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Analytical expression for the standing wave intensity in photoresist

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When a thin dielectric film placed between two semi-infinite media is irradiated with monochromatic plane waves, a standing wave is produced in the film. An analytical expression for the standing wave intensity within the film is derived. This expression is then expanded to include the effects of other dielectric films on either side of the film or an inhomogeneous film. Applications of these expressions are given for photolithographic modeling.

I. Introduction

When a thin dielectric film placed between two semi-infinite media (e.g., a thin coating on a reflecting substrate) is exposed to monochromatic light, standing waves are produced in the film. This effect has been well documented for such cases as antireflection coatings and photoresist exposure.[1–5] In the former, the standing wave effect is used to reduce reflections from the substrate. In the latter, standing waves are an undesirable side effect of the exposure process. Unlike the antireflection application, photolithography applications require knowledge of the intensity of the light within the thin film itself. Previous work[4,5] on determining the intensity within a thin photoresist film has been limited to numerical solutions. This paper presents an analytical expression for the standing wave intensity within a thin film. This film may be homogeneous or of a known inhomogeneity. The film may be on a substrate or between one or more other thin films. Finally, applications of this expression are given for photoresist exposure.

II. Standing Wave Effect

Consider a thin film of thickness D and complex index of refraction $\mathbf{n}_2$ deposited on a thick substrate with complex index of refraction $\mathbf{n}_3$ in an ambient environment of index $\mathbf{n}_1$. An electromagnetic plane wave is normally incident on this film. Let E_1, E_2, and E_3 be the electric fields in the ambient, thin film, and substrate, respectively (see Fig. 1). Assuming monochromatic illumination, the electric field in each region is a plane wave or the sum of two plane waves traveling in opposite directions (i.e., a standing wave). Maxwell's equations require certain boundary conditions to be met at each interface: specifically, E_j and the magnetic field H_j are continuous across the boundaries $z = 0$ and $z = D$. Solving the resulting equations simultaneously, the electric field in region 2 can be shown to be (see Appendix)

$$E_2(x,y,z) = E_I(x,y)\tau_{12}\frac{\exp(-ik_2z) + \rho_{23}\tau_D^2\exp(ik_2z)}{1 + \rho_{12}\rho_{23}\tau_D^2}, \qquad (1)$$

where $E_I(x,y)$ = the incident wave at $z = 0$;
$\rho_{ij} = (\mathbf{n}_i - \mathbf{n}_j)/(\mathbf{n}_i + \mathbf{n}_j)$, the reflection coefficient;
$\tau_{ij} = 2\mathbf{n}_i/(\mathbf{n}_i + \mathbf{n}_j)$, the transmission coefficient;
$\tau_D = \exp(-ik_2D)$, the internal transmittance of the resist film;
$k_j = 2\pi\mathbf{n}_j/\lambda$, the propagation constant;
$\mathbf{n}_j = n_j \pm i\kappa_j$, the complex index of refraction; and
λ = vacuum wavelength of the incident light.

For a weakly absorbing film, the imaginary parts of ρ_{12} and τ_{12} can be neglected, and the intensity can be calculated from

$$I(z) = I_0T_{12}\exp(-az)\frac{1 + g(D-z) + |\rho_{23}|^2\exp[-a2(D-z)]}{1 + \rho_{12}g(D) + \rho_{12}^2|\rho_{23}|^2\exp(-a2D)}, \qquad (2)$$

where $g(\Delta) = 2\exp\{-\alpha\Delta[\mathrm{re}\{\rho_{23}\}\cos(4\pi n_2\Delta/\lambda) + \mathrm{im}\{\rho_{23}\}\sin(4\pi n_2\Delta/\lambda)]\}$;
$T_{12} = \tau_{12}\tau_{21}$, the transmittance of the interface between mediums 1 and 2; and
$\alpha = 4\pi\kappa_2/\lambda$, the absorption coefficient of medium 2.

