Convergence properties of critical dimension measurements by spectroscopic ellipsometry on gratings made of various materials

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Spectroscopic ellipsometry (SE) in the visible/near-UV spectral range is applied to monitor optical critical dimensions of quartz, Si, and Ta gratings, namely, the depth, linewidth, and period. To analyze the SE measurements, the rigorous coupled-wave theory is applied, whose implementation is described in detail, referred to as the Airy-like internal reflection series with the Fourier factorization rules taken into account. It is demonstrated that the Airy-like series implementation of the coupled-wave theory with the factorization rules provides fast convergence of both the simulated SE parameters and the extracted dimensions. The convergence properties are analyzed with respect to the maximum Fourier harmonics retained inside the periodic media and also with respect to the fineness of slicing imperfect Ta wires with paraboloidally curved edges. © 2006 American Institute of Physics.

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I. INTRODUCTION

Specular-mode spectroscopic ellipsometry (SE) has become perhaps the most important technique within optical scatterometry, especially for its precision, sensitivity, applicability for in situ, and other advantages over the conventional critical-dimension measurement techniques such as scanning electron microscopy or atomic force microscopy. In recent years scatterometry of diffraction gratings based on SE has widely spread owing to considerable progress in computation scopes that are necessary for the effective analysis of experimental diffraction-response data, particularly for the real-time process monitoring. Moreover, progress in theoretical algorithms with improving convergence properties enabled researchers to refine the correspondence between surface-relief profiles monitored optically and profiles visible by conventional scanning probe methods. In particular, the introduction of Li’s Fourier factorization rules for electromagnetic fields propagating inside media with periodic discontinuous permittivity remarkably enhanced the convergence of the algorithms.

Among many diffraction theories in literature, the coupled-wave theory is the mostly used method for scatterometry, widely referred to as the rigorous coupled-wave analysis. Authors presenting various implementations of the theory usually focus their numerical analyses to single-wavelength numerical experiments on hypothetical gratings that are considered perfectly known, and present convergence properties according to the number of Fourier harmonics retained inside a periodic medium. On the other hand, authors of scatterometric analyses on real samples do not provide details of algorithms they use, thereby not clarifying the effectiveness of their methods. For this reason, we devote this paper to the complete description of the optical-scatterometric technique based on SE, including the detailed description of our implementation of the coupled-wave theory, its convergence properties with respect to extracting the dimensions and topographic data, and the comparison of results obtained on gratings made of transparent quartz, semiconductive silicon, and metallic tantalum.

After the appearance of original papers on coupled waves initially implemented as the numerically unstable transfer-matrix approach, the method was revised several times to obtain algorithms usable for general structures, particularly with respect to higher depths of patterning and
II. MATHEMATICAL CALCULATION OF THE ELLIPSOMETRIC PARAMETERS

A. Formulation of the diffraction problem

In order to clearly demonstrate the Airy-like series implementation of the coupled-wave theory, we devote this section to a detailed description of diffraction of a polarized plane wave by a layer with periodic permittivity \( \varepsilon^{(1)}(y) \) sandwiched between two semi-infinite ambient media, a superstrate with uniform permittivity \( \varepsilon^{(0)} \) and a substrate with uniform permittivity \( \varepsilon^{(2)} \). The geometrical configuration of the problem is depicted in Fig. 1 including the denomination of the Cartesian coordinates, two principal polarizations, and directional wave vectors of plane waves, \( \hat{k}^i \) that is incident and \( \hat{k}_s^i \) and \( \hat{k}_t^i \) that are reflected and transmitted into the \( n \)th diffraction order, respectively. We assume the planar-diffraction mounting and the far-field Fraunhofer-diffraction approximation throughout this paper. Owing to the symmetry properties of the mounting, the diffraction response preserves the \( s \) polarization of a transverse-electric incident wave; the direction of the \( s \) polarization is here identical to the direction of the \( x \) axis. We introduce unit vectors \( \hat{x} = \hat{\mathbf{s}} \), \( \hat{y} \), and \( \hat{z} \), parallel to the Cartesian coordinates. Similarly, in the case of a transverse-magnetic incident wave with \( p \) polarization, whose direction is perpendicular to both the \( \hat{s} \) and \( \hat{k}^i \) vectors (i.e., \( \hat{p}^i = \hat{k}^i \times \hat{\mathbf{s}} \)), all the diffracted waves are \( p \) polarized as well provided that the normalized polarization vector of the \( n \)th diffraction order is defined as \( \hat{p}_n^i = \hat{k}_n^i \times \hat{\mathbf{s}} \).

For the sake of simplicity, we first limit our demonstration to the \( s \) polarization. Furthermore, we assume the \( e^{i\omega t} \) time dependence throughout this paper, and the space coordinates scaled by the \( 2\pi/\lambda \) factor, \( \lambda \) being the wavelength in vacuum. With these assumptions we can formulate the problem of finding the reflected and transmitted amplitudes of the electric field, denoted \( f_n^s \) and \( f_n^t \), respectively, corresponding to the \( n \)th diffraction order. By means of Rayleigh’s expansion, the incident, reflected, and transmitted electric fields are written

\[
E'(y,z) = \hat{x} f_0^s \exp[-i(q_0y + s_0^s z)], \quad (1a)
\]

\[
E'(y,z) = \hat{\mathbf{s}} \sum_{m=-\infty}^{+\infty} f_n^s \exp[-i(q_ny + s_n^s z)], \quad (1b)
\]

\[
E'(y,z) = \hat{x} \sum_{m=-\infty}^{+\infty} f_n^t \exp[-i(q_ny + s_n^t z)], \quad (1c)
\]

respectively, where the \( x \) dependence is omitted owing to the planar-diffraction mounting and where the components of the wave vectors are defined as follows:

\[
q_n = \sin \vartheta_t + nq, \quad (2a)
\]

\[
s_n^J = \sqrt{e^{(J)} - q_n^2}, \quad (2b)
\]

\[
q = \frac{\lambda}{\Lambda}, \quad (2c)
\]

where \( \vartheta_t \) and \( \Lambda \) denote the angle of incidence and the period of the function \( e^{(1)}(y) \), respectively, with \( J \) indexing here the uniform media 0 and 2.

