An Electromagnetic Crystal Green Function Multiple Scattering Technique for Arbitrary Polarizations, Lattices, and Defects

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Abstract—A generalized electromagnetic crystal (EC) Green function (GF) multiple scattering technique (MST) that permits the simulation of transverse electric and magnetic waves in 2-D EC devices created by replacing crystal cylinders by nonconforming ones is presented. The EC may be defined on a square or triangular lattice. Both EC and nonconforming devices can be of arbitrary shape and composition. Integral equations in terms of equivalent currents residing on circular surfaces centered about the nonconforming cylinders are constructed using GFs innate to the background EC. Contrary to the (conventional) free-space GF MST, the proposed generalized EC GF MST yields sparse systems of equations that can be solved efficiently by multifrontal methods. A combination of the generalized EC GF MST with a volume integral-equation- and/or finite-element-based scheme to calculate scattering matrices of noncircular/inhomogeneous/plasmonic cylinders yields a very powerful tool that permits simulating wave propagation in a very broad class of EC devices. The generalized EC GF MST is applied to the analysis of a wide variety of practical EC devices, including a third-order Chebyshev bandpass filter, a pair of power dividers, two channel drop filters, a large multiplexer–demultiplexer, a set of bended waveguides, and waveguide filters comprising noncircular or plasmonic cylinders.

Index Terms—Numerical analysis, periodic structures, photonic band gap waveguides, photonic crystals.

I. INTRODUCTION

In recent years, many computational schemes for simulating wave propagation in complex 2-D electromagnetic crystal (EC) devices have been proposed (see [1] and references therein). The EC Green function multiple scattering technique (EC GF MST), which is a new integral-equation-based technique presented in [2], distinguishes itself from its predecessors in terms of its computational efficiency and accuracy. The EC GF MST permits the fast analysis of 2-D EC devices that are obtained by “removing” circular crystal elements from doubly periodic, defectless, and infinite ECs comprising identical homogeneous dielectric/magnetic circular cylinders. Just like the conventional free-space GF MST [3], the EC GF MST solves integral equations in terms of equivalent currents that reside on circular cylindrical surfaces. However, contrary to the conventional free-space GF MST, which associates unknowns with the surfaces of all physical cylindrical elements that define the EC device and then subsequently describes their interactions using a free-space GF, the EC GF MST considers equivalent currents that reside on the cylindrical surfaces of the voids left by removed cylinders and then models their interaction via a GF innate to the surrounding infinite EC. For frequencies in the EC band gap, this EC GF can be precomputed easily using the free-space GF MST by considering a centrally excited, finite, and small EC.

When compared to conventional free-space MSTs for analyzing EC devices, the EC GF MST has four advantages of note. All four relate to the nature of the linear system of equations that results upon discretizing the integral equations considered. First, for the vast majority of EC devices, the number of voids/removed cylinders is much smaller than the number of physical cylinders, which translates to smaller linear systems. Second, the EC GF MST’s system of equations is essentially sparse, whereas that produced by the free-space GF MST is dense; indeed, for frequencies in the EC band gap, the EC GF decays exponentially with distance, and each and every removed cylinder only interacts with its near neighbors. Third, the EC GF MST’s sparse systems of equations can be solved rapidly by multifrontal methods [4], thereby avoiding the excessive iteration counts associated with the iterative solution of the free-space GF MST’s dense systems of equations [5]. Fourth, the EC GF MST is ideally suited to extract an EC device’s S parameters as it enables the implementation of exact modal excitations and absorbing boundary conditions.

