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van Beurden, M.C.; Zacharopoulou, T.; van Kraaij, M.G.M.M.

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A spectral-domain integral equation for scattering by periodic birefringent dielectric objects embedded in a birefringent layered medium

Martijn C. van Beurden¹, Thomai Zacharopoulou², and Mark G.M.M. van Kraaij²

Abstract — We consider electromagnetic scattering from periodic dielectric objects in a layered medium, where both the layered medium and the dielectric objects can exhibit birefringence in the permittivity oriented along the direction of stratification. To compute reflection and transmission coefficients, we employ a volume integral equation formulated in the spectral domain, containing a normal-vector-field framework. We briefly illustrate the impact of birefringence on the formulation and implementation of the volume integral equation, we indicate ways to test the correctness of the implementation, and we provide numerical results.

1 INTRODUCTION

In modern integrated-circuit lithography, more and more exotic materials are being used, among which materials with birefringent properties, such as amorphous carbon [1]. This form of anisotropy can be a result of the deposition process in the form of e.g. thermomechanical stresses [2]. The presence of birefringent materials needs to be taken into account in forward electromagnetic modeling tools for wafer metrology, to properly characterize the scattering behavior of metrology targets that contain or are embedded in such materials.

2 FORMULATION OF A SPECTRAL-DOMAIN VOLUME INTEGRAL EQUATION

The general form of a volume integral equation formulated in the spectral domain constitutes of two parts, i.e. the integral representation for the electric field, \( E \), in terms of the contrast current density, \( J \), and the field-material interaction that defines the contrast current density in terms of the electric field. Below, we discuss these two parts in more detail.

2.1 Incident field and Green function

The spectral domain is particularly useful for the expression of the electric field in terms of the contrast current density, the incident field and the Green function, owing to the availability of the Green function for layered media in this domain. For periodic configurations, the spectral domain is discrete and we indicate the discrete modes of the electric field by \( E_m(z) \), where \( m \) is a two-dimensional index that runs over all Fourier modes (or harmonics) and \( z \) is the direction of stratification of the layered medium. Similarly, we indicate the spectral constituents of the contrast current density by \( j_m \). To complete the integral representation, we split the electric field into two contributions, i.e. the incident field \( E_m(z) \) that is the field in the presence of the layered background medium in absence of the dielectric objects and the scattered field \( E_m(z) \) due to the scattering by the objects. The resulting relation per spectral component is then given by

\[
e_m(z) = e_m(z) - \int_{z_{min}}^{z_{max}} G_m(z,z') j_m(z') dz',
\]

where it is assumed that the contrast current density, and therefore the dielectric objects, are confined to the interval \([z_{min}, z_{max}]\). The Green function \( G_m \) is a 3×3 matrix function acting on the Cartesian components of the vector fields. For a layered background medium with birefringence in the \( z \) direction versus the \( xy \) direction, the Green function separates into an s- and p-polarized contribution that can be determined independently. However, these polarization directions depend on the two-dimensional mode index \( m \). Each of these polarization states has its own propagation coefficient in a birefringent layer, whereas these are the same for an isotropic layer, and its own set of reflection and transmission coefficients for the entire stack of layers. For the incident field, the polarization states also need to be separated and propagated along the stack of layers, identical to the way in which the Green function is determined. Since the polarization basis for s- and p-polarization depends on \( m \), we choose to keep the basis for the electric field and the contrast current density in the Cartesian basis.

The integration along the \( z \) direction in Eq. (1) can take place in \( O(N) \) steps for \( N \) piecewise linear functions for each component of \( j_m \) along the \( z \) direction, similar as in the case of isotropic media [3], albeit the different propagation coefficients for s- and p-polarization require that the vectorial components of the contrast current density are decomposed according to the type of polarization that they generate. The same holds if we employ a discretization based on Chebyshev polynomials, which can be executed in \( O(N \log N) \) steps for \( N \) polynomials [4].

