On the solution of a metrology problem in semiconductor manufacturing using shape analysis

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Abstract. This paper presents an efficient numerical technique to reconstruct the profile of one-dimensional gratings from ellipsometry measurements, that is, the ratio of reflection coefficients between the two basic polarizations. The basic idea is to use gradient-based optimization methods to create a minimizing sequence of profiles by iteratively changing its geometric parameters. The gradients with respect to the parameters are computed efficiently using adjoints of the electromagnetic fields. One possible application of this technique is in semiconductor metrology.

1. Introduction
The evolution of integrated circuit (IC) technology has been characterized by a constant decrease in device dimensions. As a result, so-called process control windows are becoming more stringent and this has created a need for tools that can rapidly and accurately measure test structures that are printed in wafers at different stages of the lithography and etch processes. The dimensions of these test structures convey important information about the process and can be used to enhance process control mechanisms.

Traditional metrology tools are based on optical gauging techniques where an image of a test structure, usually a grating, is obtained using, for example, a scanning electron microscope. Then an automatic image-processing technique is applied to infer certain feature sizes which are known as critical dimensions. Nevertheless, critical three-dimensional information cannot be obtained with these tools since they operate on aerial images.

In recent years, optical techniques based on the spectral analysis of reflected light have been developed to address these needs. One set of tools [2, 3, 8] is based on the analysis of ellipsometry measurements. In its classical form, ellipsometry can measure the optical properties and thickness of thin transparent films or stacks of films. By combining this technique with an accurate electromagnetic diffraction model it is possible to extend its applicability and infer other three-dimensional information from samples. This reconstruction process is usually carried out by constructing off-line a large database of shapes of grating sections that could be the result of deviations in manufacturing conditions. The corresponding ellipsometry signal is matched against measurements using pattern-matching algorithms. Although fast, such an approach has a caveat: the database has to be carefully constructed to contain all possible deviations to the profile caused by the process.

Alternatively, one could solve this inverse scattering problem using gradient-based optimization techniques. Starting from an expected profile, change the geometric parameters...
until the simulated signal matches the measurements in some norm. For a large number of parameters, this approach has been deemed impractical as the main cost of each iteration is in the computation of the gradient, usually from a finite-difference approximation. As a consequence, multiple diffraction problems would have to be solved at each iteration. In this manuscript, a different technique is proposed that addresses this issue: using adjoint equations and shape analysis all the derivatives are computed at the cost of an extra diffraction simulation, making the optimization approach feasible.

The remaining part of this manuscript is organized as follows. In the following section, ellipsometry is briefly presented and the corresponding electromagnetic scattering model is discussed. Section 2.2 presents the technique used to compute the derivatives with respect to geometric parameters. These derivatives are called shape derivatives. The technique is similar to that developed for acoustic scattering problems in [1]. The adjoint equations necessary to evaluate these derivatives are also presented in this Section. An example showing the accuracy of these computations is presented in Section 3. The solution of a representative inverse problem using synthetic data is also presented.

2. Optical metrology as an inverse problem

2.1. Preliminaries: ellipsometry

Ellipsometry is a measurement technique that uses the change in polarization of light reflected from or transmitted through a sample to characterize its optical properties. Figure 1 shows a schematic representation of a type of spectroscopic ellipsometer, where measurements over a range of optical frequencies are obtained using a broadband light source. The apparatus consists of a series of optical elements that are arranged in the path of the light beam altering its polarization state. First, the beam passes through a polarizer, which is typically a quartz or calcite crystal. The outgoing beam is linearly polarized, i.e. the electric vector field oscillates in a well-defined plane characterized by the orientation of the crystal. The beam then strikes the surface of the sample, which for the purpose of the following analysis is assumed to be planar and the index of refraction of the sample is assumed to be homogeneous. Upon reflection, the resulting electromagnetic field becomes in general elliptically polarized, i.e. the components of the electric field parallel and perpendicular to the incidence plane have a shift in phase. The reflected beam then passes through a rotating polarizer, also known as an analyzer, whose axis rotates at a constant angular velocity $\omega$. The emerging polychromatic beam is dispersed by a quartz prism or a diffraction grating onto the surface of a diode array. As a result, each diode will receive light of a slightly different wavelength than its neighbors. The intensity of each beam, which has a sinusoidal form of angular frequency $2\omega$, is then recorded on a computer.

