Copyright 2004 by the Society of Photo-Optical Instrumentation Engineers.


The International Society for Optical Engineering

This paper was published in the proceedings of Optical Microlithography XVII, SPIE Vol. 5377, pp. 1475-1486. It is made available as an electronic reprint with permission of SPIE.

One print or electronic copy may be made for personal use only. Systematic or multiple reproduction, distribution to multiple locations via electronic or other means, duplication of any material in this paper for a fee or for commercial purposes, or modification of the content of the paper are prohibited.

# Methods for Benchmarking Photolithography Simulators: Part II 

Mark D. Smith ${ }^{*}$, Jeffrey D. Byers, Chris A. Mack<br>KLA-Tencor Corp.


#### Abstract

Numerical simulation has become an indispensable tool for the design and optimization of photolithographic processes. Because the semiconductor industry now relies heavily on these tools, it is necessary to be able to benchmark their accuracy - as feature sizes continue to shrink, the numerical error in these simulators must decrease as well.

In a previous paper, we proposed benchmarks for aerial image calculation that were drawn from the optics literature. Because these benchmarks were closed-form solutions, we could use these results as an absolute standard for determining the numerical accuracy of an aerial image calculation. In the current study, we continue this effort by presenting closed-form solutions that can serve as benchmarks for the resist response to the projection optics. Benchmarks are proposed for film stack reflectivity and image in resist. Specific results will be presented for PROLITH.


Keywords: Lithography simulation, numerical accuracy, PROLITH

## 1 INTRODUCTION

As numerical simulation becomes more important to the design and optimization of photolithographic processes, it becomes vital that simulators provide accurate results. A simulator must not only be accurate, it must become more accurate with each design node [1]. The metrology concept of the $\mathrm{P} / \mathrm{T}$ ratio (precision to tolerance) is very appropriate for simulators as well - a 5 nm error might seem insignificant when engineering a 0.5 micron process, but it is a significant fraction of the error budget for a 65 nm process.

Benchmarking the accuracy of a simulator should be an important part of an "acceptance test" for all simulation software. A P/T ratio of 0.1 to 0.2 is typical for metrology tools, so perhaps it would be reasonable for simulators as well. Benchmarking should be performed if you have purchased a commercial simulator (such as PROLITH) or if you are using a code that you or your colleagues have written for internal use at your company. Although it is obvious that software must be free of bugs or algorithm problems in order to make quantitative engineering decisions, few users of simulation software actually perform a quantitative study of the accuracy of their simulator.

One of the reasons relatively few quantitative accuracy studies are performed is that for the end-user of a simulator, it is often difficult to make a judgment regarding the accuracy of a simulator beyond whether a particular result is "reasonable". Of course, it is possible to compare one simulator with the results calculated with another simulator, but if the results do not agree, how do you decide which one is correct? In addition, both simulators could agree and still be incorrect. The approach taken in the current study is to find closed-form solutions from the research literature, and to use these solutions as an absolute standard for benchmarking lithography simulators. This is similar to the approach taken by Brunner [2] and Gordon [3].

The current work is an extension of our previous paper [4], where we proposed standard benchmark problems for aerial image calculations. The benchmarks presented here are for film stack reflectivity and image in resist. The outline of this paper is as follows: in Section 2, we review the definition of intensity, transmissivity, and reflectivity in order to understand how the results predicted by a photolithography simulator are related to thin-film results presented in a typical optics textbook. Next, we present benchmarks for resist and substrate reflectivity with non-absorbing materials in Section 3, and for transmissivity of absorbing materials in Section 4. In Section 5, we present benchmarks for image in resist for a simple two-beam imaging system.

[^0]

Figure 1: Diagram of the incident, transmitted, and reflected electric fields at an interface between two materials.