B. Electromagnetic waves in a periodic medium

Defining \( \vec{H} = c \mu_0 \vec{H} \), with \( c \), \( \mu_0 \), and \( \vec{H} \) representing the light velocity in vacuum, the magnetic permeability in vacuum, and the magnetic field vector in the Système International (SI) units, respectively, we write Maxwell’s equations inside periodic medium 1 in a concise, time-independent form

\[
\nabla \times \vec{E} = -i \vec{H}, \quad (3a)
\]
\[ \nabla \times \mathbf{H} = i \epsilon^{(1)}(y) \mathbf{E}. \]  

(3b)

In the case of a rectangular grating patterned in a homogeneous layer, displayed in Fig. 2, we adopt the terminology of periodic "wires" commonly used for metallic gratings. Then the permittivity is a periodic function of only one lateral coordinate \( y \) with periodicity \( \Lambda \), assuming two values,

\[ \epsilon^{(1)}(y) = \begin{cases} 
\epsilon^{(1)}_w, & y \in (0, W) \\
\epsilon^{(1)}_b, & y \in (W, \Lambda),
\end{cases} \]

(4)

where \( \epsilon^{(1)}_w \) denotes the permittivity of wires, \( \epsilon^{(1)}_b \) the permittivity of the medium between wires, and \( W \) the width of wires. Note that the boundary point between the wire and the space \( (y=W) \) as well as the limit points of the periodicity interval \( (0, \Lambda) \) are not important for evaluating the Fourier series of the function (4).

Assuming \( s \) polarization, we may rewrite Eqs. (3) into a scalar wave equation for the single component \( E^{(1)} = E_z^{(1)} \) as follows:

\[ [\epsilon^{(1)}(y) + \kappa^2]E^{(1)}(y,z) = -\partial_z^2 E^{(1)}(y,z), \]

(5)

in which \( \partial_y \) and \( \partial_z \) represent partial derivatives with respect to the scaled space coordinates. Next we transform Eq. (5) into a matrix eigenvalue problem by expanding the permittivity function and the electric-field function into the Fourier and pseudo-Fourier series, respectively, i.e.,

\[ E^{(1)}(y) = \sum_{n=-\infty}^{+\infty} \epsilon^{(1)}_n e^{-iny}, \]

(6a)

\[ E^{(1)}(y,0) = \sum_{n=-\infty}^{+\infty} \epsilon^{(1)}_n e^{-in\Lambda}, \]

(6b)

where we have utilized Floquet's theorem.

Looking for a propagation eigenmode \( E^{(1)}(y) \) with the dependence

\[ E^{(1)}(y,z) = E^{(1)}(y,0)e^{-iz}, \]

(7)

(assuming only propagation in the direction of the increasing \( z \) coordinate), we obtain from Eq. (5) using Eqs. (6) and (7) the following:

\[ \sum_{k=-\infty}^{+\infty} \epsilon^{(1)}_{n-k} f^{(1)}_k - (q_n)^2 f^{(1)}_n = s^2 f^{(1)}_n, \]

(8)

which we transform to an eigenvalue equation of a matrix \( C^{(1)} \) with eigenvalues \( \mu^{(1)}_j \) and eigenvectors \( f^{(1)}_j \),

\[ C^{(1)} f^{(1)}_j = \mu^{(1)}_j f^{(1)}_j, \]

(9a)

\[ C^{(1)} = \epsilon^{(1)} - q^2, \]

(9b)

\[ \mu^{(1)}_j = |s_j|^2, \]

(9c)

where \( \epsilon^{(1)} = \| \epsilon^{(1)} \| \)

(10)

is a Toeplitz matrix composed of the Fourier coefficients \( \epsilon^{(1)}_n \) of the permittivity function \( \epsilon^{(1)}(y) \) truncated for the purpose of numerical evaluation,

\[ q = \text{diag}[-q_2, q_1, q_0, q_1, q_2, \ldots], \]

(11)

and with \( f^{(1)}_j \) being column vectors composed of the pseudo-Fourier coefficients \( f^{(1)}_n \). The subscript \( j \) indexes all the eigenvalue-eigenvector solutions of Eq. (9a).

Let \( F^{(1)}(0) \) be a column vector of the pseudo-Fourier coefficients from Eq. (6b) in the plane \( z=0 \), and let \( F^{(1)}(d) \) be an analogous column vector corresponding to the plane \( z=d \). Then we can describe the propagation of waves between the two planes as a matrix transform

\[ F^{(1)}(d) = P^1 F^{(1)}(0), \]

(12)

in which the propagation matrix \( P^1 \) is defined as

\[ P^1 = T^1 \]

(13)

where \( T^1 \) is the transformation matrix between the Fourier and eigenmode representations in medium 1; the columns of \( T^1 \) are the eigenvectors of \( C^1 \), and for brevity, we denote \( s^{(1)}_j = s_j \).

