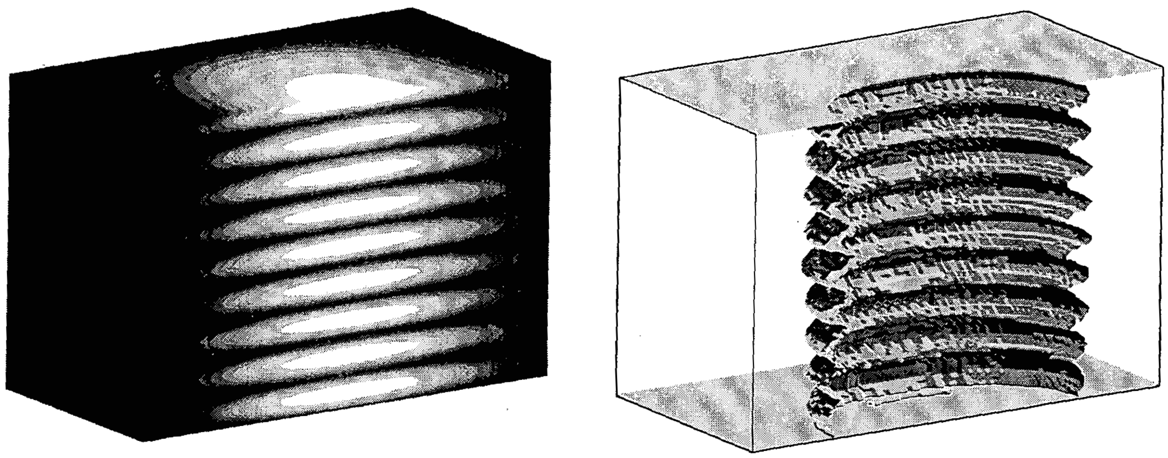

Figure 1: Simulation over a planar substrate. The oval contours are caused by standing waves within the resist, which result from substrate reflections.

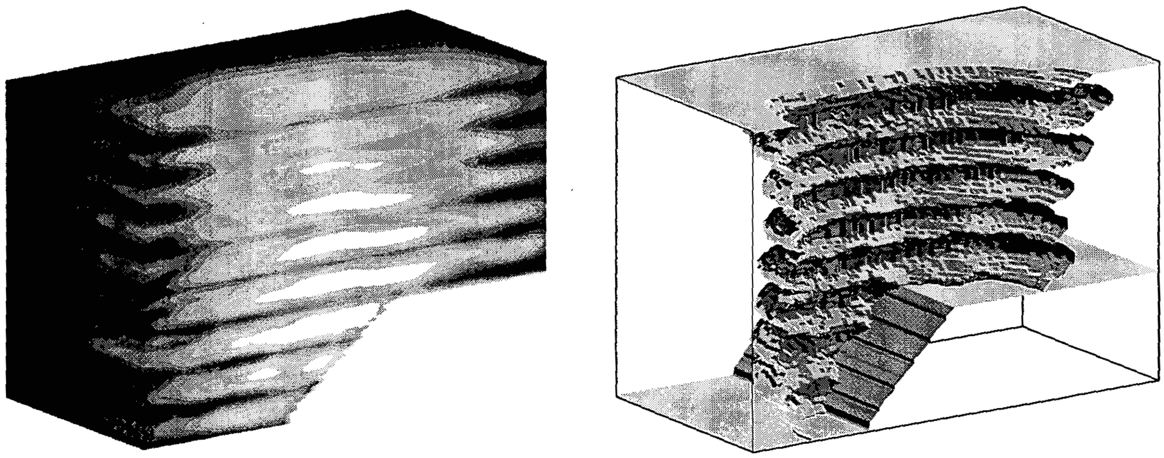

Figure 2: Simulation over a stepped substrate. Due to the variation in optical thickness the oval contours are distorted.Therefore certain regions within the resist are overexposed.

Acknowledgments. Our work is significantly supported by Austria Mikro Systeme AG, Unterpremstätten, Austria; and Christian Doppler Gesellschaft, Vienna, Austria.