## 2 DEFINITION OF INTENSITY, REFLECTIVITY, AND TRANSMISSIVITY

Consider light intersecting the plane interface between two materials, numbered 1 and 2 as shown in Figure 1, with an incident electric field $\boldsymbol{E}_{I}$, a reflected electric field $\boldsymbol{E}_{R}$, and a transmitted electric field $\boldsymbol{E}_{T}$. The reflection and transmission coefficients are given by the Fresnel formulae, which depend on the polarization of the light and the angle of incidence, $\theta_{1}$ :

$$
\begin{align*}
& \rho_{12, s}=\frac{E_{R, s}}{E_{I, s}}=\frac{\mathbf{n}_{1} \cos \left(\theta_{1}\right)-\mathbf{n}_{2} \cos \left(\theta_{2}\right)}{\mathbf{n}_{1} \cos \left(\theta_{1}\right)+\mathbf{n}_{2} \cos \left(\theta_{2}\right)} \\
& \rho_{12, p}=\frac{E_{R, p}}{E_{I, p}}=\frac{\mathbf{n}_{2} \cos \left(\theta_{1}\right)-\mathbf{n}_{1} \cos \left(\theta_{2}\right)}{\mathbf{n}_{2} \cos \left(\theta_{1}\right)+\mathbf{n}_{1} \cos \left(\theta_{2}\right)}  \tag{1}\\
& \tau_{12, s}=\frac{E_{T, s}}{E_{I, s}}=\frac{2 \mathbf{n}_{1} \cos \left(\theta_{1}\right)}{\mathbf{n}_{1} \cos \left(\theta_{1}\right)+\mathbf{n}_{2} \cos \left(\theta_{2}\right)} \\
& \tau_{12, p}=\frac{E_{T, p}}{E_{I, p}}=\frac{2 \mathbf{n}_{1} \cos \left(\theta_{1}\right)}{\mathbf{n}_{2} \cos \left(\theta_{1}\right)+\mathbf{n}_{1} \cos \left(\theta_{2}\right)}
\end{align*}
$$

The subscript s indicates the s-polarization, which is also called the TE (or transverse electric) polarization, where the electric field vector is perpendicular to the page in Figure 1. The subscript p indicates the p-polarization, which is also called the TM (or transverse magnetic) polarization, where the electric field vector lies within the page in Figure 1. The angle $\theta_{2}$ can be found by Snell's law:

$$
\begin{equation*}
\mathbf{n}_{1} \sin \theta_{1}=\mathbf{n}_{2} \sin \theta_{2} \tag{2}
\end{equation*}
$$

In equations (1) and (2), both the index of refraction and the angle can be complex numbers for absorbing media.
It is interesting to look at the impact of direction that the light is traveling on the definitions of equation (1). Completely reversing the direction of the light in Figure 1, if light approaches the interface through material 2 at an angle $\theta_{2}$, the resulting reflection and transmission coefficients become

$$
\begin{align*}
& \rho_{21}=-\rho_{12}  \tag{3}\\
& \tau_{21}=\frac{\boldsymbol{n}_{2} \cos \left(\theta_{2}\right)}{\boldsymbol{n}_{1} \cos \left(\theta_{1}\right)} \tau_{12} \tag{4}
\end{align*}
$$

where these relationships hold for either polarization.
The quantity of interest in photochemistry is the intensity, which we shall define as the magnitude of the (time averaged) Poynting vector, the energy per second crossing a unit area perpendicular to the direction of propagation of the light. It is given by

$$
\begin{equation*}
I=n|E|^{2} \tag{5}
\end{equation*}
$$

Note that the definition given in equation (5) may differ by a constant multiplicative factor depending on the units used.
On the other hand, the quantity of interest when engineering a film stack, such as optimizing the thickness an antireflective coating, is the reflectivity. The reflectivity of a surface is defined in terms of the irradiance. The difference between intensity and irradiance is a subtle one. For our purposes, the irradiance is the projection of the intensity onto a surface which may not be normal to the direction that the light is traveling. When determining the intensity or irradiance transmitted into a material at an oblique angle, it is very important to differentiate between the two.

The reflectivity and transmissivity, for either polarization, are derived by considering a unit area on the interface between the two materials. Consider the irradiance, J , of the incident light along the surface of the interface between the materials.

$$
\begin{equation*}
J_{I}=I_{I} \cos \left(\theta_{I}\right) \tag{6}
\end{equation*}
$$

Likewise, the irradiances of the reflected and transmitted light along this surface are

$$
\begin{align*}
J_{R} & =I_{R} \cos \left(\theta_{I}\right) \\
J_{T} & =I_{T} \cos \left(\theta_{T}\right) \tag{7}
\end{align*}
$$

Now the irradiance reflectivity and transmission coefficients can be defined

$$
\begin{align*}
& R_{12}=R_{21}=R=\frac{J_{R}}{J_{I}}=\left|\rho_{12}\right|^{2}  \tag{8}\\
& T_{12}=T_{21}=T=\frac{J_{T}}{J_{I}}=\frac{n_{2} \cos \left(\theta_{T}\right)}{n_{1} \cos \left(\theta_{I}\right)}\left|\tau_{12}\right|^{2} \tag{9}
\end{align*}
$$