Similar to Eq. (7), we can look for propagation modes in the opposite direction (backward modes) \( E^{(1)-j}(y,z) = E^{(1)-j}(0) e^{+i\Lambda}, \) which leads to an analogous matrix formula \( f^{(1)-j}_{\text{back}}(d) = (P^1)^{-1} f^{(1)-j}_{\text{back}}(0). \) By inverting the propagation matrix we may conclude that the propagation in the opposite direction is described by the same matrix transform, i.e.,

\[ f^{(1)-j}_{\text{back}}(0) = P^1 f^{(1)-j}_{\text{back}}(d). \]
FIG. 3. Diffraction on the interface between media 0 and 1. In general, incident, reflected, and transmitted waves are identified with column vectors \( f_i, f_r, \) and \( f_t \), respectively, whose elements are the components of the pseudo-Fourier series of the corresponding electric fields. The diffraction response is then described by linear transforms between those vectors, \( R^{01} \) for reflection and \( T^{01} \) for transmission.

C. Boundary conditions

The conditions on the boundary between two periodic media or between a periodic and a homogeneous medium can be expressed as the requirement for the continuity of the tangential components of the electric and magnetic fields. For the case of \( s \) polarization, we require the continuity of the components \( E(y, z) \) and \( H_y(y, z) \), the latter of which follows from Eq. (3a) for any of the \( J \)th medium,

\[
\vec{H}^{(J)}(y, z) = \frac{i\sigma}{\epsilon} \vec{E}^{(J)}(y, z) .
\]

For the propagation mode proportional to \( e^{-i\omega_c} \), we get

\[
\vec{H}^{(J)}(y, z) = i\epsilon E^{(J)}(y, z)
\]

which, after the pseudo-Fourier expansion

\[
\vec{H}^{(J)}(y, z) = \sum_{n=-\infty}^{\infty} i \epsilon_s^{(J)} e^{-i\omega_n y},
\]

becomes a matrix transform

\[
g^{(J)}(z_0) = D^{(J)} f^{(J)}(z_0),
\]

where \( f^{(J)}(z_0) \) and \( g^{(J)}(z_0) \) are the column vectors of the pseudo-Fourier coefficients of the fields \( E^{(J)}(y, z_0) \) and \( H_y^{(J)}(y, z_0) \) in any plane \( z = z_0 \). Here

\[
D^{(J)} = T^{(J)} [s_1 0 0 \cdots 0 s_2 0 \cdots \cdots] (T^{(J)})^{-1}
\]

represents the so-called dynamical matrix of the \( J \)th medium.

For the illustration of applying the boundary conditions, we first calculate the diffraction response of the interface between media 0 and 1, which is symbolically depicted in Fig. 3. Let \( f_1 \) and \( f_2 \) be the column vectors of the pseudo-Fourier coefficients of the incident and reflected waves, respectively, and \( f_3 \) of the field transmitted into the periodic medium. All of the three vectors are evaluated in the plane \( z = 0 \). Using the matrix formalism, we express the continuity of the electric and magnetic field at the interface as

\[
f'_1 + f'_r = f'_t ,
\]

\[
D^{01}(f_1 - f'_r) = D^{01} f'_t ,
\]

respectively, from which we derive the reflection and transmission matrix transforms at the interface 0-1 as

\[
f' = R^{01} f, \]

\[
f' = T^{01} f,
\]

On the base of Eqs. (19), the reflection and transmission matrices can be defined as

\[
R^{01} = - [I + (D^{01})^{-1} D^{01}]^{-1} [I - (D^{01})^{-1} D^{01}]
\]

\[
T^{01} = I + R^{01},
\]

respectively, where \( I \) denotes the unit matrix.

D. Airy-like internal reflection series

The essence of our implementation of the coupled-wave theory is based on decomposing the electromagnetic field inside the periodic medium into a series of multiple internal reflections and propagations, as depicted in Fig. 4. The total reflected and transmitted field of the sandwich structure is thus expressed as a sum of contributions

\[
f' = f'_0 + f'_1 + f'_2 + \cdots
\]

\[
f' = f'_0 + f'_2 + f'_3 + \cdots
\]

The corresponding reflection and transmission matrices then become

\[
R^{02} = R^{01} + T^{01} P^{01} R^{12} P^{10} T^{01}
\]

\[
+ T^{01} P^{01} R^{12} (P^{10} R^{12} P^{01}) T^{01} + \cdots
\]
where the bracketed term is repeated with an increasing exponent. If we apply the formula for the geometric series $\sum_{j=0}^{\infty} Q^j = (1 - Q)^{-1}$, the result will be expressed in a concise form

$$R^{02} = R^{01} + T^{10} R^{10} R^{12} P^{1} T^{01},$$

(24a)

$$T^{02} = T^{12} P^{1} T^{01} + T^{12} (P^{1} R^{10} P^{1} R^{12}) P^{1} T^{01} + \cdots,$$

(23b)

where $Q = P^{1} R^{10} P^{1} R^{12}$ is the matrix coefficient of the geometric series.

E. Recursiโฃп algorithm for a sliced nonrectangular relief

So far we have assumed only a rectangular-relief grating, identified by depth $d$ and one periodic permittivity function $\varepsilon^{(1)}(y)$ corresponding to the first layer. In order to describe more general relief profiles by means of periodic permittivity, we must slice the relief into $N$ sufficiently thin layers so that the artificial roughness thereby produced can be neglected, as depicted in Fig. 5. The relief is then identified by a set of depths $d_j$ and a corresponding set of periodic permittivity functions $\varepsilon^{(j)}(y)$, each of those with the same period $\Lambda$; $j$ indexes the sublayers from 1 to $N$ and the ambient media numbered 0 and $N+1$.

