

A Review of Integral-equation Methods for the Analysis of Scattering by All-dielectric Gratings

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Abstract—Integral-equation methods treating boundary-value problems of electromagnetic wave scattering by all-dielectric isotropic gratings are reviewed. The presented methods include boundary-integral-equation and volume-integral-equation methods, analytical regularization methods, and the extended boundary condition method. They can, in principle, provide accurate solutions in a limited computational time and, hence, assist substantially in optimizations of the grating's parameters to achieve desired operational characteristics.

I. INTRODUCTION

The first occurrence of diffraction gratings dates back to Hopkinson and Rittenhouse in the eighteenth century [1]. Their applications are well known for many decades now, spanning, indicatively, from spectroscopy to light polarizers [2], solar absorbers [3], and grating couplers [4]. Surveys on traditional as well as industrial applications of optical diffraction by gratings can be found in [5] and [6].

The rise of metamaterials and metasurfaces gave new birth to modern applications of gratings and necessitated the need for fast and accurate modeling of their electromagnetic behavior. Particularly, in the last decade, completely transparent and high-refractive-index dielectric building blocks have been extensively applied in nanophotonic design. In this way, the class of all-dielectric metamaterials emerged which has shown to overcome limitations of relevant structures incorporating metallic parts [7]. High-contrast all-dielectric gratings, realized as subwavelength arrays of free-standing cylinders with a large refractive index contrast, have been shown to exhibit extraordinary properties, like, e.g., achieving tunable coloration or being used in holograms, modulators, and optical switches [8]. Besides, metagratings were introduced in [9] as periodic arrays of realizable inclusions yielding light manipulation and wave front engineering with unitary efficiency and overcoming fundamental limitations of continuously gradient metasurfaces.

Scattering by gratings has been analyzed by various different methods ranging from simple and intuitive techniques to rigorous full-wave approaches. Nevertheless, the mathematical analysis of grating structures still constitutes a challenging research topic serving the increasing needs for optimizations of complex structures incorporating gratings. To this end, integral equation methods play a key role since they can provide guaranteed convergence of their solutions and can be fast and efficiently implemented in computer programs. In this contribution, the following established and widely used integral equation methods for all-dielectric isotropic gratings are reviewed: (i) boundary integral equation methods, (ii) volume integral equation methods, (iii) method of analytical regularization, and (iv) extended boundary condition method.

II. BOUNDARY INTEGRAL EQUATION METHODS

Boundary integral equation (BIE) methods discretize only the interfaces (in case of piecewise homogeneous materials) and can achieve high-order accuracy. Moreover, they do not need artificial boundary conditions on a truncated computational domain since they satisfy directly the radiation condition for the scattered field [10]. BIEs can be classified as Fredholm integral equations of the form [11]

$$\alpha u(\mathbf{r}) - \int_S K(\mathbf{r}, \mathbf{r}') u(\mathbf{r}') d\mathbf{s}(\mathbf{r}') = v(\mathbf{r}), \quad (1)$$

with S the surface of a 3-D diffracting object or the cross-section boundary of a 2-D object. In Eq. (1), u is the unknown function, while v and K are known functions. A first and a second kind Fredholm integral equation is obtained, respectively, when $\alpha = 0$ and $\alpha = 1$.

In a simple setting, the BIE formulation employs single-layer potential representations for the field below the grating, while above the grating Green's theorem is applied for the scattered field. Imposing the transmission boundary conditions on the boundary of the grating yields the single integral equation (involving single- and double-layer potentials) [12]

$$[\mathcal{V}^+(\mathcal{I} - \mathcal{L}^-) + (\mathcal{I} + \mathcal{K}^+)\mathcal{V}^-] w(P) = -2E_z^{\text{inc}}(P), \quad P \in \Gamma, \quad (2)$$

where w is the unknown density, and Γ denotes the part of the grating lying inside the unit cell. Numerical solutions proceed from the discretization of the single integral equation (2).

Besides, BIE methods can be viewed as a special case of boundary element methods (BEM) applied to boundary value problems for the Helmholtz equation [13]. Discretization schemes and quadrature rules of BEM need to be considered.