2.2 Field-material interaction for birefringence

The choice for the spectral domain benefits the construction of the Green function in layered media, but it significantly complicates the relation that

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¹ Electromagnetics group, Department of Electrical Engineering, Eindhoven University of Technology, Eindhoven, The Netherlands, e-mail: m.c.v.beurden@tue.nl
² ASML, Veldhoven, The Netherlands
expresses the contrast current density in terms of the electric field, due to the presence of concurrent jumps in the electric field and the permittivity function that describes the presence of a dielectric object. Such concurrent jumps are the root cause of convergence problems in the spectral domain when the field-material interactions are straightforwardly implemented according to the Laurent rule, i.e. as convolutions. To overcome these obstacles, we employ the normal-vector-field formalism introduced in [5]. The normal-vector-field framework introduces an auxiliary field, $F$, that is composed of the continuous components of the electric field and electric flux density. Additionally, two anisotropic operators, $C_\epsilon$ and $\varepsilon C_\epsilon$, are introduced that relate the electric field and flux density to the auxiliary field and the permittivity, which are stated in the spatial domain as

$$E = C_\epsilon \cdot F, \quad (2a)$$

$$D = \varepsilon C_\epsilon \cdot F, \quad (2b)$$

$$J = j\omega (\varepsilon C_\epsilon - \varepsilon_b) F, \quad (2c)$$

where $\varepsilon_b$ denotes the permittivity tensor of the background, which is constant as a function of $x, y$.

We employ a further refinement in terms of local normal-vector fields as introduced in [6], in which the normal-vector field and the pertaining Fourier integrals are only evaluated on the support of the dielectric objects, even in the presence of general anisotropy, thus allowing for geometrical flexibility at the cost of more complicated expressions for the Fourier integrals that need to be evaluated. Here we restrict the discussion to piecewise-homogeneous dielectric objects.

For birefringent media with the optical axis in the $z$ direction, the general form of the Fourier integrals for $C_\epsilon$ are given by

$$C_{i,j} = \int \frac{n_i n_j}{1 + \eta^2} \exp(-jk \cdot r_T) dr_T, \quad (3)$$

where $i, j \in \{x, y, z\}$ and $n_i$ denotes a Cartesian component of the normal-vector field, which is in general a function of $x, y$ and $z$. Further, $k_T$ is the two-dimensional Fourier parameter, $r_T$ denotes the location vector in the $xy$ plane, and $\eta$ denotes the ratio of the permittivity of the object in the ordinary and extraordinary directions. The general situation for Eq. (3) yields rather complicated Fourier-integrals to compute. Therefore, it is convenient to consider two special cases for the shapes and corresponding normal-vector fields of the dielectric objects:

- a) shapes consisting of vertical material boundaries only, i.e. binary gratings or gratings with stair-cased boundaries along $z$ for which the normal-vector field is entirely $xy$ directed,
- b) shapes with non-stair-cased boundaries for which the normal-vector field has a constant but nonzero $z$ component.

Both these cases make the denominator in Eq. (3) constant. For category a), we note that the Fourier integrals are not impacted at all compared to the isotropic case. For category b), we observe a straightforward scaling of the expressions for the isotropic case. This class includes polyhedrons and bodies of revolution, where the rotation axis is parallel to the $z$-axis.

### 3 Numerical Results

The first test case is a 1D-periodic configuration. A schematic overview of the input can be found in Figure 1. The superstrate and substrate halfspaces are both isotropic with refractive indices $(n_0, k_0) = (1.0, 0.0)$ and $(n_2, k_2) = (4.5, 0.1)$ respectively. The grating layer 1 containing the birefringent materials can be modeled in four different ways:

- i) isotropic background with refractive index equal to upper halfspace. Layer 1 contains two sloped birefringent lines, 1a and 1b, filling the entire unit-cell with refractive indices as mentioned in the table.
- ii) birefringent background with refractive index equal to birefringent line 1a. Layer contains one sloped birefringent line 1b.
- iii) birefringent background with refractive index equal to birefringent line 1b. Layer contains one sloped birefringent line 1a.
- iv) similar to i) but now with an anisotropic background $(n_{1,o}, k_{1,o}) = (1.6, 0.3)$ and $(n_{1,e}, k_{1,e}) = (2.0, 0.5)$.

![Figure 1: Grating input of first configuration. Subscripts o and e are used for the ordinary and extra-ordinary components, respectively. Dimensions are specified in nanometers and the wavelength of the incident field is 425 nm.](image)

The incident field is TM polarized (recall that TE polarization is not affected by the extra-ordinary component) and arrives at an angle of 30 degrees at a wavelength $\lambda$ of 425 nm. We take $2M + 1$ harmonics per transverse direction and $N$ Chebyshev polynomials in the longitudinal direction into account.