To evaluate the optical response of the multilayer, we utilize Eqs.(24) recursively. Assuming we have evaluated the reflection and transmission matrices $R^{0j}$, $R^{10}$, $T^{0j}$, and $T^{10}$ of a partial system of first $J$ layers for both incidences from the top and bottom, we may simply regard this partial system as a pseudointerface fully described by these matrices. Then we apply the Airy-like series to the $J+1$ 1st layer [cf. Eqs. (23) and (24)], i.e.,

$$R^{0,j+1} = R^{0,j} + T^{10} P^{1} R^{1,j+1} (1 - Q^{j+1})^{-1} P^{1} T^{0,j},$$

(25a)

$$T^{0,j+1} = T^{1,j+1} (1 - Q^{j+1})^{-1} P^{1} T^{0,j},$$

(25b)

with $Q^{j} = P^{1} R^{10} P^{1} R^{1,j+1}$, and similarly for $R^{1+1,0}$ and $T^{1+1,0}$, until we obtain the matrices with $J=N$, corresponding to the total structure.

F. Transverse-magnetic ($p$) polarization

The evaluation of the diffracted amplitudes for the $p$ polarization follows the lines analogous to the above case of $s$ polarization. We apply the duality transformation and replace the electric and magnetic fields with each other to obtain formulas formally identical to the case of $s$ polarization, but with different meaning of individual components. Now the magnetic field is the fundamental quantity treated inside a periodic medium, while the electric field being the derived quantity helps us to determine the boundary conditions.

The wave equation for the single component of the magnetic field $\tilde{H} = \tilde{H}_x$, following from Eqs. (3), becomes

$$\exp\left(\frac{1}{\beta_j} \frac{\partial}{\partial y} \int_{y_0}^{y} \frac{1}{\varepsilon^{(j)}(y)} \partial_j \tilde{H}(y,z) \right) = - \beta_j \tilde{H}(y,z),$$

(26)

where the superscript $j$ indicates that we are treating the $j$th periodic layer. Instead of Eqs. (1), (6b), (7), (8), (9b), (14)–(16), and (18) we now write

$$\tilde{H}^{(j)}(y,z) = \tilde{H}^{(j)}(y,0) \exp(-i q_y y - s^{(0)}_m z),$$

(27a)

$$\tilde{H}^{(j)}(y,z) = \tilde{H}^{(j)}(y,0) \exp(-i q_y y - s^{(0)}_n z),$$

(27b)

$$\tilde{H}^{(j)}(y,z) = \tilde{H}^{(j)}(y,0) \exp(-i q_y y - s^{(12)}_n z),$$

(27c)

$$\tilde{H}^{(j)}(y,0) = \sum_{n=-\infty}^{+\infty} f^{(j)}_n e^{-i q_y n},$$

(28)

$$\tilde{H}^{(j)}(y,z) = \tilde{H}^{(j)}(y,0) e^{-iz},$$

(29)

$$\sum_{k=-\infty}^{+\infty} \left( e^{(j)}_{n-k} - \sum_{m=-\infty}^{+\infty} e^{(j)}_{n-m} g_{m,k} e^{(j)}_{m-k} \right) f^{(j)}_k = s^{(j)}_n,$$

(30)

$$C^{(j)} = e^{(j)} - e^{(j)} q [e^{(j)}]^{-1} q,$$

(31)

$$E^{(j)}(y,z) = - \frac{i}{\varepsilon^{(j)}(y)} \partial_j \tilde{H}^{(j)}(y,z),$$

(32)

$$E^{(j)}(y,z) = - \frac{s}{\varepsilon^{(j)}(y)} \tilde{H}^{(j)}(y,z),$$

(33)

$$E^{(j)}(y,0) = \sum_{n=-\infty}^{+\infty} g^{(j)}_n e^{-i q_y n},$$

(34)
\[
\begin{bmatrix}
 s_1 & 0 & 0 & \cdots \\
 0 & s_2 & 0 & \cdots \\
 0 & 0 & s_3 & \cdots \\
 \vdots & \vdots & \vdots & \ddots \\
\end{bmatrix}^{-1}
\begin{bmatrix}
 s_1 & 0 & 0 & \cdots \\
 0 & s_2 & 0 & \cdots \\
 0 & 0 & s_3 & \cdots \\
 \vdots & \vdots & \vdots & \ddots \\
\end{bmatrix}
\]
(35)

Otherwise, the remaining formulas for determining the diffracted amplitudes \( f_n^s \) and \( f_n^p \) stay same.

**G. Fourier factorization**

Appropriate transformation of Eq. (26) into a matrix formula requires particular treatment of discontinuous periodic functions, known as the Fourier factorization rules introduced by Li.\(^6\) According to his three factorization theorems, instead of Eqs. (30) and (31) we obtain

\[
\sum_{k=\infty}^{+\infty} \left[\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right]^{-1} \sum_{m=-\infty}^{+\infty} q_m \left[\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right]^{-1} f_k = s^2 f_n,
\]

(36)

\[
C^{(j)} = \tilde{\epsilon}^{(j)} - \tilde{\epsilon}^{(j)} q \left[\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right]^{-1} q,
\]

(37)

where we have defined \( \tilde{\epsilon}^{(j)} = [1/\epsilon^{(j)}]^{-1} \). For an arbitrary periodic function \( F(y) \), the symbol \([F]\) like in Eq. (10), denotes the Toeplitz matrix composed of its Fourier coefficients.

Several authors described more general rules usable for relief gratings with large slopes of edges of wires, referred to as the “fast Fourier factorization” method.\(^7\) In this paper, however, we limit our analyses to rectangular and quasi-rectangular gratings, so such generalization would not be necessary.