From these two equations it is easy to show that $R+T=1$ for each polarization, which is a consequence of conservation of energy. An alternate form for equations (8) and (9), making use of the reverse direction definitions of reflection and transmission coefficients in equations (3) and (4), are
$R=\left|\rho_{12} \rho_{21}\right|$
$T=\left|\tau_{12} \tau_{21}\right|$

Consider a unit intensity plane wave incident on the plane boundary between material 1 and 2 at an incident angle $\theta_{\mathrm{I}}$ and with intensity $I_{I}$. From equation (5) the magnitude of the incident electric field must be

$$
\begin{equation*}
\left|E_{I}\right|=\sqrt{\frac{I_{I}}{n_{1}}} \tag{11}
\end{equation*}
$$

The transmitted electric field is then

$$
\begin{equation*}
\left|E_{T}\right|=\left|\tau_{12} E_{I}\right|=\left|\tau_{12}\right| \sqrt{\frac{I_{I}}{n_{1}}} \tag{12}
\end{equation*}
$$

The transmitted intensity (i.e., the intensity in material 2) is found by applying the definition of intensity to equation (12).

$$
\begin{equation*}
I_{T}=n_{2}\left|E_{T}\right|^{2}=\frac{n_{2}}{n_{1}}\left|\tau_{12}\right|^{2} I_{I} \tag{13}
\end{equation*}
$$

By comparing equation (13) with equation (9), the non-intuitive result below is obtained.

$$
\begin{equation*}
I_{T}=T \frac{\cos \left(\theta_{1}\right)}{\cos \left(\theta_{2}\right)} I_{I} \tag{14}
\end{equation*}
$$

As can be seen in equation (14), the transmittance $T$ is not the ratio of the intensities $I_{T}$ and $I_{I}$. The difference comes from the change in the direction of the energy flow caused by refraction. This result will be useful for comparing solutions for the transmissivity from the optics literature to the intensity calculations in PROLITH.

## 3 REFLECTIVITY AND TRANSMISSIVITY OF NON-ABSORBING FILM STACKS

The first benchmark is a straightforward application of the Fresnel formulae for the reflection and transmission coefficients at an interface between two materials, given by equation (1), combined with the definition of reflectivity, equation (8). In order to provide a specific example, we will consider the following simulator settings:

## Film Stack:

$$
\begin{array}{ll}
\text { Photoresist: } & \mathrm{n}=1.0+0.0 \mathrm{i} \\
\text { Substrate: } & \mathrm{n}=1.563117+0.0 \mathrm{i} \text { (similar to silicon dioxide) }
\end{array}
$$

Imaging Tool:
Wavelength: $\quad 193 \mathrm{~nm}$
Numerical Aperture: 0.8
Reduction Ratio: $\quad 1.0$
Source Shape: Coherent Monopole at location ( $\mathrm{S}_{\mathrm{x}}, \mathrm{S}_{\mathrm{y}}$ )
Immersion Liquid: $\quad \mathrm{n}=1.0$ (air)
Vector image calculation mode
The incident angle is related to the monopole location by the equation

$$
\begin{equation*}
\theta=\arcsin \left(\frac{N A}{n_{1}} \sqrt{S_{x}^{2}+S_{y}^{2}}\right) \tag{15}
\end{equation*}
$$



Figure 2: Comparison of the substrate reflectivity calculated by PROLITH and by equations (1) and (8) for a coherent monopole source located at $\left(\mathrm{S}_{\mathrm{x}}, 0\right)$.

We will test both s and p polarizations, which correspond to y -polarized and x -polarized vector imaging modes in PROLITH. PROLITH reports the substrate reflectivity, which can be compared directly with the reflectivity calculated using equations (1) and (8). Results are shown in Figure 2, and the PROLITH result agrees with the analytic expressions within $10^{-6}$, which corresponds to the number of significant figures reported by PROLITH.

