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A New Vector Model for Photoresist Bleaching in Optical Lithography

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Abstract

This paper describes a two-dimensional model for photoresist bleaching in optical lithography. The bleaching model incorporates an existing imaging simulator, METRO, with the vector *waveguide* method to calculate the electric field amplitudes within arbitrary structures upon a substrate being exposed by actinic light. Dill's model for positive photoresists is used to determine the changing photoactive compound concentrations within photoresist throughout the exposure. The resulting bleaching model comes considerably closer than current models to satisfying the simulation needs of process engineers.

1 Introduction

Better understanding of the exposure process in optical lithography is a key to developing smaller structure sizes reliably in semiconductor manufacture. The most important part of lithography simulation is the bleaching step. Bleaching defines the changes in photoresist chemistry caused by the electric fields of incident light. The four requirements for useful simulation are accessibility, speed, accuracy, and flexibility. To perform useful simulation we have combined the flexible imaging model from the alignment and metrology simulator, METRO[1], with the fast and accurate *waveguide* method for calculation of electric field amplitudes within photoresists. Dill's model[2] is used to compute the changes in photoresist solubility occurring during the exposure process.

2 Background

Simulation of the lithography process is necessary because conducting laboratory experiments is costly and time consuming. As process engineers generally do not have free use of supercomputers or massively parallel computers, useful simulations must be able to run on engineering workstations. Because many simulations must be performed to understand a problem or manufacturing trend, individual results need to be obtained quickly. High sensitivity to process parameters requires that simulations be accurate. Simulators must also be flexible to handle the wide range of topographic process styles, material types and imaging schemes encountered.

Currently, popular approaches to lithography simulation fall into two classes, supercomputer simulations and scalar models. Numerical methods for solving Maxwell's equations within

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arbitrary topographies on a supercomputer or massively parallel computer are flexible, accurate and often fast[3]. However, this class of simulators is expensive and not readily available. Scalar (pseudo 2-D) models such as SAMPLE[4], PROLITH[5] and DEPICT[6] run quickly on standard engineering workstations. The drawback of these methods is that they approximate the physical lithography environment as having planar surfaces in which light travels only vertically. They do not take into account diffraction effects within the wafer structure or fully simulate the effects of non-vertically incident light. Thus, they have poor flexibility and provide low accuracy when attempting to model complex situations. Therefore, no present simulator adequately fulfills the needs of the process engineer.

3 Simulation Method

The *waveguide* method was originated by Burckhardt[7] in 1966 for the study of holograms. Yuan used the method to calculate the reflected and transmitted light amplitudes for METRO, an optical metrology and alignment simulator. Yuan extended the *waveguide* method to rigorously solve Maxwell's equations for both polarizations of light incident upon non-planar substrate structures from arbitrary directions[8]. We have further extended the method to calculate the electric field amplitudes within arbitrarily shaped substrate structures.

The model simulates a true 2-D lithography system, dividing the photoresist bleaching problem into three parts. These parts are the simulation of the incident light pulse, the calculation of light intensity within the wafer structure and the modeling of the changes in local resist solubility. METRO's imaging simulator, which is based upon Abbe's imaging theory, computes the shape of the incident light pulse. This pulse is then discretized into a set of incoming spatial frequencies. The *waveguide* method computes the relative amplitudes of the spatial frequencies within photoresist structures approximated in a *Manhattan geometry* format (See Fig. 1). When combined with the input frequency amplitudes, the absolute internal amplitudes necessary for bleaching simulation can be obtained.

The function of the dielectric constant versus horizontal position in layer j of a structure, $\epsilon(x)$, can be described by its Fourier series:

$$\epsilon^j(x) = \sum_q \epsilon_q^j \exp(i2\pi qbx).$$

b is the inverse of the structure period P, where $P >> \lambda_o$, the wavelength in air of the imaging light.

The electric field amplitudes E_i^j's of the internal waves for any layer j and any spatial frequency i for the TE mode are to be calculated using Yuan's notation[8]. The Maxwell's equation governing the electric field $\mathbf{E}^j(x,z)$ $(= \hat{y}E^j(x,z))$ for layer j is:

$$\nabla^2\mathbf{E}^j - \mu_o\epsilon_o\epsilon^j(x)\frac{\partial^2\mathbf{E}^j}{\partial t^2} + \nabla\left(\mathbf{E}^j \cdot \frac{\nabla\epsilon^j(x)}{\epsilon^j(x)}\right) = 0.$$