The reflection coefficient obtained with the isotropic background in i) will be the reference, the other 3 cases should produce the same reflection.
coefficient. The match is obtained in the limit of $M$ and $N$ to infinity. Figure 2 shows that by increasing the number of harmonics the difference between the cases ii), iii), iv) and the reference obtained with i) gets smaller. However, at approximately 10 harmonics the error levels off at around $1e-5$, which is still much larger than the iterative solver tolerance of $1e-10$ used in these simulations. By increasing the number of points in the Chebyshev discretization from 30 to 60 we are able to lower the error further to about $1e-7$ as can be seen from Figure 3.

Figure 2: Absolute error in reflection coefficient $R_p$ for fixed Chebyshev discretization $N=30$.

![Figure 2](image2.png)

Figure 3: Absolute error in reflection coefficient $R_p$ for fixed Chebyshev discretization $N=60$.

The second test case is a 2D-periodic configuration of a grating consisting of a square hole in an amorphous Carbon background layer, which is modeled as a birefringent material [7]. A schematic overview of the side and top view of the geometry can be found in Figure 4. We consider two incident fields: one s-polarized and one p-polarized and both arrive at angles $\theta$ and $\varphi$, which are defined with respect to the $z$- and $x$-axis, respectively. The superstrate and substrate halfspaces are isotropic with refractive indices $(n_0, k_0) = (1.0, 0.0)$ and $(n_3, k_3) = (4.5, 0.1)$, respectively. The refractive indices of the remaining materials are displayed in Table 1.

![Figure 4](image4.png)

Table 1: Refractive indices of materials of the second configuration. Subscripts $o$ and $e$ are used for the ordinary and extra-ordinary components respectively.

<table>
<thead>
<tr>
<th></th>
<th>$n_o$</th>
<th>$k_o$</th>
<th>$n_e$</th>
<th>$k_e$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>1.9</td>
<td>0.4</td>
<td>2.9</td>
<td>0.4</td>
</tr>
<tr>
<td>1b</td>
<td>1.0</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>1.5</td>
<td>0.0</td>
<td>1.5</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Firstly, the input geometry is simulated under a varying incident wave with wavelength $\lambda=633$ nm. The angle of incidence $\varphi$ is fixed at $10^\circ$, whereas the angle $\theta$ varies in the range $[0^\circ, 90^\circ)$. The discretization settings for Chebyshev polynomials $N$ and number of harmonics $M$, as well as the grating width are kept constant. Figure 5 shows the absolute value of the reflection coefficients for the $(0,0)^{th}$ order.

![Figure 5](image5.png)

To demonstrate the impact of birefringence on the reflection coefficient $|R_{pp}|$, we set the extraordinary refractive index of the material 1a equal to the
ordinary refractive index, i.e., \((n_x, k_x) = (n_y, k_y)\). The absolute values of the reflection coefficient and their absolute difference are shown in Figure 6.

![Figure 6: Absolute difference of (0,0)th order reflection coefficient \(R_{pp}\) for a background material modeled as either birefringent or isotropic, as well as for fixed Chebyshev discretization \(N=30\), harmonics along both directions \(M=7\), \(w=158.25\) nm, and \(\phi=10^\circ\).](image)

Secondly, the input geometry is simulated under a varying width \(w\) of the hole, in the range \([\lambda/10, \lambda]\), while the input wave arrives at fixed angles \(\theta=45^\circ\) and \(\phi=10^\circ\). The discretization settings for Chebyshev polynomials \(N\) and the number of harmonics \(M\) remain fixed. Figure 7 shows the absolute values of the reflection coefficients for the (0,0)th order. It is clear that the cross-polarized terms \(|R_{sp}|\) and \(|R_{ps}|\) approach zero for a grating occupying the entire unit cell, i.e. \(w=633\) nm, because the geometry is then constant in the \(xy\) plane. In a further study (not shown here), the reflection coefficients for \(w=633\) nm were compared to an independent reference in which the grating occupied the entire unit cell, i.e. \(w=633\) nm, and the background material of the grating was replaced by an arbitrary isotropic material. In particular, for the background material of the grating we chose \((n_1, k_1) = (2.0, 0.0)\), while keeping the discretization settings the same as in Figure 7. The comparison resulted in an absolute error in the reflection coefficients in the same order as the level of the iterative solver tolerance.

4 CONCLUSIONS

We have discussed the implications due to the presence of birefringent materials in a periodic setup of dielectric layers and objects in terms of the formulation of a spectral-domain volume integral equation. We have discussed the consequences for the implementation and we have given suggestions for testing the implementation, illustrated by numerical results.

References