Unfortunately, the formulation of the EC GF MST in [2] was quite narrow, thereby unnecessarily limiting its applicability to EC devices that exactly fit the preceding mold. In reality, many EC devices comprise cylindrical elements that are noncircular, inhomogeneous, plasmonic, etc. In addition, many EC devices cannot be constructed by simply removing cylindrical elements from an otherwise defectless and infinite EC as they contain other types of defects, i.e., elements that do not conform to those of the EC background. In [2], the EC GF MST was applied successfully to EC devices comprising a “small” number of irregular circular defects, e.g., circular cylinders with center positions, radii, and/or material parameters that do not conform to those of the EC background. The EC GFs that reflect the presence of the irregular defects were obtained as
This paper describes a "generalized" EC GF MST that broadens the scheme's applicability to virtually arbitrary EC configurations and excitations while retaining the original scheme's benefits. Specifically, the proposed scheme efficiently handles EC devices that are defined on square or triangular lattices supporting both transverse magnetic and electric polarized fields and that are obtained by "replacing" cylindrical elements from a defectless EC with cylindrical elements that "do not conform to those of the EC background." These cylindrical elements can be of arbitrary shape and composition. Contrary to the scheme of [2], which considers only equivalent currents on circular cylindrical surfaces centered about "removed cylindrical elements," the generalized scheme considers equivalent currents on circular cylindrical surfaces centered around "all defects." Although for every type of defect, another type of EC GF is required, the precomputation of all these GFs can be achieved rapidly once a few template EC GFs are known. If combined with volume integral-equation- and/or finite-element-based schemes (e.g., the unimoment method [7], [8]) to calculate the scattering parameters, the proposed algorithm applies to both transverse magnetic and electric to $z$ (TM$_z$ and TE$_z$) fields. Starting from the field-equivalence principle [9], two sets of integral equations in terms of equivalent electric and magnetic currents residing on circular cylindrical surfaces centered about all physical cylindrical elements are derived. The second (interior) set of integral equations permits the elimination of one type of current. For circular and homogeneous cylindrical elements, this relationship can be found in closed form. For arbitrarily shaped and/or composed elements, this relationship has to be established via a volume integral-equation- or finite-element-based method. Upon substituting this relationship in the first (exterior) set of integral equations, the free-space GF is defined, and a dense linear system of equations is obtained.

Consider a finite 2-D EC device comprising $N_c$ infinite $z$-invariant dielectric/magnetic cylindrical elements residing in a homogeneous background medium with constitutive parameters $(\epsilon_b, \mu_b)$ (permittivity, permeability) [Fig. 1(a)]. The cylindrical elements can be of arbitrary shape and material composition. The following nomenclature and terminology are used.

- All sources and fields are assumed to be time harmonic with angular frequency $\omega$; temporal dependencies $e^{j\omega t}$ ($j = \sqrt{-1}$) are suppressed.
- $\rho_j$, $(\rho, \phi)$, and $(\rho, \phi)$ denote the global position vectors, cylindrical coordinates, and cylindrical unit vectors, respectively.
- $\rho_j$ and $(\rho_j, \phi_j)$ denote the position vector and cylindrical coordinates of the center of cylindrical element $j$, $j = 1, \ldots, N_c$, respectively.
- $\rho_j$, $(\rho_j, \phi_j)$, and $(\rho_j, \phi_j)$ denote the position vector, cylindrical coordinates, and cylindrical unit vectors in the coordinate system centered about $\rho_j$, respectively.

This section details a generalized free-space GF MST [2], [3] for characterizing finite EC devices that comprise arbitrarily positioned and arbitrarily shaped dielectric/magnetic cylindrical elements. First, it is shown that by casting Maxwell's equations in terms of generalized fields, currents, and constitutive parameters, the proposed algorithm applies to both transverse magnetic and electric to $z$ (TM$_z$ and TE$_z$) fields. Starting from the field-equivalence principle [9], two sets of integral equations in terms of equivalent electric and magnetic currents residing on circular cylindrical surfaces centered about all physical cylindrical elements are derived. The second (interior) set of integral equations permits the elimination of one type of current. For circular and homogeneous cylindrical elements, this relationship can be found in closed form. For arbitrarily shaped and/or composed elements, this relationship has to be established via a volume integral-equation- or finite-element-based method. Upon substituting this relationship in the first (exterior) set of integral equations, the free-space GF is defined, and a dense linear system of equations is obtained.

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- $\rho_j$, $(\rho_j, \phi_j)$, and $(\rho_j, \phi_j)$ denote the position vector, cylindrical coordinates, and cylindrical unit vectors in the coordinate system centered about $\rho_j$, respectively.
• $(\varepsilon(\rho)\mu(\rho))$ denote the permittivity and permeability at $\rho$, respectively.

• $k_b = \omega \sqrt{\varepsilon_b \mu_b}$ represents the wavenumber in the homogeneous background medium.

• $r_j$, $j = 1, \ldots, N_c$, is the radius of the smallest circle centered about $\mathbf{r}_j^c$ circumscribing circular element $j$.