After substituting for $\epsilon^j(x)$ and omitting the universal constants μ_o and ϵ_o for simplicity, the wave equation above can be decomposed into two ordinary differential equations using separation of variables (i.e., $E^j(x,z) = X^j(x)Z^j(z)$):

$$\frac{\partial^2 X^j}{\partial x^2} + \left[k_o^2 \sum_q \epsilon_q^j \exp(i2\pi qbx) + \left(\alpha^j\right)^2\right] \cdot X^j = 0, \tag{1}$$

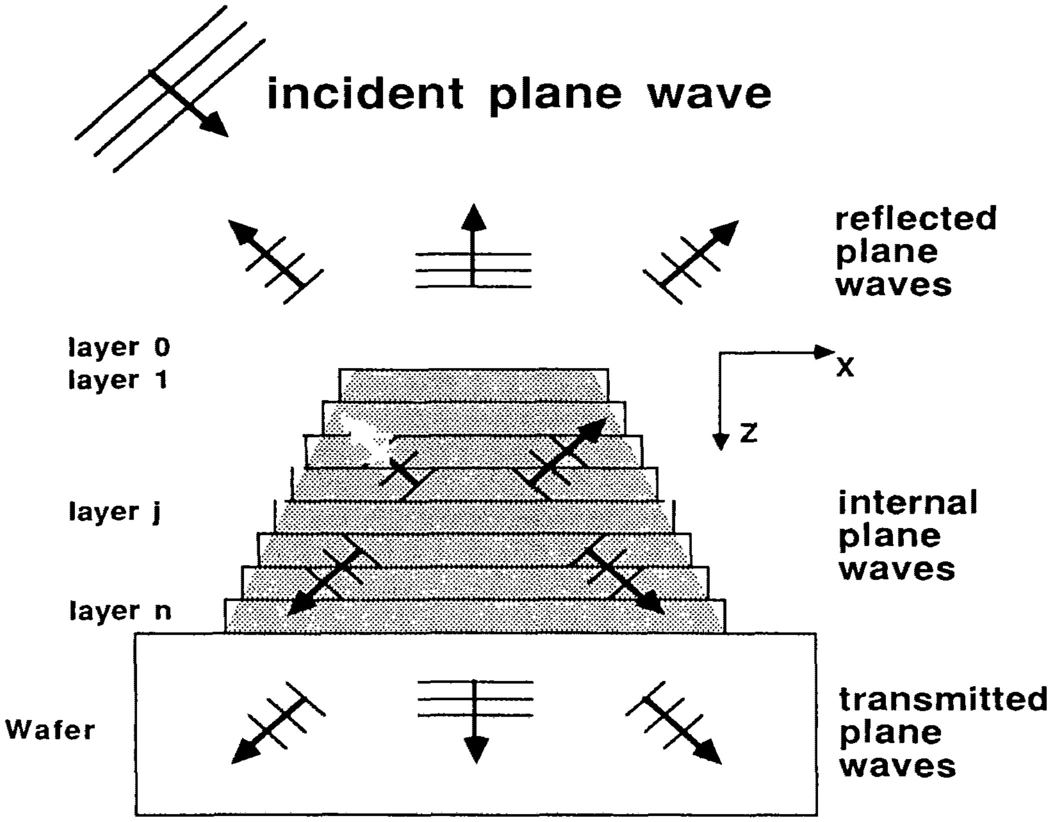

Figure 1: Diagram of Internal Light Waves.

$$\frac{\partial^2 Z^j}{\partial z^2} - \left(\alpha^j\right)^2 Z^j = 0, \tag{2}$$

The solution of $X^j(x)$ has the general form

$$X^j(x) = \sum_l B_l^j \exp(i2\pi lbx), \tag{3}$$

according to the Floquet theorem. By inserting Eq. 3 into Eq. 1, we obtain the eigenvalue problem for each layer

$$\mathbf{D}^j\mathbf{B}^j = \left(\alpha^j\right)^2 \mathbf{B}^j$$

After solving Eq. 2 for Z^j, the E field can then be expressed by:

$$E_y^j = \sum_{m=-L}^{+L} \left[\left(A_m^j \exp\left(\alpha_m^j z\right) + A_m'^j \exp\left(-\alpha_m^j z\right)\right) \sum_{l=-L}^{+L} B_{l,m}^j \exp(i2\pi lbx)\right] \tag{4}$$

Physically, the E field can be thought of as linear combinations of waves with discrete wave-guide modes of spatial frequency α_m. Eq. 4 is used for calculating the internal electric field amplitudes at a position (x,z), however, all the coefficients still need to be determined by employing boundary conditions. The amplitudes for the TM mode are obtained in a similar manner.