**H. Ellipsometric parameters**

For the purposes of this paper, we evaluate the two relevant ellipsometric parameters \( \Psi \) and \( \Delta \) in the specular mode, i.e., in the zeroth diffraction order of reflection. We assume each of the incident \( s \)- and \( p \)-polarized waves, respectively, with the dependence

\[
\exp[-i(q_{0s} + \sqrt{q_{0s}^2 - \Delta^2})z],
\]

(38)

which can be expressed in a matrix form of the Fourier representation at \( z=0 \) as

\[
\begin{bmatrix}
 0 & 0 & \cdots \\
 1 & 0 & \cdots \\
 0 & 0 & \cdots \\
 \vdots & \vdots & \ddots \\
\end{bmatrix}
\]

(39)

The vectors of reflected and transmitted waves can then be calculated as

\[
f^{(s)}_n = R^{(s)}_{0,N+1} f^{(s)}_n,
\]

(40a)

\[
f^{(p)}_n = R^{(p)}_{0,N+1} f^{(p)}_n,
\]

(40b)

where the superscripts \([s]\) and \([p]\) represent independent calculations corresponding to the \( s \) and \( p \) polarizations, respectively.

Finally, the ellipsometric parameters follow from the complex-number ratio

\[
\tan \Psi \exp i\Delta = \frac{R_{0,N+1}^{[p]}}{R_{0,N+1}^{[s]}},
\]

(41)

where \( R_{0,N+1}^{[s]} \) and \( R_{0,N+1}^{[p]} \) denote the \([0,0]\) element of the matrices \( R_{0,N+1}^{[s]} \) and \( R_{0,N+1}^{[p]} \) according to the pseudo-Fourier expansions \([Eqs. (1) and (27)]\). The minus sign on the right hand side of Eq. (41) is because \( R_{0,N+1}^{[p]} \) represents the transformation matrix for the magnetic field, whereas in ellipsometry we evaluate the electric one.

**III. SAMPLES AND EXPERIMENTAL PROCEDURES**

Three sets of samples were analyzed, made as (A) rectangular-relief gratings patterned on a fused-quartz substrate, (B) rectangular-relief gratings patterned on a Si substrate, and (C) rectangular-relief gratings patterned in a Ta thin film deposited on a fused-quartz substrate. For the purposes of this paper we have chosen one sample from each set, with their fabrication parameters summarized in Table I. The Ta film of sample C was deposited by means of rf sputtering. The patterning was made by means of x-ray lithography.

The SE measurements on samples A and C were performed on a four-zone null spectroscopic ellipsometer with the polarizer-sample-compensator-analyzer configuration,\(^23\) covering the wavelength range of 230–840 nm, and with an adjustable angle of incidence \( \theta_i \). Here we report on measurements at \( \theta_i=70^\circ \). To avoid the influence of incoherent back-reflections from the transparent quartz substrates for which the specular-mode SE is highly sensitive, we utilized the liquid solution procedure whose details are described in Ref. 17. For the present samples we used the same glycerin solution.

The SE measurements on sample B were performed on a rotating-analyzer ellipsometer in the polarizer-sample-analyzer configuration with a measurement spot diameter of 30 \( \mu \)m, covering the wavelength range of 300–800 nm, and with a fixed angle of incidence \( \theta_i=65.45^\circ \). The technical details of the apparatus are described in Ref. 24. Since the measurement on an ellipsometer in the polarizer-sample-
IV. DATA PROCESSING

Optical scatterometry is a measurement technique based on analyzing the experimental optical response of laterally patterned structures in order to determine their material and/or geometrical properties, particularly optical critical dimensions. The principle of determining unknown grating parameters, known as fitting, is minimizing the difference between simulated and measured values. This error is here evaluated as the angular distance between the measured and simulated points plotted on Poincaré’s sphere. This distance is specified by the azimuthal angle 2Ψ and the polar angle Δ, i.e.,

\[
\cos \Delta_j = \mathbf{S}_{e,j} \cdot \mathbf{S}_{m,j},
\]

where  \( \mathbf{E}_j \) represents the error of the \( j \)th value, while  \( \mathbf{S}_{e,j} \) and  \( \mathbf{S}_{m,j} \) denote the three-dimensional normalized Stokes vectors,

\[
\mathbf{S}_{e,j} = \begin{bmatrix}
\sin 2\Psi_{e,j} \cos \Delta_{e,j} \\
\sin 2\Psi_{e,j} \sin \Delta_{e,j} \\
\cos 2\Psi_{e,j}
\end{bmatrix},
\]

\[
\mathbf{S}_{m,j} = \begin{bmatrix}
\sin 2\Psi_{m,j} \cos \Delta_{m,j} \\
\sin 2\Psi_{m,j} \sin \Delta_{m,j} \\
\cos 2\Psi_{m,j}
\end{bmatrix},
\]

of the \( j \)th experimental [Eq. (43a)] and modeled [Eq. (43b)] ellipsometric values, respectively, in an ideal nondepolarizing system. The dot on the right hand side of Eq. (42) denotes the scalar product.

In the case of fitting, the sum of the squares of differences  \( \sum_{j=1}^{M} \mathbf{E}_j^2 \) is minimized. In tables, however, the averaged error over \( M \) experimental values  \( \tilde{\mathbf{E}} = (1/M) \sum_{j=1}^{M} \mathbf{E}_j \) is listed. To evaluate errors of values measured by rotating-analyzer ellipsometry (sample B), which only provides \( \text{Re}(e^{i\Delta_{e,j}}) = \cos \Delta_{e,j} \) instead of the complete information on phase \( \Delta_{e,j} \), we simply complete that information by defining

\[
\sin \Delta_{e,j} = \sin[\arccos(\cos \Delta_{e,j})],
\]

\[
\sin \Delta_{m,j} = \sin[\arccos(\cos \Delta_{m,j})],
\]

to substitute in Eqs. (43).