![Figure 1. Schematic representation of a spectroscopic ellipsometer.](image1)

![Figure 2. Planar diffraction from periodic grating.](image2)
Using the Jones formalism of optics, an expression for the normalized voltage $V(t)$ measured by each diode (normalized with respect to the DC component) can be derived. It is given by the following expression

$$V(t) = 1 + \frac{|\rho|^2 - (\tan P)^2}{|\rho|^2 + (\tan P)^2} \cos 2\omega t + \frac{2\text{Re}(\rho) \tan P}{|\rho|^2 + \tan P} \sin 2\omega t. \quad (1)$$

$P$ is the angle between the axis of polarization of the polarizer and the plane of incidence. $\rho$ is the ratio of reflection coefficients: $R_{TM}$ for the $p$-polarization or TM-polarization (polarization in the plane of incidence) and $R_{TE}$ for the $s$-polarization or TE-polarization (polarization perpendicular to the plane of incidence)

$$\rho = \frac{R_{TM}}{R_{TE}}. \quad (2)$$

For the case of a bulk isotropic sample, the quantity $\rho$ is a function

$$\rho = \rho(\theta_0, n_0, n_1), \quad (3)$$

of the angle $\theta_0$ between the incident beam and the normal to the planar interface, of the index of refraction $n_0$ of the medium where the incident beam propagates and the index of refraction $n_1$ of the sample. Since $\theta_0$, $n_0$ and $P$ are known, equation (1) gives the unknown index of refraction $n_1$ from measurements of the normalized voltage $V(t)$. The expression for (3) is obtained by solving Maxwell’s equations for this particular geometry. In this case, $R_{TM}$ and $R_{TE}$ are the Fresnel reflection coefficients

$$R_{TM} = \frac{n_1 \cos \theta_0 - n_0 \cos \theta_1}{n_1 \cos \theta_0 + n_0 \cos \theta_1}, \quad (4)$$

$$R_{TE} = \frac{n_0 \cos \theta_0 - n_1 \cos \theta_1}{n_0 \cos \theta_0 + n_1 \cos \theta_1}, \quad (5)$$

and Snell’s law relates the angles $\theta_0$ and $\theta_1$ and the indices of refraction $n_0$ and $n_1$,

$$n_0 \sin \theta_0 = n_1 \sin \theta_1. \quad (6)$$

If a thin planar film of thickness $a$ and index of refraction $n_1$ is deposited over a substrate with index of refraction $n_2$ an expression for $\rho$ can also be constructed: in this case the reflection coefficients for the TM- and TE-polarizations are given by

$$R = \frac{R_{01} + R_{12} \exp(2i\beta)}{1 + R_{01}R_{12} \exp(2i\beta)}, \quad (7)$$

where $R_{01}$ and $R_{12}$ are the Fresnel reflection coefficients (for the appropriate polarization) between mediums 0 and 1, and 1 and 2, respectively. $\beta$ is the so-called phase thickness of the film and is given by

$$\beta = 2\pi \frac{a}{\lambda} n_1 \cos \theta_1, \quad (8)$$

where $\lambda$ is the wavelength relative to vacuum. Expressions (7) and (8) show that in this case the parameter $\rho$ is a function $\rho(\theta_0, n_0, n_1, n_2, a)$ that depends on each index of refraction as well as the thickness, a geometric parameter. Assuming that the indices of refraction are known, then this expression can be used to determine the thickness of the film using (1).

The classic ellipsometry technique can be extended to infer more complex geometric information, such as, for example, the dimensions of cross sections of optical gratings. Assume
that a one-dimensional grating is illuminated by the ellipsometer as shown schematically in Figure 2. The period of the grating is \( d \) and, for the purpose of the following analysis, each medium has a uniform index of refraction: \( n_1 \) for the medium where the incident beam propagates, \( n_II \) for the substrate and \( n_{III} \) for the grating lines. The curve \( \Sigma \) separates the three media. The grating and the illumination (here modeled as a plane wave) are invariant in the \( z \)-direction so Figure 2 is showing a cross section of the grating.