As can be seen from Eq. (2), the intensity within the thin film varies sinusoidally with a period of $\lambda/2n_2$. There will be a minimum intensity at the film–substrate interface ($z = D$) for a reflecting substrate (ρ_{23}

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negative). This minimum will be zero for a perfectly reflecting substrate ($\rho_{23} = -1$). The factor $\exp(-\alpha z)$ accounts for absorption by the film. Of course, an exact expression for the intensity may be obtained by squaring the magnitude of E_2 in Eq. (1).

III. Multiple Films

It is very common to have more than one film coated on a substrate. The problem then becomes that of two or more absorbing thin films on a substrate. An analysis similar to that shown above for one film yields the following result for the electric field in the top layer of an $m - 1$ layer system:

$$E_2(x,y,z) = E_I(x,y)\tau_{12}\,\frac{\exp(-ik_2z) + \rho'_{23}\tau_{D2}^2\exp(ik_2z)}{1 + \rho_{12}\rho'_{23}\tau_{D2}^2}\,, \tag{3}$$

where

$$\rho'_{23} = \frac{n_2 - n_3X_3}{n_2 + n_3X_3}\,,$$

$$X_3 = \frac{1 - \rho'_{34}\tau_{D3}^2}{1 + \rho'_{34}\tau_{D3}^2}\,,$$

$$\rho'_{34} = \frac{n_3 - n_4X_4}{n_3 + n_4X_4}\,,$$

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$$X_m = \frac{1 - \rho_{m,m+1}\tau_{Dm}^2}{1 + \rho_{m,m+1}\tau_{Dm}^2}\,,$$

$$\rho_{m,m+1} = \frac{n_m - n_{m+1}}{n_m + n_{m+1}}\,,$$

$$\tau_{Dj} = \exp(-ik_jD_j);$$

and all other parameters are defined previously. The parameter ρ'_{23} is the effective reflection coefficient between the thin film and what lies beneath it.

If the thin film in question is not the top film (layer 2), the intensity can be calculated in layer j from

$$E_j(x,y,z) = E_{I(\mathrm{eff})}\tau^*_{j-1,j}\,\frac{\exp(-ik_jz_j) + \rho'_{j,j+1}\tau_{Dj}^2\exp(ik_jz_j)}{1 + \rho^*_{j-1,j}\rho'_{j,j+1}\tau_{Dj}^2}\,, \tag{4}$$

where $\tau^*_{j-1,j} = 1 + \rho^*_{j-1,j}$,

$$\rho^*_{j-1,j} = \frac{n_{j-1}Y_{j-1} - n_j}{n_{j-1}Y_{j-1} + n_j}\,;$$

$$Y_{j-1} = \frac{1 + \rho^*_{j-2,j-1}\tau_{Dj-1}^2}{1 - \rho^*_{j-2,j-1}\tau_{Dj-1}^2}\,;$$

$$\cdot$$

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$$\rho^*_{23} = \frac{n_2Y_2 - n_3}{n_2Y_2 + n_3}\,;$$

$$Y_2 = \frac{1 + \rho_{12}\tau_{D2}^2}{1 - \rho_{12}\tau_{D2}^2}\,;$$

$$\rho_{12} = \frac{n_1 - n_2}{n_1 + n_2}\,;$$

$$E_{I(\mathrm{eff})} = E_I\,\frac{\tau_{12}\tau_{D2}}{1 + \rho_{12}\tau_{D2}^2}\,\frac{\tau^*_{23}\tau_{D3}}{1 + \rho^*_{23}\tau_{D3}^2}$$

$$\cdots\frac{\tau^*_{j-2,j-1}\tau_{Dj-1}}{1 + \rho^*_{j-2,j-1}\tau_{Dj-1}^2}\,;$$

and z_j is the distance into layer j. The effective reflection coefficient ρ^* is analogous to the coefficient ρ' looking in the opposite direction.