Next, we test the transmittance calculation in PROLITH. This test is a little more complicated because PROLITH does not directly report transmissivities. Instead, we will calculate the intensity within a non-absorbing resist layer on an optically matched substrate and then use equation (14) to convert between intensity and transmissivity. For this test, we will use the following simulator settings:

Film Stack:

$$
\begin{array}{ll}
\text { Photoresist: } & \mathrm{n}=1.8+0.0 \mathrm{i} \\
\text { Substrate: } & \mathrm{n}=1.8+0.0 \mathrm{i} \text { (matched to resist layer) }
\end{array}
$$

## Mask:

Space with width equal to the pitch (open frame)
Imaging Tool:

| Wavelength: | 193 nm |
| :--- | :--- |
| Numerical Aperture: | 0.8 |
| Reduction Ratio: | 1.0 |
| Source Shape: | Coherent Monopole at location $\left(\mathrm{S}_{\mathrm{x}}, \mathrm{S}_{\mathrm{y}}\right)$ |
| Immersion Liquid: | $\mathrm{n}=1.44$ (water) |

Vector image calculation mode


Figure 3: Comparison of the intensities calculated by PROLITH and by equations (1) and (13) for a coherent monopole source located at $\left(\mathrm{S}_{\mathrm{x}}, 0\right)$.

The imaginary part of index of refraction in the resist layer is set to zero by selecting the Dill absorbance parameters A and B to be zero. Note also that this test uses an immersion refractive index (1.44) above the film stack in order to test the immersion capabilities in PROLITH. For an open frame calculation with a reduction ratio of 1.0 , the intensity of the incident wave is set to 1.0 regardless of the index of the immersion liquid. Results are shown in Figure 3, and the PROLITH result agrees with the analytic expressions within $2 \times 10^{-6}$, which corresponds to the number of significant figures reported by PROLITH.

## 4 TRANSMISSIVITY OF ABSORBING FILM STACKS

The next test is for a planar, absorbing film between two non-absorbing films, as shown in Figure 4. The transmissivity of this film stack is calculated as an example in the textbook by Born and Wolf, "An absorbing film on a transparent substrate", found in Section 13.4.1 of the $6^{\text {th }}$ edition [5]. Although the solution of this problem is fairly straightforward, the resulting equations are algebraically complicated, so we will not present the solution here. Instead, we will present results for a specific test problem in Table 1, so that the interested reader can reproduce our results directly (via the table) or by using the equations in Born and Wolf.

The procedure for this test will be very similar to the intensity calculation in the previous test - the transmissivity is given by the analytic solution while the intensity in the bottom layer is given by PROLITH. We can convert the calculated transmissivity into an intensity value by following a derivation similar to the one presented in Section 2, except that here we have three layers instead of two:
$I_{T}=T \frac{\cos \left(\theta_{1}\right)}{\cos \left(\theta_{3}\right)} I_{I}$
Snell's law, equation (2), can be used to calculate the angle $\theta_{3}$.


Figure 4: Diagram of a three-layer film stack where the middle layer is absorbing while the top and bottom layers are non-absorbing. The transmissivity for this geometry is calculated as an example problem in Born and Wolf [5].

For this test, we will use the following simulator settings:
Film Stack:

| Top Coat: | $\mathrm{n}=1.8+0.015 \mathrm{i}$, | (typical of a photoresist layer) |
| :--- | :--- | :--- |
|  | 300 nm thickness |  |
| Photoresist: | $\mathrm{n}=1.563117+0.0 \mathrm{i}$ | (typical of silicon oxide) |
| Substrate: | $\mathrm{n}=1.563117+0.0 \mathrm{i}$ | (typical of silicon oxide) |

Mask:
Space with width equal to the pitch (open frame)
Imaging Tool:
Wavelength: $\quad 193 \mathrm{~nm}$
Numerical Aperture: 0.8
Reduction Ratio: $\quad 1.0$
Source Shape: Coherent Monopole at location ( $\mathrm{S}_{\mathrm{x}}, \mathrm{S}_{\mathrm{y}}$ )
Immersion Liquid: $\quad \mathrm{n}=1.44$ (water)
Vector image calculation mode
The optical properties of the film stack have been chosen to be typical of an immersion system, except we have assigned optical properties of a photoresist to the top coat and then assigned optical properties of silicon oxide to the photoresist and substrate layers (see film stack description, above). As in the previous test, we will compare the intensity in resist output from PROLITH to the transmissivity prediction from Born and Wolf. Results are shown in Table 1. Again, errors are quite small - the largest discrepancy is less than $3 \times 10^{-6}$. This again is within the number of significant figures reported by PROLITH.