Let $E^{\text{inc}}(\rho)$ and $H^{\text{inc}}(\rho)$ denote the incident electric and magnetic fields radiated by impressed sources (assumed to reside outside all cylindrical elements) in the absence of any cylindrical elements, respectively. In the presence of the cylindrical elements, the total fields $E^{\text{tot}}(\rho)$ and $H^{\text{tot}}(\rho)$ are observed. The difference between the total and incident fields defines the scattered fields $E^{\text{ sca}}(\rho)$ and $H^{\text{ sca}}(\rho)$. To describe the total and scattered fields, two fields $(\alpha = 1, 2)$ of equivalent electric and magnetic currents $(J^{\alpha}(\rho), K^{\alpha}(\rho))$ residing on the circular surface $S_j$ with radius $r_j$ centered about $\mathbf{r}_j^c$, $j = 1, \ldots, N_c$, are introduced [Fig. 1(b) and (c)]. These currents relate to the total fields on $S_j$ as

\begin{align}
J^{\alpha}(\rho) &= s_{\alpha} \mathbf{r}_j \times H^{\text{tot}}(\rho)|_{\rho \in S_j} \delta(\rho - r_j) \\
K^{\alpha}(\rho) &= -s_{\alpha} \mathbf{r}_j \times E^{\text{tot}}(\rho)|_{\rho \in S_j} \delta(\rho - r_j)
\end{align}

with $s_1 = 1$ and $s_2 = -1$. To analyze wave propagation in 2-D EC devices, it suffices to consider the two noninteracting TM$_2$ and TE$_2$ polarizations. Because of duality, the same formulation applies to both polarizations if Maxwell’s equations are cast in terms of generalized fields $(F^{\tau}(\rho), G^{\tau}(\rho))$ ($\tau = \text{inc}, \text{tot}, \text{ sca}$), currents $(P^{\alpha}(\rho), Q^{\alpha}(\rho))$, and constitutive parameters $(\kappa(\rho), \theta(\rho))$. For the TM$_2$ polarization, these generalized fields, currents, and constitutive parameters are

\begin{align}
F^{\tau}(\rho) &= F^{\tau}(\rho) \hat{z} = E^{\tau}(\rho) \hat{z} \\
G^{\tau}(\rho) &= G^{\tau}(\rho) \hat{\rho}_j + G^{\tau}(\rho) \hat{\phi}_j \\
&= H^{\tau}(\rho) \hat{\rho}_j + H^{\tau}(\rho) \hat{\phi}_j \\
P^{\alpha}(\rho) &= P^{\alpha}(\rho) \hat{z} = J^{\alpha}(\rho) \hat{z} \\
Q^{\alpha}(\rho) &= Q^{\alpha}(\rho) \hat{\phi}_j = K^{\alpha}(\rho) \hat{\phi}_j \\
\kappa(\rho) &= \epsilon(\rho) \\
\theta(\rho) &= \mu(\rho)
\end{align}

while for the TE$_2$ polarization, these are

\begin{align}
F^{\tau}(\rho) &= F^{\tau}(\rho) \hat{z} = -H^{\tau}(\rho) \hat{z} \\
G^{\tau}(\rho) &= G^{\tau}(\rho) \hat{\rho}_j + G^{\tau}(\rho) \hat{\phi}_j \\
&= E^{\tau}(\rho) \hat{\rho}_j + E^{\tau}(\rho) \hat{\phi}_j \\
P^{\alpha}(\rho) &= P^{\alpha}(\rho) \hat{z} = -K^{\alpha}(\rho) \hat{z} \\
Q^{\alpha}(\rho) &= Q^{\alpha}(\rho) \hat{\phi}_j = J^{\alpha}(\rho) \hat{\phi}_j \\
\kappa(\rho) &= \mu(\rho) \\
\theta(\rho) &= \epsilon(\rho).
\end{align}

All other field components vanish. From here on forward, the generalized free-space and EC GF MST will be described in terms of these generalized fields, currents, and constitutive parameters, thereby simultaneously covering both the TM$_2$ and TE$_2$ polarizations.

The following two facts are derived from the field-equivalence theorem (Fig. 1):

1) The currents $\sum_{j=1}^{N_c} P^\alpha_j(\rho) \hat{z}$ and $\sum_{j=1}^{N_c} Q^\alpha_j(\rho) \hat{\phi}_j$, when radiating alongside the impressed sources in an unbounded medium with constitutive parameters $(\kappa_b, \theta_b)$, generate zero fields inside each surface $S_j$ centered about $\mathbf{r}_j^c$ and the total fields $F^{\text{tot}}(\rho) \hat{z}$ and $G^{\text{tot}}(\rho) \hat{\phi}_j + \tilde{G}^{\text{tot}}(\rho) \hat{\phi}_j$ outside all $S_j$.