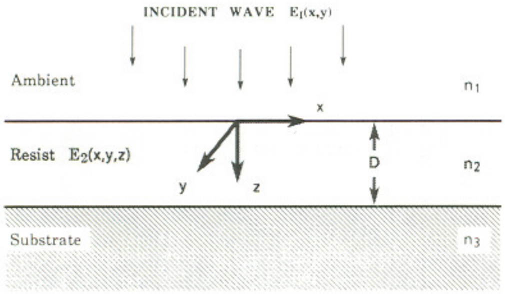

Fig. 1. Geometry used in the derivation of the standing wave intensity.

IV. Inhomogeneous Films

If the film in question is not homogeneous, the equations above are in general not valid. Let us, however, examine one special case in which the inhomogeneity takes the form of variations in the imaginary part of the index of refraction of the film, leaving the real part constant. In this case, absorbance A is no longer simply αz but becomes

$$A(z) = \int_0^z \alpha(z')dz'. \tag{5}$$

It can be shown that Eqs. (1)–(4) are still valid if the anisotropic expression for absorbance (5) is used. For example, Eq. (2) will become

$$I(z) = I_0T_{12}\exp[-A(z)]\,\frac{1 + g(D - z) + |\rho_{23}|^2\exp[-2A(D - z)]}{1 + \rho_{23}g(D) + \rho_{12}^2|\rho_{23}|^2\exp[-2A(D)]}\,, \tag{6}$$

where $g(\Delta) = 2\exp[-A(\Delta)][\mathrm{re}\{\rho_{23}\}\cos(4\pi n_2\Delta/\lambda) + \mathrm{im}\{\rho_{23}\}\sin(4\pi n_2\Delta/\lambda)]$. Thus $I(z)$ can be found if the absorption coefficient is known as a function of z.

Table I. Typical Parameters for Photoresist Projection Printing. $\lambda = 436$ nm

Layer	Index of refraction	Thickness (μm)
Ambient: air	1.0	—
Layer 2: AZ1350	$1.65-i0.02$	0.85
Layer 3: SiO_2	1.47	0.10
Substrate: silicon	$4.7-i0.08$	—

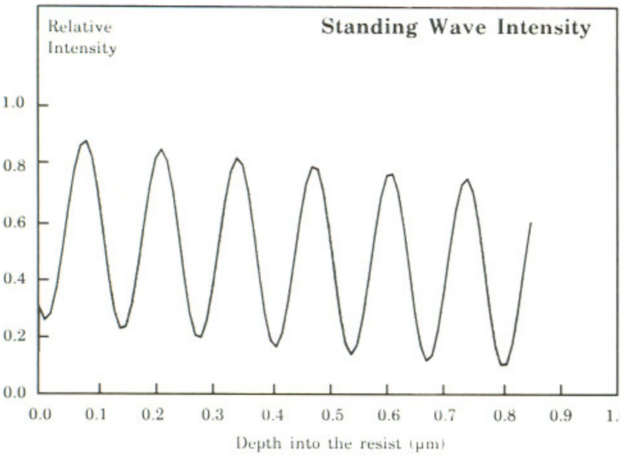

Fig. 2. Standing wave intensity within a photoresist film at the start of exposure (calculated using the parameters given in Table I). The intensity shown is relative to the incident intensity I_0.

V. Applications to Photolithography

When a photoresist is exposed during fabrication of an integrated circuit via projection printing, the light which arrives at the wafer is nearly a plane wave. Thus Eqs. (1)–(4) are directly applicable. A typical set of parameters for photoresist exposure is given in Table I with the results of Eq. (3) graphed in Fig. 2. Recently, use of a thin contrast-enhancement layer on top of the photoresist has been shown to improve resolution.[6] This type of resist system can be modeled with the use of Eq. (4).