| $\mathrm{S}_{\mathrm{x}}$ | $\mathrm{T}_{\mathrm{s}}(\mathrm{B} \& \mathrm{~W})$ | $\mathrm{T}_{\mathrm{p}}(\mathrm{B} \& \mathrm{~W})$ | $\mathrm{I}_{\mathrm{s}}(\mathrm{B} \& \mathrm{~W})$ | $\mathrm{I}_{\mathrm{p}}(\mathrm{B} \& \mathrm{~W})$ | $\mathrm{I}_{\mathrm{s}}($ PROLITH $)$ | $\mathrm{I}_{\mathrm{p}}($ PROLITH $)$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0.0 | 0.726635 | 0.726635 | 0.726635 | 0.726635 | 0.726635 | 0.726634 |
| 0.1 | 0.726148 | 0.726335 | 0.725978 | 0.726165 | 0.725979 | 0.726166 |
| 0.2 | 0.724723 | 0.725493 | 0.724038 | 0.724808 | 0.724041 | 0.724810 |
| 0.3 | 0.722476 | 0.724282 | 0.720919 | 0.722721 | 0.720917 | 0.722719 |
| 0.4 | 0.719062 | 0.722994 | 0.716847 | 0.720169 | 0.716847 | 0.720170 |
| 0.5 | 0.716715 | 0.722009 | 0.712224 | 0.717485 | 0.712222 | 0.717483 |
| 0.6 | 0.714298 | 0.721671 | 0.707637 | 0.714941 | 0.707634 | 0.714939 |

Table 1: Transmissivities and intensities from Born and Wolf (B\&W) and from PROLITH for the three-layer film stack test problem for both the s and p polarization.

## 5 TWO-BEAM IMAGING IN AN ABSORBING MEDIA ON A MATCHED SUBSTRATE

In this test problem, we calculate two-beam imaging in a semi-infinite slab of absorbing material, so the geometry for this problem is the similar to that shown in Figure 1, except there are two incoming beams, separated by the same incident angle from the surface normal, $\theta_{i}$. This benchmark problem is the same as presented in the report by Brunner [2], although the presentation here closely follows Section 6.6 in the text by Fowles [6].

Consider a plane wave traveling through non-absorbing media incident on an absorbing material. The incident wave $\boldsymbol{E}_{\boldsymbol{I}}$ (and the reflected wave) can be represented as an ordinary plane wave with wave number $k_{\mathrm{I}}$. However, because the index of refraction for material 2 is complex, the transmitted wave $\boldsymbol{E}_{\boldsymbol{T}}$ must be described as an inhomogeneous wave, which means that the wave has a complex propagation vector:

$$
\begin{aligned}
& \mathbf{E}_{I}=E_{I} \exp \left(i\left(\mathbf{k}_{I} \cdot \mathbf{r}-\omega t\right)\right) \mathbf{e}_{1} \\
& \mathbf{E}_{T}=E_{T} \exp \left(i\left(\mathrm{~K}_{T} \cdot \mathbf{r}-\omega t\right)\right) \mathbf{e}_{T} \\
& \mathbf{K}_{T}=\mathbf{k}_{T}+i \mathbf{a}_{T}
\end{aligned}
$$

where $\mathbf{e}_{\mathrm{I}}$ and $\mathbf{e}_{\mathrm{T}}$ represent the appropriate unit vectors for s or p polarizations. The vector $\mathbf{r}=\mathbf{e}_{x} x+\mathbf{e}_{\mathrm{y}} y+\mathbf{e}_{z} z$ is the position vector. The vector $\mathbf{k}_{\mathbf{T}}$ will be normal to surfaces of constant phase, while the vector $\mathbf{a}_{\mathbf{T}}$ will be normal to surfaces of constant amplitude. We can derive a relationship between the wave numbers of the incident wave and the transmitted wave by matching the phase of the waves at the interface:

$$
\mathbf{k}_{I} \cdot \mathbf{r}=\left(\mathbf{k}_{T}+i \mathbf{a}_{T}\right) \cdot \mathbf{r}
$$

Equating real and imaginary parts yields
$\mathbf{k}_{I} \cdot \mathbf{r}=\mathbf{k}_{T} \cdot \mathbf{r}$
$0=\mathbf{a}_{T} \cdot \mathbf{r}$

