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THREE-DIMENSIONAL SIMULATION OF LIGHT-SCATTERING OVER NONPLANAR SUBSTRATES IN PHOTOLITHOGRAPHY

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A key step in photolithography simulation is a rigorous three-dimensional modeling of the exposure/bleaching of the resist's photoactive compound (PAC). Thereby electromagnetic (EM) scattering of light caused by the nonlinear resist as well as by a nonplanar topography has to be considered. We present a novel three-dimensional approach, based on a numerical solution of the Maxwell equations. Furthermore, we give a physically rigorous description of scattering effects as necessary for sub-micrometer-photolithography. A similar method in two dimensions was first proposed in the simulation of diffraction gratings [1] and adapted for photolithography in [2].

According to Dill's exposure/bleaching model the dependency between the PAC and the EM field is described by coupled nonlinear partial differential equations (PDEs) [3]. The quasi-static approximation of these PDEs assumes a steady-state field distribution within a time step, i.e. the EM field is time harmonic, e.g. $\mathcal{E}(\mathbf{x};t) = \mathrm{Re}\{\mathbf{E}(\mathbf{x})\exp(-j\omega t)\}$, and obeys the Maxwell equations in the form of

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

We solve (1) under the following two assumptions: (i) the simulation domain is one period of a laterally periodical geometry containing the resist and all nonplanar layers (cf. *Fig. 1*); (ii) the incident light is quasi-periodic and the period is identical to that of the geometry. Hence, the inhomogeneous permittivity $\varepsilon_r(\mathbf{x})$ in (1) can be expanded in a Fourier series,

$$\varepsilon_r(x,y,z) = \sum_n \sum_m \varepsilon_{nm}(z)e^{j2\pi(nx/a+my/b)}. \tag{2}$$

Furthermore, the EM field in the resist is also quasi-periodic. Consequently, we write

$$\mathbf{E}(x,y,z) = \sum_n \sum_m \mathbf{E}_{nm}(z)e^{j(k_{x,n}x+k_{y,m}y)}, \qquad \mathbf{H}(x,y,z) = \sum_n \sum_m \mathbf{H}_{nm}(z)e^{j(k_{x,n}x+k_{y,m}y)} \tag{3}$$

with $k_{x,n} = k_x^{in} + n2\pi/a$ and $k_{y,m} = k_y^{in} + m2\pi/b$. For oblique illumination k_x^{in} and k_y^{in} are nonzero and determined by the angle of the incident waves. Next, we insert (2) and (3) into (1) and transform the PDEs 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 with the Rayleigh expansion. Matching these expansions with the ODEs yields the boundary conditions on top and at the bottom of the resist. Finally, the two sums in (3) are truncated and the resulting finite-dimensional system of ODEs is solved numerically with the shooting method [4].

An inherent advantage of the proposed method is the possibility to run three- as well as two-dimensional simulations. In the latter case only one summation index occurs in (2) and (3). In *Fig. 2* and *Fig. 3* we demonstrate the capability of our approach. In both figures a contour plot of the PAC is shown.

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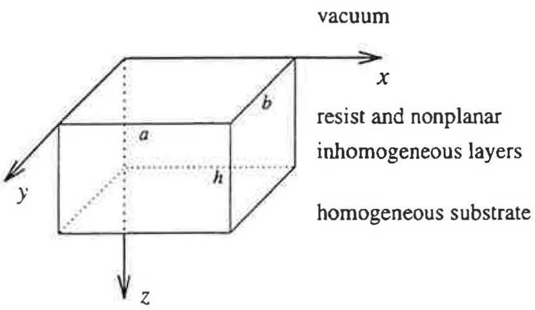

Fig. 1: The simulation domain is a rectangular prism ($a \times b \times h$) containing the resist and all nonplanar layers. Laterally the geometry is periodical with periods a and b in $x-$ and $y-$direction respectively. Above the resist ($z < 0$) we have vacuum, below ($z > h$) we assume an infinitely extended homogeneous substrate.

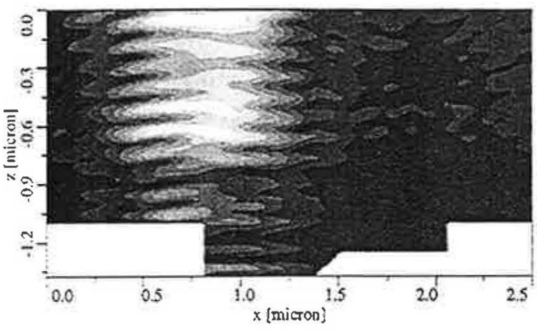

Fig. 2: Two-dimensional simulation over a bumpy substrate. Contours are shown for PAC = 0.2, 0.3, ..., 1.0. The 0.7 μm wide mask-opening is centered above the sharp edge at $x = 0.8\,\mu m$. The used wavelength is 0.365 μm, the exposure-dose is 120 mJ/cm^2. Due to the variation in optical thickness the oval contours which are typical for standing waves over planar substrates are distorted into interleaved fingers. Therefore certain regions within the resist are overexposed.

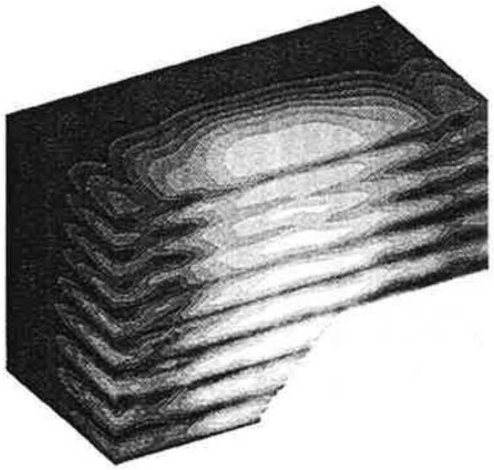

Fig. 3: Three-dimensional simulation over a stepped substrate. Contours are shown for PAC = 0.1, 0.2, ..., 1.0. The 0.75 $\mu m \times 0.75\,\mu m$ wide mask-opening is in the center of the $1.5\,\mu m \times 1.5\,\mu m \times 1.0\,\mu m$ large simulation domain. The used wavelength is 0.365 μm, the exposure-dose is 120 mJ/cm^2. Compared to *Fig. 2* the distortion of the oval contours is less significant, because the optical thickness of the sloped step varies continuously.