The electric field intensities are used to calculate the destruction of the photoactive compound (PAC) in photoresists at a rate given by Dill's model. The local PAC concentrations determine the local solubility of the photoresist to a developer solution. The final output of this simulator is these PAC concentration values. Because the destruction of PAC alters the dielectric function within photoresists, the electric field and PAC concentrations calculations are repeated for a small number of time steps during the exposure simulation. For each time step the changes in PAC concentration and the related changes in optical properties of the photoresist are kept small. Keeping the changes per step to less than 20% of the original PAC value (ie. five or more time steps in all) is a useful guideline[9].

4 Results

The model has shown excellent agreement with electromagnetic theory. However, only results for uncomplicated structures may be verified theoretically. Implementation has shown its usability on a standard engineering workstation. Simulation results for planar structures agree well with those of DEPICT-2 from TMA Inc. The limitations of DEPICT and other scalar models can be examined visually in Figures 2 and 3. Figure 2 shows PAC concentrations within a planar photoresist structure for both DEPICT and our vector model. Figure 3 shows examples of equal light intensity curves within non-planar structures from the model. These structures could be a result of non-planar topography underneath or the defects in a photoresist layer. Scalar models such as SAMPLE, PROLITH and DEPICT are unable to perform these types of complicated simulations[10].

The quickest simulations take only a few minutes on a DECstation 3100. Longer simulations can take approximately 100 minutes for a six time step run. However, the matrix calculations are performed in a relatively inefficient direct manner. Yuan has shown a that a factor of ten speedup is possible by using iteritive matrix solution methods. The model is also capable of simulating the effects of thick, non-uniform exposure masks upon the lithography process. The model described in this report is an accurate, reasonably fast, highly flexible and usable bleaching simulator. It comes much closer than present methods for meeting the requirements of process engineers for useful simulations.

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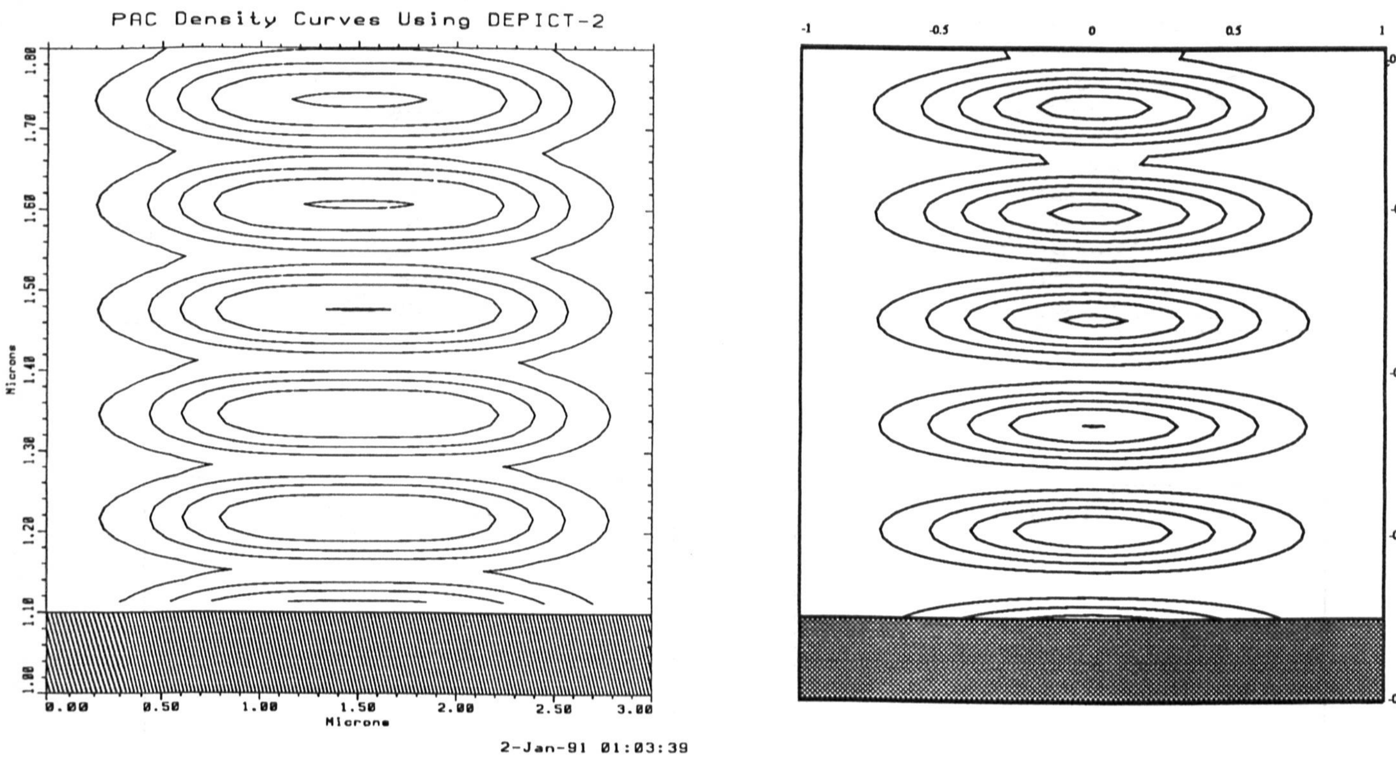

Figure 2: Comparison with DEPICT of PAC Concentrations in a Planar Structure Consisting of 0.7μ of Photoresist Above 0.1μ of SiO_2.