The first part of Equation (17) gives Snell's law in a modified form:

$$
\begin{equation*}
\frac{2 \pi n_{I}}{\lambda_{0}} \sin \theta_{I}=k_{T} \sin \phi_{T} \tag{18}
\end{equation*}
$$

where $\phi_{\mathrm{T}}$ is the angle formed between the vector $\mathbf{k}_{\mathbf{T}}$ and the surface normal, and $\mathrm{k}_{\mathrm{T}}$ represents the magnitude of the vector $\mathbf{k}_{\mathrm{T}}$. Note that this equation is different from Equation (2) because all of the values are real numbers. The original form of Snell's law given by Equation (2) uses complex index of refraction values and can lead to complex angles. The
second half of Equation (17) indicates that the vector $\mathbf{a}_{\mathrm{T}}$ is perpendicular to the interface, so $\phi_{\mathrm{T}}$ is also the angle between $\mathbf{k}_{\mathrm{T}}$ and $\mathbf{a}_{\mathrm{T}}$.

In order to find the value of $k_{T}$, we revisit the wave equation written in terms of the complex index of refraction:
$\nabla^{2} \mathbf{E}=\frac{\left(n_{2}+i \kappa_{2}\right)^{2}}{c^{2}} \frac{\partial^{2} \mathbf{E}}{\partial t^{2}}$
Substitution of the inhomogeneous wave equation for $\mathbf{E}_{\mathrm{T}}$ into the above wave equation yields
$\left(\mathbf{k}_{T}+i \mathbf{a}_{T}\right) \cdot\left(\mathbf{k}_{T}+i \mathbf{a}_{T}\right) \mathbf{E}_{T}=\frac{\left(n_{2}+i \kappa_{2}\right)^{2}}{c^{2}} \omega^{2} \mathbf{E}_{T}$
If we equate the real and imaginary parts of the coefficients in the above equation and recall that $\omega / c=2 \pi / \lambda_{0}$ we obtain

$$
\begin{align*}
& {k_{T}}^{2}-{a_{T}}^{2}=\left(n_{2}^{2}-\kappa_{2}^{2}\right)\left(\frac{2 \pi}{\lambda_{0}}\right)^{2}  \tag{19}\\
& \mathbf{k}_{T} \cdot \mathbf{a}_{T}=k_{T} a_{T} \cos \phi_{T}=n_{2} \kappa_{2}\left(\frac{2 \pi}{\lambda_{0}}\right)^{2} \tag{20}
\end{align*}
$$

We will solve Equations (2), (18), (19), and (20) numerically for the three unknown values $\theta_{\mathrm{T}}, \phi_{\mathrm{T}}, \mathrm{k}_{\mathrm{T}}$, and $\mathrm{a}_{\mathrm{T}}$. Thus, for a single plane wave, the electric field in the absorbing media is given by

$$
\begin{align*}
& \mathbf{E}_{s}=E_{I} \tau_{12, s}\left(\theta_{I}, \theta_{T}\right) \exp \left(-a_{T} z\right) \exp \left(i k_{T}\left(\sin \phi_{T} x+\cos \phi_{T} z\right)\right) \mathbf{e}_{s} \\
& \mathbf{E}_{p}=E_{I} \tau_{12, p}\left(\theta_{I}, \theta_{T}\right) \exp \left(-a_{T} z\right) \exp \left(i k_{T}\left(\sin \phi_{T} x+\cos \phi_{T} z\right)\right) \mathbf{e}_{p} \tag{21}
\end{align*}
$$

Note that the transmissivities are calculated from the Fresnel equations, (1), and that the complex angle $\theta_{\mathrm{T}}$ must be found by Snells law, equation (2). The first exponential in equation (21) describes the decay of the amplitude of the wave due to absorption, while the complex exponential describes the propagation of the phase of the wave. We have also introduced the vectors $\mathbf{e}_{\mathrm{s}}$ and $\mathbf{e}_{\mathrm{p}}$, which are unit vectors pointing in the s and p polarization directions:
$\mathbf{e}_{s}=\mathbf{e}_{y}$
$\mathbf{e}_{p}\left(\phi_{T}\right)=\mathbf{e}_{x} \cos \phi_{T}-\mathbf{e}_{z} \sin \phi_{T}$