For a generic shape \( \Sigma \) the reflection coefficients for each polarization can not be determined analytically as in the case of a bulk sample or a planar film, and \( \rho \) has to be computed with a numerical technique. The electromagnetic field is found by solving two uncoupled boundary-value problems: one for the \( E_z \) component of the electric field (\( s \)-polarization, TE problem) and another for the \( H_z \) component of the magnetic field (\( p \)-polarization, TM problem). The TE problem is

\[
\nabla^2 E_z + k^2 E_z = 0 \quad \text{in } \mathbb{R}^2 - \Sigma, \tag{9}
\]

\[
[E_z] = 0 \quad \text{on } \Sigma, \tag{10}
\]

\[
[\nabla E_z \cdot \nu] = 0 \quad \text{on } \Sigma, \tag{11}
\]

where \( \nu \) is the normal to the curve \( \Sigma \), \( k(x, y) = k_0 n(x, y) \), \( k_0 = 2\pi/\lambda \) is the wavenumber in vacuum and \( n(x, y) \) is the appropriate index of refraction at \( (x, y) \in \mathbb{R}^2 \). The TM problem is given by

\[
\nabla^2 H_z + k^2 H_z = 0 \quad \text{in } \mathbb{R}^2 - \Sigma, \tag{12}
\]

\[
[H_z] = 0 \quad \text{on } \Sigma, \tag{13}
\]

\[
\left[ \frac{1}{\varepsilon} \nabla H_z \cdot \nu \right] = 0 \quad \text{on } \Sigma, \tag{14}
\]

where \( \varepsilon(x, y) = n(x, y)^2 \) is the electric permittivity. Problems (9)–(11) and (12)–(14) are complete with the specification of radiation conditions and the incident fields. The incident field in each case is given by a plane wave with wavevector \( k_1 = k_0 n_1 (\sin \theta, -\cos \theta) \). Given the periodicity of the structure in the \( x \)-direction, it is possible to show that the electric and magnetic fields in the region \( y > a \) above the grating are given by the following decompositions (see [7]),

\[
E_z(x, y) = \exp(i(\alpha_0 x - \beta_{10} y)) + \sum_{m=-\infty}^{+\infty} R_{\text{TE},m} \exp(i(\alpha_m x + \beta_{1m} y)) \quad \text{for } y > a, \tag{15}
\]

\[
H_z(x, y) = \exp(i(\alpha_0 x - \beta_{10} y)) + \sum_{m=-\infty}^{+\infty} R_{\text{TM},m} \exp(i(\alpha_m x + \beta_{1m} y)) \quad \text{for } y > a, \tag{16}
\]

where

\[
\beta_{1m} = \left( k_0^2 n_1^2 - \alpha_m^2 \right)^{1/2} \tag{17}
\]

\[
\alpha_m = k_0 n_1 \sin \theta + m \frac{2\pi}{d}. \tag{18}
\]

These expressions satisfy the radiation conditions. The unknown coefficients \( R_{\text{TE},m} \) and \( R_{\text{TM},m} \), which are the reflection coefficients for each spectral order \( m \), are determined by the numerical method.

Finally, the ellipsometry parameter \( \rho \) for the generic structure shown in Figure 2 is given by

\[
\rho = \frac{R_{\text{TM},0}}{R_{\text{TE},0}}. \tag{19}
\]
Assuming that the index of refraction of each material is known, the previous development shows that the ellipsometry parameter is a function of the grating shape and the wavelength which is indicated by the notation \( \rho = \rho(\Sigma, \lambda) \). The procedure to obtain the geometry of the grating from measurements of \( \rho \) is conceptually straightforward: search for the geometric parameters that define \( \Sigma \) that minimize, for example, \[ f(\Sigma) = \sum_{\lambda \in [\lambda_i, \lambda_f]} |\rho(\Sigma, \lambda) - \rho_m(\lambda)|^2 \] over a discrete set of wavelengths in the range \([\lambda_i, \lambda_f]\). The geometric parameters can be, for example, control points of a B-spline that generates \( \Sigma \). \( \rho_m \) is the measured ellipsometry parameter obtained from (1).

In [8], the authors, who were among the original proponents of ellipsometry for metrology of grating lines, solve this inverse problem using a pattern-matching algorithm. The search space is created off-line, that is, a large, but limited set of \( \rho \)’s is preloaded into a database. Although the number of iterations in the search procedure may be large, the cost of each iteration is negligible as the diffraction problems are pre-computed. Certainly, if the true shape is very different from those available in the library, this search procedure will fail.

An alternative is to create the search space “dynamically” using, for example, a gradient-based algorithm to solve the minimization problem. Derivatives with respect to geometric parameters can be computed efficiently using the adjoint method. This is discussed in the next Section. The mathematical expression for the derivatives is obtained with the shape differentiation technique of Murat and Simon (see [6] and [9]). This technique is of interest in this work as it effectively decouples the expression of the derivative from the choice of geometric parameters used to represent \( \Sigma \). As a result, different geometric representations can be used in the software. Furthermore, the computation of derivatives is independent of the numerical method used to solve the TE and TM problems.