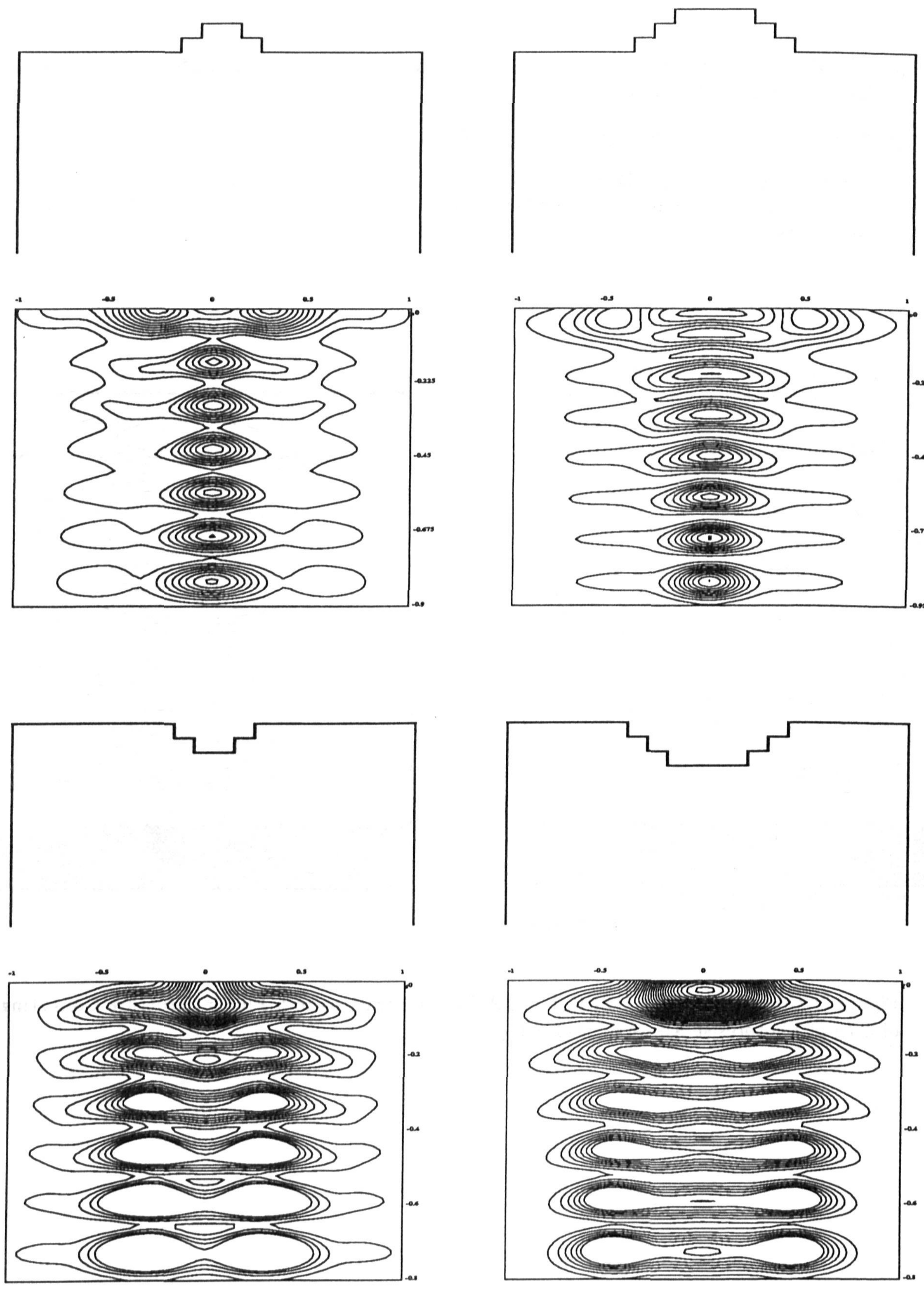

Figure 3: Equal Light Intensity Curves Within Non-Planar Photoresist Above Planar 0.1 Micron Silicon Dioxide layer. The Surfaces of the Photoresists are Shown Above the Curves.