Note that $\mathbf{e}_{\mathrm{s}}$ is a constant, while $\mathbf{e}_{\mathrm{p}}$ is a function of the transmitted angle $\phi_{\mathrm{T}}$. To form the image in resist, we use two incident plane waves, and we set the amplitude $E_{\mathrm{I}}$ for each wave equal to the Fourier coefficients representing the -1 and +1 diffraction orders of the mask. Here we will use an alternating phase shift mask with equal lines and spaces. The Fourier coefficients are then normalized with the pitch of the mask, so that an open frame calculation would give a zero order diffraction coefficient of unity. This leads to the following formula for the Fourier coefficients for the phase shift mask:

$$
\begin{aligned}
& f_{-1}=\frac{\sqrt{2}}{\pi} i \\
& f_{1}=-\frac{\sqrt{2}}{\pi} i
\end{aligned}
$$

Combining the above equations leads to

$$
\begin{aligned}
& \mathbf{E}_{s}=i \frac{\sqrt{2}}{\pi} \tau_{12, s}\left(\theta_{I}, \theta_{T}\right) \exp \left(-a_{T} z\right) \exp \left(i k_{T} \cos \left(\phi_{T}\right) z\right)\left\{\exp \left(i k_{T} \sin \phi_{T} x\right)-\exp \left(-i k_{T} \sin \phi_{T} x\right)\right\} \mathbf{e}_{y} \\
& \mathbf{E}_{p}=i \frac{\sqrt{2}}{\pi} \tau_{12, p}\left(\theta_{I}, \theta_{T}\right) \exp \left(-a_{T} z\right) \exp \left(i k_{T} \cos \left(\phi_{T}\right) z\right) . \\
& \left\{\exp \left(i k_{T} \sin \phi_{T} x\right)\left(\mathbf{e}_{x} \cos \phi_{T}+\mathbf{e}_{z} \sin \phi_{T}\right)-\exp \left(-i k_{T} \sin \phi_{T} x\right)\left(\mathbf{e}_{x} \cos \phi_{T}-\mathbf{e}_{z} \sin \phi_{T}\right)\right\}
\end{aligned}
$$

We determine $\theta_{\mathrm{I}}$ by applying Bragg's law to the mask, which determines the angle of the incident beam,
$n_{1} \sin \theta_{I}=\frac{\lambda_{0}}{p}$
where $p$ is the pitch of the mask. We can also combine this equation with Equation (18) to eliminate the quantity $\mathrm{k}_{\mathrm{T}}$ from the equations. Finally, we calculate the intensity according to Equation (5) for each polarization:

$$
\begin{align*}
& I_{s}=n_{2} \mathbf{E}_{s} \cdot \mathbf{E}_{s}^{*}=\frac{4 n_{2}}{\pi^{2}} \tau_{12, s}\left(\theta_{I}, \theta_{T}\right) \tau_{12, s}\left(\theta_{I}, \theta_{T}\right)^{*} \exp \left(-2 a_{T} z\right)\left(1-\cos \left(\frac{4 \pi x}{p}\right)\right)  \tag{22}\\
& I_{p}=n_{2} \mathbf{E}_{p} \cdot \mathbf{E}_{p}{ }^{*}=\frac{4 n_{2}}{\pi^{2}} \tau_{12, p}\left(\theta_{I}, \theta_{T}\right) \tau_{12, p}\left(\theta_{I}, \theta_{T}\right)^{*} \exp \left(-2 a_{T} z\right)\left(1-\cos 2 \phi_{T} \cos \left(\frac{4 \pi x}{p}\right)\right) \tag{23}
\end{align*}
$$

For this test, we will use the following simulator settings, and we will examine the intensity at the resist/substrate interface:

Film Stack:

| Photoresist: | $\mathrm{n}=1.8+0.015 \mathrm{i}$ <br> Thickness 200nm | (typical resist material) |
| :--- | :--- | :--- |
| Substrate: | $\mathrm{n}=1.8+0.015 \mathrm{i}$ |  |$\quad$ (matched to resist material)

Mask:
Alternating Phase-shift with 75 nm lines and spaces
Imaging Tool:
Wavelength: 193nm
Numerical Aperture: 0.8
Reduction Ratio: $\quad 1.0$
Source Shape: Coherent illumination
Immersion Liquid: $\quad \mathrm{n}=1.44$ (water)
Vector imaging calculation mode
We solve numerically for the following results using Mathematica, version 5.0 [7]:


Figure 5: Comparison of the relative intensity given by PROLITH and the analytical solutions at the bottom of a 200nm resist coating on a matched substrate. The relative intensity is the intensity given by Equations (22) and (23) divided by the refractive index of the immersion liquid.

| $\theta_{\mathrm{I}}:$ | $0.4631397 \ldots$ radians |
| :--- | :--- |
| $\theta_{\mathrm{T}}:$ | $0.3654619 \ldots-0.00318877 \mathrm{i} \ldots$ radians |
| $\tau_{12, \mathrm{~s}}:$ | $0.8676877 \ldots-0.00469308 \mathrm{i}$ |
| $\tau_{12, \mathrm{p}}:$ | $0.8718405 \ldots-0.00444311 \mathrm{i}$ |
| $\phi_{\mathrm{T}}:$ | $0.3654885 \ldots$ radians |
| $\mathrm{a}_{\mathrm{T}}:$ | $5.228635 \ldots \times 10^{-4} \mathrm{~nm}^{-1}$ |

One additional note is that PROLITH reports the relative intensity by dividing the results in Equations (22) and (23) by the refractive index of the immersion liquid. Once this is taken into consideration, a comparison can be made. Results for this benchmark problem are shown in Figure 5, and the largest error is smaller than $2 \times 10^{-5}$.

## 6 SUMMARY AND CONCLUSIONS

In this study we have presented benchmark problems for film stack reflectivity and transmissivity calculations and for image in resist calculations. For all cases, PROLITH agreed with the analytic results within a fraction of a percent. In the Introduction, we noted that a typical $\mathrm{P} / \mathrm{T}$ ratio is 0.1 to 0.2 . The $\mathrm{P} / \mathrm{T}$ ratio for the intensity calculations presented here can be estimated by considering the impact on an error in the intensity. First, write a Taylor series for the intensity as a function of position:
$I=I_{0}+\frac{d I}{d x} d x+\ldots$

With a little manipulation, we use this expression to estimate the CD error in an aerial image threshold model due to a small error in the intensity.

$$
\begin{aligned}
& \frac{I-I_{0}}{I_{0}} \cong \frac{C D}{I_{0}} \frac{d I}{d x} \frac{d x}{C D} \cong \frac{N I L S}{2} \frac{\Delta C D}{C D} \\
& \frac{\Delta C D}{C D} \cong \frac{2}{N I L S} \frac{I-I_{0}}{I_{0}}
\end{aligned}
$$

The final equation show that the relationship between the CD error and an intensity error depends on the NILS. In fact, this equation is very similar to the relationship between the NILS and exposure latitude. If we assume that a viable process has a NILS of at least 2 , then for errors of around $10^{-5}$, the relative CD error is also around $10^{-5}$. If one has a CD error budget of $10 \%$, then this gives a $\mathrm{P} / \mathrm{T}$ ratio of $10^{-4}$ - three orders of magnitude lower than the $\mathrm{P} / \mathrm{T}$ ratio of 0.1 to 0.2 mentioned in the introduction. Of course, there are sources of error in a photolithography simulator other than intensity errors.

Combined with our previous report and the work of others such as Brunner and Gordon, there is now a comprehensive suite of reference solutions that can be used to determine the accuracy of the optics calculations within a simulator on planar substrates. Future work in this area would include calculations of the impact of standing waves and benchmark calculations for downstream processes, such as PEB and develop.

## 7 REFERENCES

1. ITRS Roadmap, 2000 Update.
2. T. Brunner, "SEMATECH Report: Benchmark tests for image simulation programs used in optical lithography", SEMATECH (1994)
3. R.L. Gordon, "Exact Computation of 2D Aerial Imagry," Proc. SPIE, Vol. 4692 (2002) pp. 517-528.
4. M.D. Smith, C.A. Mack, "Methods for Benchmarking Photolithography Simulators", Proc. SPIE, Vol. 5040 (2003) pp. 57-68.
5. M. Born and E. Wolf, Principles of Optics, $6^{\text {th }}$ edition, Pergamon Press (Oxford, 1980).
6. G.R. Fowles, Introduction to Modern Optics, $2^{\text {nd }}$ edition, Dover Publications (New York, 1989).
7. Mathematica version 5.0 is produced by Wolfram Research, Inc., http://www.wolfram.com

[^0]:    * mark.d.smith@kla-tencor.com; phone 1-512-381-2318; 8834 North Capital of Texas Highway, Suite 301, Austin, TX 78759