In order to perform a topographical analysis on the samples, we parametrize the geometrical relief profile by expanding the \( z \) dependence of the filling factor into a Taylor series up to the second order, i.e.,

\[
w(z) = w_1 + w_2 \left( \frac{2z}{d} - 1 \right) + w_3 \left( \frac{2z}{d} - 1 \right)^2,
\]

where \( d \) is the depth of the relief structure and \( w_j \) represents parameters of the relief profile. The function  \( w(z) = W(z)/\Lambda \) depends on the normal coordinate \( z \) and has its domain of definition between 0 and \( d \). For rectangular gratings, only  \( w_1 = W/\Lambda \) is nonzero, where \( W \) is the linewidth constant within depth. Trapezoidal-wire gratings are characterized by

\[
w_1 \text{ and } w_2 \text{ that are related to the top linewidth by } W(0) = w_1 - w_2 \text{ and to the average linewidth } W(d/2) = w_1. \text{ In a special case of wires with paraboloidal edges, the grating is characterized by } w_1 \text{ and } w_2 \text{ that are related to the top linewidth by } W(0) = w_1 - w_2 \text{ and to the maximum linewidth } W(d/2) = w_1. \text{ Finally, a general profile is characterized by all the } w_j \text{ parameters in Eq. (45), or more when assuming a polynomial approximation of higher order.}

For the purpose of the application of the Airy-like series, we slice the relief profile into \( N \) sublayers and correspondingly evaluate \( N \) discrete values of Eq. (45) as

\[
w^{(j)} = w_1 + w_2 \left( \frac{2j - (1/2)}{N} - 1 \right) - w_3 \left( \frac{2j - (1/2)}{N} - 1 \right)^2
\]

for each \( j \)th sublayer. In the case of sample C, the top layer corresponds to a native Ta\(_2\)O\(_5\) overlayer assumed present on the top of wires, and hence the relief slices are indexed from 2 to \( N+1 \).

The convergence properties are in this paper presented either according to the increasing number of slices \( N \) or according to the maximum diffraction order \( n_{\text{max}} \) retained in the Rayleigh, Floquet, and Fourier expansions in Eqs. (1), (6), (27), and (28), where the infinite sum is replaced with \( \sum_{n = n_{\text{max}}}^{n_{\text{max}}} \). This means that the field in the periodic medium as well as in the sandwiching media is being described by the so-called \( (2n_{\text{max}}+1) \)-wave approximation, the value of which corresponds to the dimension of the column vectors and to the order of the matrices of the linear-algebraic equations in Sec. II. The dependences of the optical critical dimensions on \( N \) and \( n_{\text{max}} \) are obtained by applying the fitting procedure described above for each pair of \( N \) and \( n_{\text{max}} \) that are fixed during fitting.

In the calculations we used optical constants of SiO\(_2\), Si, and Ta\(_2\)O\(_5\) published in references.\(^ {25,26} \) To obtain the constants of Ta, however, we analyzed optical experiments carried out on a thin-film reference sample prepared with the same conditions as a nonpatterned version of sample C but with a shorter deposition time to facilitate measurement in the transmission mode. A joint analysis of the SE and energy transmittance measurements yielded the refractive index and extinction coefficient of the Ta (Fig. 6) as well as the thickness \( t_{\text{Ta}_2\text{O}_5} = 4.5 \text{ nm} \) of the native oxide overlayer assumed present on the top of the Ta film.

V. RESULTS AND DISCUSSION

In the case of samples A and B, the simulation corresponding to rectangular gratings, that assume a single slice (\( N = 1 \)), adequately interprets the SE experimental data. The dependences of extracted dimensions on increasing \( n_{\text{max}} \) are summarized in Table II, together with dimensions assuming an ideal rectangular-wire grating profile of sample C as well. The corresponding fitted SE parameters, \( \Psi(\lambda) \) and \( \Delta(\lambda) \), are displayed for a few demonstrative examples of \( n_{\text{max}} \) in Fig. 7 for sample A, in Fig. 8 for sample B, and in Fig. 9 for sample C.
As clearly visible from Fig. 7, the SE response of the transparent sample in the spectral range of interest is perfectly described by the three-wave approximation since the curves corresponding to \( n_{\text{max}} = 1 \) are almost overlapped with those of the 21-wave approximation (corresponding to \( n_{\text{max}} = 10 \)). It is nearly surprising that the three-wave approximation is capable of simulating with high accuracy not only the two interference oscillations below 500 nm of wavelength but also Wood's anomaly appearing near Rayleigh's wavelength of 504 nm at which the minus first diffraction order of reflection passes off.\(^1\)

What has been stated about sample A can analogously be repeated for the case of sample B except that instead of three waves we need the five-wave approximation to interpret the SE measurement correctly. This is evident in Fig. 8 where we compare two fits, with \( n_{\text{max}} \) equal to 2 and 10. In particular, the three-wave approximation would be insufficient in the near-UV spectral range where Si is more absorbing. Slight discrepancies between the measured and fitted SE values in the peripheral parts of the spectral range can be explained by the presence of a TECH SPEC™ heat absorbing glass filter within the rotating-analyzer ellipsometer. The filter cuts off the intensity of light out of the range 300–800 nm and hence increases the noise and systematic errors of SE measurement near the limit points.