2.2. Solving the inverse problem using shape analysis and adjoint equations

The inverse problem is solved using a technique similar to that presented in [1]. A gradient-based method is used to solve the optimization problem, creating a sequence of curves \( \Sigma \) that minimize the error, in this case given by (20). At every iteration, the method computes the gradient of this function with respect to the geometric parameters that define \( \Sigma \). To compute the expression of the gradient, the shape differentiation technique of Murat and Simon (see [9]) is used. This is done as follows. Starting with a shape \( \Sigma_0 := \Sigma \), a uniparametric family of transformations \( \varphi_\tau : \Sigma_0 \rightarrow \Sigma_\tau \) is constructed

\[ \varphi_\tau(x) = x + \tau V(x), \quad x \in \Sigma, \tau \in \mathbb{R}. \]  

The shape derivative of the function \( f(\Sigma_\tau) \) in the direction defined by the deformation field \( V \), computed at \( \Sigma \) is the derivative of the mapping \( \tau \rightarrow f(\Sigma_\tau) \) at \( \tau = 0 \),

\[ D f(\Sigma)[V] = \left. \frac{d}{d\tau} f(\Sigma_\tau) \right|_{\tau=0}. \]  

The geometric parametrization chosen for \( \Sigma \) defines the basis of the vector field \( V \).

A straightforward calculation shows that the shape derivative of \( f(\Sigma) \) depends on the shape derivatives of the square of the magnitudes of the reflection coefficients \( R_{\text{TE},0} \) and \( R_{\text{TM},0} \). The expression of these derivatives involves the adjoints of the TE and TM fields. Using adjoints, the cost of computing the derivatives becomes independent of the number of parameters used.
to represent $\Sigma$. The reader is referred to [1] for a detailed description of the technique. Here, only the main results for the case of ellipsometry are described.

The problem is reduced to the differentiation of the functions

$$f_1(\Sigma) = |R_{\text{TE},0}|^2 \quad \text{and} \quad f_2(\Sigma) = |R_{\text{TM},0}|^2.$$  

The derivatives of these functions are

$$Df_1(\Sigma)[V] = \text{Re} \left( - \int_{\Sigma} k_0^2 \left[ n^2 \right] \lambda_1^* E_z \cdot V \, d\Sigma \right),$$  

$$Df_2(\Sigma)[V] = \text{Re} \left( \int_{\Sigma} \left[ \frac{\partial \lambda_2^*}{\partial n} \cdot \frac{1}{n^2} \frac{\partial H_z}{\partial n} - \frac{\partial \lambda_2}{\partial n} \cdot \frac{1}{n^2} \frac{\partial H_z}{\partial n} \right] V \cdot \nu \, d\Sigma \right).$$  

The asterisk indicates the operation of conjugation and $\text{Re}(\cdot)$ indicates the real part of a complex number. $\nu$ and $t$ are the unit normal and tangential vectors to $\Sigma$, respectively. The notation $[g]$ indicates the jump of the quantity $g$ across $\Sigma$: $[g](x) := \lim_{\delta \to 0^+} [g(x - \delta \nu) - g(x + \delta \nu)]$. The scalar fields $\lambda_1^*$ and $\lambda_2^*$ are the solutions of the adjoint problems for $E_z$ and $H_z$, respectively. For example, $\lambda_1^*$ can be shown to satisfy equations (12)–(14) but with the incident field depending on the magnitude of the reflection coefficient $R_{\text{TM},0}$. Furthermore, the incident waves in the adjoint problems strike the grating at an angle $-\theta$ (in the notation of Figure 2), that is, the incident waves are being “back-propagated” from the detector. The general form of the adjoint fields $\lambda_1^*$ and $\lambda_2^*$, for $y > a$, is

$$\lambda_1^*(x, y) = \frac{R_{\text{TE},0}^*}{i\hat{\beta}_{1,0}} \exp i(\hat{\alpha}_0 x - \hat{\beta}_{1,0} y) + \sum_{m=-\infty}^{+\infty} A_m \exp i(\hat{\alpha}_m x + \hat{\beta}_{1,m} y),$$  

$$\lambda_2^*(x, y) = \frac{n_1^2 R_{\text{TM},0}^*}{i\hat{\beta}_{1,0}} \exp i(\hat{\alpha}_0 x - \hat{\beta}_{1,0} y) + \sum_{m=-\infty}^{+\infty} B_m \exp i(\hat{\alpha}_m x + \hat{\beta}_{1,m} y).$$  

The factors $A_m$ and $B_m$ are determined numerically and

$$\hat{\beta}_{1,m} = (k_0^2 n_2^2 - \hat{\alpha}_m^2)^{1/2},$$  

$$\hat{\alpha}_m = k_0 n_1 \sin(-\theta) + m \frac{2\pi}{d}.$$  

The $-\theta$ in the definition (29) of the $x$–component of the wave vectors indicates that the incident fields are coming from the detector.