The condition that the photoresist be homogeneous is true only at the start of exposure. Once exposed, the resist changes composition at a rate proportional to the light received. (This anisotropy is essential giving rise to the resist's imaging properties.) Thus Eq. (6) can be applied if the absorption coefficient $\alpha(z)$ can be determined. For an AZ-type positive photoresist, the absorption coefficient is related to the concentration of light sensitive material within the resist[5]

$$\alpha(z) = Am(z) + B, \tag{7}$$

where A and B are measurable constants, and $m(z)$ is the relative concentration of the photoactive compound (PAC). Furthermore, $m(z)$ can be calculated for a given light intensity from[5]

$$m(z) = \exp[-cI(z)t], \tag{8}$$

where c = exposure constant,
t = exposure time, and

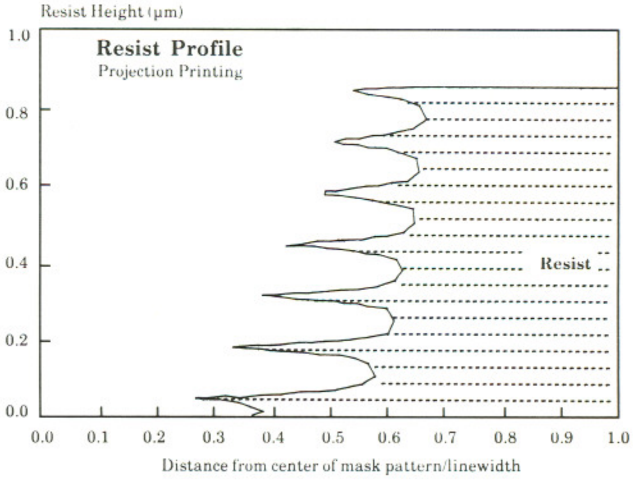

Fig. 3. Predicted resist profile using the standing wave intensity shown in Fig. 2 (calculated using the model PROLITH[7]).

$I(z)$ = light intensity as calculated from Eqs. (1), (2), (3), (4), or (6).

Thus knowledge of the homogeneous standing wave intensity $I(z)$ enables one to predict the chemical changes that take place in the resist as a result of exposure [i.e., calculating $m(z)$]. An iterative approach can then be used to solve Eqs. (5)–(8) for a given exposure time and incident intensity.[7]

VI. Conclusion

An exact solution has been given for the intensity of light within a thin film irradiated by normally incident monochromatic plane waves. This film may be homogeneous or of a known inhomogeneity and may be layered between other films. These solutions can be applied to semiconductor photolithography, in particular, to projection printing of positive images. Numerical calculations of the standing wave intensity given by other authors[4,5] yield comparable results. This analysis of the standing wave intensity has been incorporated into a comprehensive optical lithography model, positive resist optical lithography (PROLITH) model,[7] which can be used to generate developed resist profiles (Fig. 3) and provide other information important to the lithographic process.

Appendix

Consider the thin film shown in Fig. 1. A monochromatic plane wave is normally incident on this film. The electric field in each region is of the form[8]

$$E_j(x,y,z) = E(x,y)[A_j \exp(-ik_jz) + B_j \exp(ik_jz)], \tag{A1}$$

where A_j,B_j = complex constants,
$k_j = 2\pi\mathbf{n}_j/\lambda$, and
$\mathbf{n}_j = n_j \pm i\kappa_j$.

The sign of imaginary part of $\mathbf{n}_j$ is negative for a wave traveling in the $+z$ direction and positive for a wave traveling in the $-z$ direction. (This describes an absorbing medium.) The magnetic field $H_j(x,y,z)$ can be written in a similar fashion:

$$H_j(x,y,z) = \frac{1}{\eta_j} E(x,y)[A_j \exp(-ik_jz) - B_j \exp(ik_jz)], \quad \text{(A2)}$$

where η_j = the intrinsic impedance of medium j,
= μ_j/n_j, and
μ_j = the magnetic permeability of medium j.