Contrary to samples A and B, the SE response of sample C in Fig. 9 cannot be correctly interpreted as a response measured on an ideal rectangular-wire grating, as is obvious from the discrepancy between the experimental data and the fits using any value of \( n_{\text{max}} \). However, carrying out the same procedure is useful to find out that the nine-wave approximation (corresponding to \( n_{\text{max}} = 4 \)) is necessary in the case of a similar but rectangular metallic grating.

Rather than a rectangular-wire grating, we identify the geometrical profile of sample C with a profile whose filling factor depends on the \( z \) coordinate as described by Eq. (45). According to various numerical experiments performed, we consider the profile as symmetric wires with paraboloidal edges, i.e., with the linear element in Eq. (45) omitted. Thus four dimensions are used to identify the profile, i.e., depth, top linewidth, maximum linewidth (in half-depth), and period. Two kinds of analyses on the convergence properties of extracted dimensions were carried out: according to increasing \( n_{\text{max}} \) while the number of slices \( N \) was fixed to 20 (Table III) and according to increasing \( N \) while \( n_{\text{max}} \) was fixed to 20 (Table IV).

**TABLE II.** Fitted critical dimensions (depth \( d \), linewidth \( W \), and period \( \Lambda \)) and errors of the fits of rectangular gratings according to increasing \( n_{\text{max}} \).

<table>
<thead>
<tr>
<th>( n_{\text{max}} )</th>
<th>Sample A</th>
<th>Sample B</th>
<th>Sample C</th>
</tr>
</thead>
<tbody>
<tr>
<td>( d ) (nm)</td>
<td>( W ) (nm)</td>
<td>( \Lambda ) (nm)</td>
<td>Error (deg)</td>
</tr>
<tr>
<td>1</td>
<td>498.18</td>
<td>102.82</td>
<td>257.84</td>
</tr>
<tr>
<td>2</td>
<td>500.44</td>
<td>102.77</td>
<td>257.51</td>
</tr>
<tr>
<td>3</td>
<td>502.36</td>
<td>101.40</td>
<td>257.72</td>
</tr>
<tr>
<td>5</td>
<td>503.68</td>
<td>102.77</td>
<td>257.84</td>
</tr>
<tr>
<td>10</td>
<td>503.86</td>
<td>100.64</td>
<td>257.91</td>
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<tr>
<td>20</td>
<td>503.90</td>
<td>100.61</td>
<td>257.91</td>
</tr>
<tr>
<td>50</td>
<td>503.90</td>
<td>100.61</td>
<td>257.91</td>
</tr>
</tbody>
</table>
The fitted SE parameters corresponding to the former case for three demonstrative examples of \( n_{\text{max}} \) are displayed in Fig. 10. In most of the spectral range, the 17-wave approximation (corresponding to \( n_{\text{max}} = 2 \)) is sufficient to fit the measurement.

The fitted SE parameters corresponding to the former case for three demonstrative examples of \( n_{\text{max}} \) are displayed in Fig. 10. In most of the spectral range, the 17-wave approximation (corresponding to \( n_{\text{max}} = 2 \)) is sufficient to perform a reliable fit. Higher value of \( n_{\text{max}} \) can slightly improve the accuracy of simulation in the short-wavelength range and at the extreme points near Rayleigh’s wavelengths, one at 388 nm where the minus first diffraction order of reflection passes off and another at 480 nm where the minus first diffraction order of transmission passes off.

The fitted SE parameters with \( n_{\text{max}} \) fixed to 20 for four demonstrative examples of \( N \) are displayed in Fig. 11. Here the agreement between experiment and fitting is improving gradually while \( N \) is increasing. Again, the short spectral ranges near Rayleigh’s wavelengths are most sensitive to insufficient slicing. We can conclude that the fit with \( N = 10 \) is satisfactory according to the error of the SE parameters defined by Eq. (42).

Finally, in Fig. 12 we present the convergence dependences of relative dimensions, i.e., parameters defined as \( p(n_{\text{max}})/p(n'_{\text{max}}) \), where \( p(n_{\text{max}}) \) denotes a dimension whose convergence properties according to increasing \( n_{\text{max}} \) are studied, while \( p(n'_{\text{max}}) \) represents a reference value obtained from a fit that assumes sufficiently high \( n'_{\text{max}} \) chosen 50 for both the rectangular-grating profiles and Ta paraboloidal-wire profiles. Thus, the subfigures depict how the dimensions are relatively approaching their approximate-limit values with high \( n_{\text{max}} \).

In Figs. 12(a)–12(c), the convergences of the relative depth, linewidth, and period are displayed as obtained on samples A, B, and C, respectively. The errors of all the dimensions of the transparent grating are less than 1% for \( n_{\text{max}} \geq 2 \) and are rapidly decreasing for higher \( n_{\text{max}} \) [Fig. 12(a)]. Note that the period converges fastest, while the line-

### TABLE III. Fitted critical dimensions (depth \( d \), top linewidth \( W_{\text{top}} \), maximum linewidth \( W_{\text{max}} \), and period \( \Lambda \)) and errors of the fits of the Ta paraboloidal-wire grating according to increasing \( n_{\text{max}} \) with a fixed number of slices \( N = 20 \).