2) The currents $P^\alpha_j(\rho) \hat{z}$ and $Q^\alpha_j(\rho) \hat{\phi}_j$, when radiating around cylindrical element $j$ placed in an unbounded medium with constitutive parameters $(\kappa_b, \theta_b)$, generate zero fields outside $S_j$ and $F^{\text{tot}}(\rho) \hat{z}$ and $G^{\text{tot}}(\rho) \hat{\phi}_j + \tilde{G}^{\text{tot}}(\rho) \hat{\phi}_j$ inside $S_j$.

If $F^{\text{ sca}}(\rho) \hat{z}$ and $Q^\alpha_j(\rho) \hat{\phi}_j$ denote the $z$-directed field radiated jointly by $P^\alpha_j(\rho) \hat{z}$ and $Q^\alpha_j(\rho) \hat{\phi}_j$ in the homogeneous medium with constitutive parameters $(\kappa_b, \theta_b)$ when $\alpha = 1$, or radiated by $P^\alpha_j(\rho) \hat{z}$ and $Q^\alpha_j(\rho) \hat{\phi}_j$ around the irregular cylinder $j$ placed in the unbounded medium with constitutive parameters $(\kappa_b, \theta_b)$ when $\alpha = 2$, then the preceding statements can be cast as

\begin{align}
F^{\text{inc}}(\rho) + \sum_{j=1}^{N_c} F^{\text{ sca}}_j(\rho) &= 0 \quad \text{if} \quad \rho \in S^\tau_i, \quad i = 1, \ldots, N_c \quad (15) \\
F^{\text{ sca}}_j(\rho) &= 0 \quad \text{if} \quad \rho \in S^\tau_j, \quad j = 1, \ldots, N_c. \quad (16)
\end{align}

Here, $S^\tau_i$ and $S^\tau_j$ denote surfaces residing just inside and outside surface $S^\tau_j$, respectively. To solve (15) and (16), $P^\alpha_j(\rho)$ and $Q^\alpha_j(\rho)$ are expanded as

\begin{align}
P^\alpha_j(\rho) &= s_{\alpha} \sum_{n=-K}^{K} \frac{P^\alpha_n}{2\pi r_j} e^{i\phi n} \delta(\rho - r_j) \\
Q^\alpha_j(\rho) &= s_{\alpha} \sum_{n=-K}^{K} \frac{Q^\alpha_n}{2\pi r_j} e^{i\phi n} \delta(\rho - r_j). \quad (17)
\end{align}

Because $r_j$ is small compared with the wavelength and because the cylindrical elements are assumed sufficiently separated from one another as well as from the impressed sources, the range of the modal index can always be restricted to $n = -K, \ldots, K$, with $K$ being a small positive integer. As detailed in the Appendix, solving (interior problem) (16) yields

\begin{align}
Q^\alpha_j(\rho) &= \sum_{n=-K}^{K} Y^\alpha_n P^\alpha_n(\rho) \quad \text{or} \quad Q^\alpha_j(\rho) = Y^\alpha P^\alpha(\rho). \quad (19)
\end{align}

This relationship permits $F^{\text{ sca}}_j(\rho) \hat{z}$, which is the $z$-directed field radiated jointly by $P^\alpha_j(\rho) \hat{\rho}_j$ and $Q^\alpha_j(\rho) \hat{\phi}_j$ in the homogeneous medium with constitutive parameters $(\kappa_b, \theta_b)$, to be expressed as

\begin{align}
F^{\text{ sca}}_j(\rho) &= \sum_{n=-K}^{K} G^\alpha_n(\rho_j) P^\alpha_n(\rho) \quad (20)
\end{align}

Quantity $G^\alpha_n(\rho_j)$ is the (generalized) free-space GF for a Huygens source with distributed components.
\[ P^I \rho = \frac{1}{2\pi r_j} e^{j m \phi_j} \delta (\rho_j - r_j) \hat{z} \quad \text{and} \quad Q^I \rho = \sum_{m=-K}^{K} (J_m^j/2\pi r_j) e^{j m \phi_j} \delta (\rho_j - r_j) \hat{f}_j, \]

where \( m, n = \frac{1}{2} \) and \( \hat{r}_j \) and \( \hat{f}_j \) denote joint radiating \( J \) and \( H \). Consider a 2-D EC device obtained by replacing \( N_c \) cylindrical elements from an infinite and defectless EC by nonconforming ones. The nomenclature in this section adheres to that of Section II, with the exception that tildes appear on symbols referring to fields, currents, and surfaces centered about irregular cylindrical elements.