III. VOLUME INTEGRAL EQUATION METHODS

A typical setting of a volume integral equation (VIE) formulation for scattering problems by layered gratings is based on integral representations of the form [14]

$$E(x, y) = E_h(x, y) + k_0^2 \iint_{\Omega_g} G(x - x', y, y') [\epsilon(x', y') - \epsilon_h(x', y')] E(x', y') dx' dy', \quad (3)$$

with Ω_g the cross section of the grating region, k_0 the free-space wavenumber, $\epsilon(x, y)$ the dielectric permittivity function of the entire structure, while E_h and G is the electric field and the Green's function of the homogeneous (grating-free) structure, respectively. Then, using Floquet's theorem, considering the Fourier integral representation of the Green's function and employing Poisson's summation formula, the

integral representation (3) is reformulated suitably on the grating's basic unit cell S . Next step involves discretization of the domain S reducing the obtained integral equation to a linear system with unknowns the fields values inside S [14]. To this direction, scattering by configurations formed by elements embedded in a stratified background was studied in [15] by employing the Green's dyadic of the background, thus, requiring only the embedded elements to be discretized. On the other hand, entire domain expansion techniques inside the grating (as, e.g., in [16], [17]) may also be employed; these approaches do not use any discretizations of the grating.

IV. METHOD OF ANALYTICAL REGULARIZATION

The Method of Analytical Regularization (MAR) refers to a family of methods converting a first-kind or strongly-singular second-kind integral equation to a second-kind integral equation with a smoother kernel [18]. Suppose that a first-kind integral equation is obtained, after applying the boundary conditions of a scattering problem, i.e.,

$$\mathcal{A}X = Y, \quad (4)$$

with X the unknown function, and operator $\mathcal{A}$ cannot be analytically inverted. According to MAR, $\mathcal{A}$ is split as

$$\mathcal{A} = \mathcal{A}_1 + \mathcal{A}_2, \quad (5)$$

such that $\mathcal{A}_1$ has a known inverse $\mathcal{A}_1^{-1}$. Then, by (4) and (5), the second-kind integral equation is obtained

$$X + \mathcal{A}_1^{-1}\mathcal{A}_2X = \mathcal{A}_1^{-1}Y. \quad (6)$$

When operator $\mathcal{A}_1^{-1}\mathcal{A}_2$ is compact on a Hilbert space and the vector $\mathcal{A}_1^{-1}Y$ lies on the same space, the resulting operator equation is of the Fredholm type, an exact solution of (6) exists and discretization schemes converge in a point-wise sense.

In [19], plane-wave scattering by dielectric strip gratings was analyzed by analytic inversion of the static part of the full-wave equations. Plasmon-assisted scattering of visible light by gratings of silver nanowires was studied in [20] by casting the matrix equation to a Fredholm second-kind type one.

V. EXTENDED BOUNDARY CONDITION METHOD

The extended boundary condition method (EBCM) is based on the integral equations stemming from the Ewald-Oseen extinction theorem [21]. Consider a scatterer defined by a domain V_i with boundary S , having a circumscribing surface S_e and an inscribing surface S_i . The sources of the incident field lie inside a region V_s outside S_e . Outside V_s , the incident fields are expanded in a suitable basis of vector wavefunctions. Outside V_i , the scattered fields are then expanded into a different set of vector wavefunctions. Enforcing the second equation of the Ewald-Oseen theorem in the interior of S_i and using the orthogonality properties of the employed vector wavefunctions leads to integral expressions for the coefficients of the incident field involving the surface fields on S . Next, enforcing the first equation of the same theorem in the exterior of S_e and applying a similar procedure, one obtains integral expressions for the unknown coefficients of the scattered fields.

Then, considering fields expansions in V_i , the T-matrix of the scattering problem is obtained connecting the scattered fields coefficients to the known ones of the incident fields.

Scattering by an isotropic dielectric grating using EBCM was studied in [22]. Extensions for a periodically corrugated slab were developed in [23].

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