<table>
<thead>
<tr>
<th>( n_{\text{max}} )</th>
<th>( d ) (nm)</th>
<th>( W_{\text{top}} ) (nm)</th>
<th>( W_{\text{max}} ) (nm)</th>
<th>( \Lambda ) (nm)</th>
<th>Error (deg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>235.84</td>
<td>71.45</td>
<td>101.46</td>
<td>190.63</td>
<td>6.72</td>
</tr>
<tr>
<td>4</td>
<td>226.75</td>
<td>52.12</td>
<td>100.44</td>
<td>198.65</td>
<td>4.80</td>
</tr>
<tr>
<td>6</td>
<td>226.88</td>
<td>59.87</td>
<td>102.94</td>
<td>198.12</td>
<td>4.70</td>
</tr>
<tr>
<td>8</td>
<td>224.73</td>
<td>53.30</td>
<td>103.37</td>
<td>198.69</td>
<td>4.70</td>
</tr>
<tr>
<td>10</td>
<td>224.64</td>
<td>56.16</td>
<td>103.14</td>
<td>198.68</td>
<td>4.39</td>
</tr>
<tr>
<td>20</td>
<td>219.27</td>
<td>49.41</td>
<td>103.79</td>
<td>199.20</td>
<td>4.01</td>
</tr>
<tr>
<td>50</td>
<td>219.01</td>
<td>50.46</td>
<td>103.42</td>
<td>199.29</td>
<td>3.87</td>
</tr>
</tbody>
</table>

### TABLE IV. Fitted critical dimensions (depth \( d \), top linewidth \( W_{\text{top}} \), maximum linewidth \( W_{\text{max}} \), and period \( \Lambda \)) and errors of the fits of the Ta paraboloidal-wire grating according to increasing number of slices \( N \) with fixed \( n_{\text{max}} = 20 \).

<table>
<thead>
<tr>
<th>( N )</th>
<th>( d ) (nm)</th>
<th>( W_{\text{top}} ) (nm)</th>
<th>( W_{\text{max}} ) (nm)</th>
<th>( \Lambda ) (nm)</th>
<th>Error (deg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>231.60</td>
<td>60.85</td>
<td>96.48</td>
<td>194.63</td>
<td>8.33</td>
</tr>
<tr>
<td>5</td>
<td>226.29</td>
<td>55.81</td>
<td>99.06</td>
<td>197.63</td>
<td>5.19</td>
</tr>
<tr>
<td>7</td>
<td>225.03</td>
<td>55.98</td>
<td>99.49</td>
<td>197.93</td>
<td>4.52</td>
</tr>
<tr>
<td>10</td>
<td>222.37</td>
<td>53.20</td>
<td>101.37</td>
<td>198.41</td>
<td>4.07</td>
</tr>
<tr>
<td>20</td>
<td>219.27</td>
<td>49.41</td>
<td>103.79</td>
<td>199.20</td>
<td>4.01</td>
</tr>
<tr>
<td>50</td>
<td>219.63</td>
<td>53.97</td>
<td>104.17</td>
<td>199.58</td>
<td>4.20</td>
</tr>
</tbody>
</table>
Width does slowest. Similarly, the errors of all the dimensions of the Si grating are less than 1% for $n_{\text{max}}/H_{33356}^4/H_{20851}^4$. In the case of the Ta grating with its wires assumed rectangular, the errors of the depth and period are less than 1% for $n_{\text{max}}/H_{33356}^3$, whereas the linewidth converges much slower. This can be explained by the inhomogeneity of the linewidth within depth or, in other words, by the incorrectness of the model applied for fitting which does not take into account all the aspects of the reality.

In Figs. 12(d) and 12(e), the convergences of the relative depth, top linewidth, maximum linewidth, and period are displayed as obtained on sample C with the number of slices $N$ assumed 3 and 20, respectively. Here the convergences of all the dimensions are slower than in the case assuming the rectangular profile. The most probable explanation follows from a partial inadequacy of the Fourier factorization rules applied here to wires with slightly curved edges, though the rules...
have been derived for rectangular-relief gratings. Nevertheless, the slopes of the wires of sample C are so small that the factorization rules should be approximately valid.

In Fig. 12(f), the convergences of the relative depth, top linewidth, maximum linewidth, and period according to increasing \( N \) are displayed as obtained on sample C with \( n_{\text{max}} \) fixed to 20. The relative parameters can now be written as \( p(N)/p(N') \), where \( p(N) \) is a parameter whose convergence properties according to increasing \( N \) are studied, while \( p(N') \) represents an approximate-limit value obtained by assuming \( N' = 50 \) slices. Just as the SE parameters do in Fig. 11, the relative dimensions gradually converge while the number of slices is increasing. We can conclude from Figs. 12(d)–12(f) that the period converges most rapidly, whereas the maximum linewidth most slowly in the case of a sliced nonrectangular profile.

VI. CONCLUSIONS

A coupled-wave implementation referred to as Airy-like series was here described in detail to increase the clarity of monitoring critical dimensions of gratings by means of optical scatterometry, particularly with respect to the convergence properties of the dimensions according to the level of approximation such as the truncation order of Fourier series, \( n_{\text{max}} \), or the number of slices \( N \) of a nonrectangular-wire grating. It was demonstrated that applying the Fourier factorization rules incredibly enhanced the convergence properties of both the simulated SE parameters and the extracted dimensions, though an improvement based on generalizing the factorization rules would provide better results for wires with curved edges. In the case of the gratings made of transparent quartz and semiconducting Si, the agreement between the experimental data and the fitted parameters was nearly perfect, obviously indicating high relevance of the model assuming a rectangular-relief structure of samples A and B. In the case of the Ta grating, however, slight discrepancies were observed in the short-wavelength part of the range of interest, even though a top native TaOx overlay and a nonideal shape of wires with curved edges were considered. The method could be improved by generalizing the model including more aspects of reality. The most important aspects are the optical constants of Ta to be monitored more precisely in a broader spectral range with an energy reflectance measurement included, the surface roughness of Ta for which SE is sensitive, the surface oxide on the edges of wires, and/or a more general shape of the Ta wires with higher-order parameters of the Taylor series in Eq. (45).

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