Maxwell's equations require certain boundary conditions to be met at each interface, specifically, E_j and H_j are continuous across a boundary. Thus, at the two boundaries $z = 0$ and $z = D$,

$$E_1(x,y,0) = E_2(x,y,0), \quad \text{(A3a)}$$

$$H_1(x,y,0) = H_2(x,y,0), \quad \text{(A3b)}$$

$$E_2(x,y,D) = E_3(x,y,D), \quad \text{(A3c)}$$

$$H_2(x,y,D) = H_3(x,y,D). \quad \text{(A3d)}$$

Using these boundary conditions on Eqs. (A1) and (A2) and assuming $\mu_j = \mu_0$,

$$A_1 + B_1 = A_2 + B_2, \quad \text{(A4a)}$$

$$n_1(A_1 - B_1) = n_2(A_2 - B_2), \quad \text{(A4b)}$$

$$A_2 \exp(-ik_2D) + B_2 \exp(ik_2D) = A_3 \exp(-ik_3D), \quad \text{(A4c)}$$

$$n_2[A_2 \exp(-ik_2D) - B_2 \exp(ik_2D)] = n_3A_3 \exp(-ik_3D). \quad \text{(A4d)}$$

These equations can now be solved simultaneously for the constants A_j and B_j. To simplify the solution let us introduce the following notation:

$\rho_{ij} = (\mathbf{n}_i - \mathbf{n}_j)/(\mathbf{n}_i + \mathbf{n}_j)$, the reflection coefficient;
$\tau_{ij} = 2\mathbf{n}_i/(\mathbf{n}_i + \mathbf{n}_j)$, the transmission coefficient;
$\tau_D = \exp(-ik_2D)$, the internal transmittance of layer 2.

The solution now becomes

$$E_2(x,y,z) = E_I(x,y)\tau_{12} \frac{\exp(-ik_2z) + \rho_{23}\tau_D^2 \exp(ik_2z)}{1 + \rho_{12}\rho_{23}\tau_D^2}, \quad \text{(A5)}$$

where $E_I(x,y) = A_1E(x,y)$, the incident wave at $z = 0$.

The same solution can be derived using a geometrical approach. A normally incident plane wave E_I is partially transmitted at the ambient–thin film interface. The transmitted wave $E_0(z)$ can be expressed as

$$E_0(z) = E_I\tau_{12} \exp(-ik_2z), \quad \text{(A6)}$$

where τ_{12} is the transmission coefficient as defined earlier. Wave $E_0(z)$ is then reflected by the substrate at $z = D$ giving rise to a new wave $E_1(z)$:

$$\begin{aligned} E_1(z) &= \rho_{23}E_0(D) \exp[ik_2(z - D)] \\ &= E_I\rho_{23}\tau_{12}\tau_D^2 \exp(ik_2z). \end{aligned} \quad \text{(A7)}$$

Similarly, $E_1(z)$ is reflected at the film–air interface to give $E_2(z)$:

$$E_2(z) = E_I\rho_{21}\rho_{23}\tau_{12}\tau_D^2 \exp(-ik_2z). \quad \text{(A8)}$$

Also,

$$\begin{aligned} E_3(z) &= E_I\rho_{21}\rho_{23}^2\tau_{12}\tau_D^4 \exp(ik_2z), \\ E_4(z) &= E_I\rho_{21}^2\rho_{23}^2\tau_{12}\tau_D^4 \exp(-ik_2z), \end{aligned} \quad \text{(A9)}$$

etc.

The total electric field within the thin film $E_T(z)$ is the sum of each $E_j(z)$. Performing this summation gives

$$E_T(z) = E_I\tau_{12}[\exp(-ik_2z) + \rho_{23}\tau_D^2 \exp(ik_2z)]S, \quad \text{(A10)}$$

where $S = 1 + \rho_{21}\rho_{23}\tau_D^2(1 + \rho_{21}\rho_{23}\tau_D^2(1 + \ldots$..

The summation S is simply a geometric series and has the value

$$S = 1/(1 - \rho_{21}\rho_{23}\tau_D^2) = 1/(1 + \rho_{12}\rho_{23}\tau_D^2). \quad \text{(A11)}$$

Thus

$$E_T(x,y,z) = E_I(x,y)\tau_{12} \frac{\exp(-ik_2z) + \rho_{23}\tau_D^2 \exp(ik_2z)}{1 + \rho_{12}\rho_{23}\tau_D^2}, \quad \text{(A12)}$$

which is identical to Eq. (A5).

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