RIGOROUS THREE-DIMENSIONAL PHOTOLITHOGRAPHY SIMULATION OVER NONPLANAR STRUCTURES

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Abstract

A rigorous three-dimensional simulation method for nonplanar substrate lithography is presented. The light propagation within the photoresist is calculated using the Maxwell equations. Our method relies on a Fourier expansion of the electromagnetic field and extends the two-dimensional differential method [1][2].

1. Introduction

Among all technologies photolithography holds the leading position in pattern transfer in today's semiconductor industry. The large cost and time necessary for experiments make simulation an important tool for further improvements. However, the reduction of the lithographic feature sizes towards the actinic wavelength places considerable demands onto the physical modeling. Our three-dimensional method is based on a numerical solution of the Maxwell equations and therefore gives a physically rigorous description of nonplanar topography effects as necessary for sub-micrometer-photolithography.

The simulation model can be summarized as follows. The exposure state of the resist is described by the photoactive compound (PAC). Part of the incident photons are absorbed and destruct the PAC. Thereby the resist's optical properties are modified. According to Dill's so-called 'ABC'-model the dependency between the PAC and the electromagnetic (EM) field is modeled by coupled nonlinear partial differential equations [3]. Because the bleaching rate is small compared to the frequency of the EM field, we apply a quasi-static approximation. Hence, we assume a steady-state field distribution within a time step, i.e. the EM field is time harmonic, e.g. $\mathcal{E}(\mathbf{x},t) = \mathrm{Re}\{\mathbf{E}_k(\mathbf{x})e^{-j\omega t}\}$, and obeys the Maxwell equations in the form of

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

The crucial point for the applicability of our simulation model is an efficient solution of the Maxwell equations (1).

2. Numerical solution of the Maxwell equations

Our solution of the Maxwell equations is based on a Fourier expansion of the EM field. A similar approach in two dimensions, the so-called differential method, was first proposed in the simulation of diffraction gratings [1] and later adapted for photolithography in [2]. The use of Fourier expansions implies a periodic nature of the EM field within the resist, which ensues from the following two assumptions: (i) the incident light is quasi-periodic or, equivalently, a periodic mask pattern is supposed; (ii) the geometry is periodic, too, and the periods a and b in $x-$ and $y-$ direction, respectively, are identical to that of the incident light. The simulation domain is one period $a \times b \times h$ of such a laterally periodic geometry, and the vertical extension h is chosen to comprise exactly the inhomogeneous resist and all nonplanar layer parts.

Lateral discretization. Consequently, the EM field inside the simulation domain can be expressed by Fourier expansions,

$$\mathbf{E}(\mathbf{x}) = \sum_n \sum_m \mathbf{E}_{nm}(z) e^{j(k_{x,n}x + k_{y,m}y)}, \quad \mathbf{H}(\mathbf{x}) = \sum_n \sum_m \mathbf{H}_{nm}(z) e^{j(k_{x,n}x + k_{y,m}y)}, \quad (2)$$

with $k_{x,n} = k_x^i + n2\pi/a$ and $k_{y,m} = k_y^i + m2\pi/b$. For off-axis illumination k_x^i and k_y^i are nonzero and determined by the angle of the incident waves. Additionally, the inhomogeneous permittivity $\varepsilon(\mathbf{x})$ and its reciprocal $\chi(\mathbf{x}) = 1/\varepsilon(\mathbf{x})$, needed for the discretization of (1), can be expanded in Fourier series,

$$\varepsilon(\mathbf{x}) = \sum_n \sum_m \varepsilon_{nm}(z) e^{j2\pi(nx/a + my/b)}, \quad \chi(\mathbf{x}) = \sum_n \sum_m \chi_{nm}(z) e^{j2\pi(nx/a + my/b)}. \quad (3)$$

Insertion of (2) and (3) into (1) transforms the partial differential equations into an infinite set of coupled ordinary differential equations (ODEs) for the Fourier coefficients of the lateral field components. The vertical components can be expressed analytically by the lateral ones. Obviously, this infinite set of ODEs cannot be solved numerically on a computer. Hence, we have to truncate the Fourier expansions (2), i.e. we consider only coefficients $\{E_{x,nm}, E_{y,nm}, H_{x,nm}, H_{y,nm}\}_{|n| \le N_x, |m| \le N_y}$ symmetrically centered around the principal incident ray $n = m = 0$. Using a matrix-vector notation the ODE system writes to

$$\mathbf{u}'(z) = \underline{\mathbf{H}}(z) \cdot \mathbf{u}(z), \qquad \mathbf{u} = [\mathbf{e}_x \ \mathbf{e}_y \ \mathbf{h}_x \ \mathbf{h}_y]^{\mathrm{T}}, \quad (4)$$

where the complex-valued $\mathbf{e}$ and $\mathbf{h}$ vectors hold the field's Fourier coefficients, and the elements of the system matrix $\underline{\mathbf{H}}(z)$ contain the Fourier coefficients of the permittivity and its reciprocal (cf. (3)). Due to the symmetric truncation of the Fourier sums each of the $\mathbf{e}$ and $\mathbf{h}$ vectors has dimension $(2N_x+1) \times (2N_y+1)$. Hence, the entire ODE system is of dimension $N_{\mathrm{ODE}} = 4 \times (2N_x+1) \times (2N_y+1)$.