3. Numerical examples

For the two numerical examples presented in this section, the TE, TM and adjoint problems are computed with the RCWA (rigorous coupled-wave analysis) method. This is one of the most commonly used methods to analyze diffraction gratings. For a detailed explanation of these methods and their numerical implementation, the reader is referred to [4, 5].

3.1. Derivatives of TM reflection coefficients: comparison with analytical solutions

As discussed in Section 2, the reflection coefficient for the case of a planar film on top of a substrate can be computed analytically using (7). Therefore, this expression can be used to check the computation of the derivative of $f(a) = |R_{\text{TM},0}|^2$ with respect to the thickness $a$ of the film using the proposed technique. Figure 3 compares the analytical (solid curve) and computed values (squares) over a range of angles for the incident field. The wavelength of the incident
radiation is $\lambda = 300$ nm, the thickness of the film is $a = 130$ nm and the indices of refraction for each medium are $n_0 = 1.0$ (vacuum), $n_1 = 3.0$ (thin film) and $n_2 = 2.0$ (substrate). Figure 4 presents the results for a fixed incident angle $\theta = 30^\circ$ and over the range of wavelengths $200$ nm $\leq \lambda \leq 1000$ nm. The agreement is excellent. In fact, the maximum relative difference between the computed and analytic values is less than $10^{-13}$.

![Figure 3](image1.png)  
**Figure 3.** Comparison between analytic (solid curve) and computed values of the derivative (squares) over a range of incidence angles.

![Figure 4](image2.png)  
**Figure 4.** Comparison between analytic (solid curve) and computed values of the derivative (squares) over a range of wavelengths.

### 3.2. Reconstruction using synthetic data

The adjoint technique is now tested on a reconstruction problem using measurements of the TE reflection coefficient. Data for this test case is produced synthetically by computing the TE response of a “target” structure with the RCWA code. 3% white Gaussian noise is added to the computed values creating a signal with a 30 dB signal-to-noise ratio. The outline of the target structure is shown in blue in Figure 5. The period is 400 nm and the region $y < 0$ represents the Si substrate. The region $0 < y < 250$ nm consists of a common photoresist with known optical properties. The variation in width along the height is for testing the method in capturing slight changes in the shape. Measurements are available for wavelengths ranging from 300 nm to 600 nm in steps of 10 nm, so a total of 31 measurements are available. The reconstructions use the Gauss-Newton algorithm to solve the optimization problems and the Jacobian or gradient is computed with the adjoint-based method described in this manuscript. The iterations stop when the relative decrease in the functional value is less than $10^{-6}$.

The reconstruction is started with the structure shown in green in Figure 5(a). The initial structure is represented with two layers of equal height in the RCWA method. The unknowns then are the widths of each layer and the height of the structure is fixed. Using only the measurements in the 500–600 nm band, the procedure converges in five iterations to the shape shown in red. Each layer of this structure is divided in two so the new structure now has four free parameters corresponding to the width of each of the four layers. The reconstruction problem is started using data in the 400–500 nm band. The new reconstruction converges in four iterations to the structure shown in red in Figure 5(b). This “frequency hopping” technique creates a good initial guess for the final reconstruction that uses the entire dataset in the range 300–600 nm. The initial structure is shown in green in Figure 5(c) and contains a total of 16 layers. Note that the converged shape, obtained in 30 iterations and shown in red, conforms closely to the target structure. Just near the top, the width of the converged and target shapes differ by less than 20 nm. This error is less than a tenth of the smallest wavelength used in the reconstruction.
Figure 5. Evolution of the profile during the reconstruction. Captions indicate the wavelength range used in each stage of the reconstruction. The target structure is shown in blue. For each stage of the reconstruction, the initial profile is shown in green and the converged profile is shown in red.

4. Conclusions
This manuscript presents a technique to rapidly compute derivatives of TE and TM reflection coefficients with respect to the geometric parameters that characterize a one-dimensional grating. The cost of computing the derivatives is independent of the number of geometric parameters. These derivatives can be used in optimization techniques to solve certain inverse scattering problems that appear in semiconductor metrology.

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