Boundary conditions. Above and below the simulation domain the EM field can be expressed by Rayleigh expansions [1]. Matching the lateral components of these expansions to the field representation (2) valid inside the simulation domain, and eliminating the unknown reflected and outgoing wave amplitudes yield the sought boundary conditions on top ($z = 0$) and at the bottom ($z = h$):

$$\underline{\mathbf{B}}_o \cdot \mathbf{u}(0) = \mathbf{e}^i, \qquad \underline{\mathbf{B}}_h \cdot \mathbf{u}(h) = \mathbf{0}. \tag{5}$$

The vector $\mathbf{e}^i$ comprises all incident wave amplitudes, which are assumed to be known as they are the output of the illumination simulation. Each of the rectangular matrices $\underline{\mathbf{B}}_o$ and $\underline{\mathbf{B}}_h$ has dimension $N_{\mathrm{ODE}}/2 \times N_{\mathrm{ODE}}$; $\mathbf{e}^i$ and $\mathbf{0}$ are $N_{\mathrm{ODE}}/2$-dimensional vectors. Hence (5) represents exactly N_{ODE} algebraic equations as necessary for the definiteness of the ODE system (4).

Vertical Discretization. Using an explicit discretization method for the two-point boundary value problem (4) and (5) yields a recursion formula like $\mathbf{u}(z_{j+1}) = \underline{\mathbf{S}}_j \cdot \mathbf{u}(z_j)$ between two adjacent mesh points [4]. In the simplest case $\underline{\mathbf{S}}_j$ equals $\underline{\mathbf{S}}_j = \underline{\mathbf{I}} + (z_{j+1} - z_j)\underline{\mathbf{H}}(z_j)$ (Euler's method). A successive evaluation of this recursion formula relates the two boundary points $z_0 = 0$ and $z_{N_z+1} = h$,

$$\mathbf{u}(h) = \left(\prod_{j=0}^{N_z} \underline{\mathbf{S}}_j \right) \cdot \mathbf{u}(0) = \underline{\mathbf{S}} \cdot \mathbf{u}(0), \tag{6}$$

where N_z is the number of vertical discretization points. Combining this equation with the boundary conditions (5) forms the final algebraic system for $\mathbf{u}(0)$,

$$\begin{bmatrix} \underline{\mathbf{B}}_o \\ \underline{\mathbf{B}}_h \, \underline{\mathbf{S}} \end{bmatrix} \cdot \mathbf{u}(0) = \begin{bmatrix} \mathbf{e}^i \\ \mathbf{0} \end{bmatrix}. \tag{7}$$

As the illuminating light is not fully coherent, the algebraic equation system has to be solved for different incoherent incoming light orders, i.e. several right hand sides $\mathbf{e}^i$ have to be considered in (7). However, the system matrix has to be calculated just once and the Fourier coefficients $\mathbf{u}(z_j)$ at the inner mesh points can be computed simultaneously for all incoherent orders.

Computational efficiency. The memory usage of our method is of order $\mathcal{O}(N_{\mathrm{ODE}}^2) \approx \mathcal{O}(256 \times N_x^2 \times N_y^2)$, e.g. for $N_x = N_y = 15$ approximately 250 MB are required assuming 16 Bytes of memory for a double precision complex number. However, this quite high memory requirement is of the same order as other rigorous three-dimensional photolithography simulation models [5].

The numerical costs are mainly determined by the evaluation of the recursion (6) and by the multiple solution of (7). Both operations are of order $\mathcal{O}(N_{\mathrm{ODE}}^3)$. Hence, the total run-time grows for N_t time steps, N_s incoherent incoming wave sets and N_z vertical discretization points with $\mathcal{O}(N_t \times (N_s + N_z) \times N_{\mathrm{ODE}}^3)$, which lies typically under a few hours on DEC-3000/600 workstation.

3. Simulation Results and Concluding Remarks

In Figure 1 and Figure 2 we demonstrate the capability of our approach showing a contour plot of the PAC for a planar and stepped topography, respectively. 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 actinic wavelength is $365\,nm$ (I-line), the exposure-dose is $120\,mJ/cm^2$. Dill's parameters are $n_o = 1.65$, $A = 0.55\,\mu m^{-1}$, $B = 0.045\,\mu m^{-1}$, $C = 0.013\,cm^2/mJ$.

We have presented a rigorous three-dimensional electromagnetic simulation method, that extends the two-dimensional differential approach [1][2]. Using Fourier expansions the Maxwell equations are transformed to ordinary differential equations. The resulting two-point boundary value problem is solved with a "shooting method" like algorithm [4]. The computational efficiency is analyzed and shown to be advantageous or at least comparable to different recently proposed methods [5]. The simulation program runs on common engineering workstations with memory requirements in the range of 250 MB.

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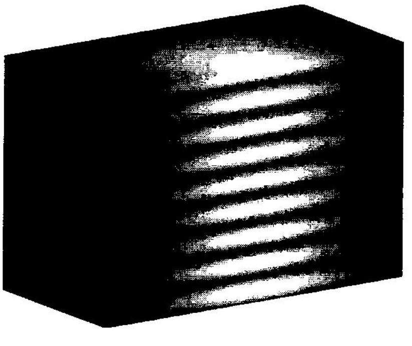

Figure 1: The oval contours are caused by standing waves within the photoresist, which result from substrate reflections.

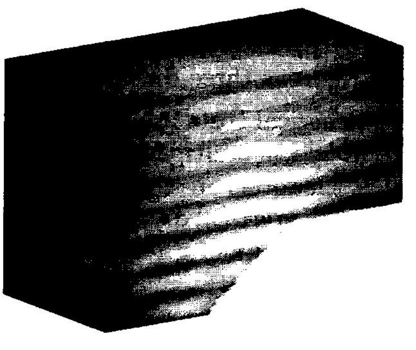

Figure 2: Due to the variation in optical thickness the oval contours are distorted and light-scattering into nominally unexposed parts of the photoresist occurs.