Furthermore, the following additional assumptions are made, and the following nomenclature/terminology is used.

- The angular frequency \( \omega \) is assumed to lie within the EC band gap.
- \( \hat{v}_1, \hat{v}_2 \) denotes lattice vectors (Fig. 3) that relate to the Cartesian unit vectors \( \hat{x}, \hat{y} \) as

\[ \hat{v}_1 = a\hat{x}, \quad \hat{v}_2 = a\hat{y} \]
for a square lattice and as
\[ \tilde{v}_1 = \frac{a}{\sqrt{2}} x \]
\[ \tilde{v}_2 = -\frac{a}{2} x + \frac{\sqrt{3}a}{2} y \]
for a triangular lattice.

- \( \tilde{\rho}_{j_1 j_2} \) and \( (\tilde{\rho}_{j_1 j_2}, \tilde{\phi}_{j_1 j_2}) \) denote the position vectors and cylindrical coordinates of the lattice sites, viz. \( \tilde{\rho}_{j_1 j_2} = l_1 v_1 + l_2 v_2, l_1, l_2 = \ldots, -1, 0, 1, \ldots \)
- \( r \) is the radius of the smallest circle centered about a lattice site and circumscribing the corresponding regular cylindrical element.
- \( \tilde{r}_j, j = 1, \ldots, N_r \) is the maximum of \( r \) and \( R \), the radius of the smallest circle centered about a lattice site and circumscribing the irregular cylindrical element \( j \).

Let \( \tilde{F}^{\text{inc}}(\rho) \) and \( \tilde{G}^{\text{inc}}(\rho) \) denote (generalized) incident fields generated by impressed sources (assumed to reside outside all cylindrical elements) that radiate "in the presence of the defectless EC," viz. the infinite EC "without any irregular cylindrical elements." Upon replacing the cylindrical elements, total fields \( \tilde{F}^{\text{tot}}(\rho) \) and \( \tilde{G}^{\text{tot}}(\rho) \) are observed. The difference between the total and incident fields defines the scattered fields \( \tilde{F}^{\text{sca}}(\rho) \) and \( \tilde{G}^{\text{sca}}(\rho) \). To describe the total and scattered fields, two sets \( (\tilde{\mathcal{P}}_\alpha(\rho), \tilde{\mathcal{Q}}_\alpha(\rho)) \) residing on the circular surface \( \tilde{S}_j \) with radius \( \tilde{r}_j \) centered about \( \tilde{\rho}_{j_1 j_2}, j = 1, \ldots, N_r \) are introduced (Fig. 2(b) and (c)). The fields \( \tilde{F}^{\text{tot}}(\rho) \) and \( \tilde{G}^{\text{tot}}(\rho) \) are defined as
\[
\tilde{F}^{\text{tot}}(\rho) = \tilde{F}^{\text{inc}}(\rho) + \tilde{F}^{\text{sca}}(\rho) = 0 \quad \text{if} \quad \rho \in \tilde{S}_j, i = 1, \ldots, N_r
\]
\[
\tilde{G}^{\text{tot}}(\rho) = \tilde{G}^{\text{inc}}(\rho) + \tilde{G}^{\text{sca}}(\rho) = 0 \quad \text{if} \quad \rho \in \tilde{S}_j, j = 1, \ldots, N_r.
\]

Here, \( \tilde{S}_j^- \) and \( \tilde{S}_j^+ \) denote surfaces residing just inside and outside surface \( \tilde{S}_j \), respectively. To solve (30) and (31), \( \tilde{\mathcal{P}}_\alpha(\rho) \) and \( \tilde{\mathcal{Q}}_\alpha(\rho) \) are expanded as
\[
\tilde{\mathcal{P}}_\alpha(\rho) = s_\alpha \sum_{n=-K}^K \tilde{G}^{\text{inc}}(\rho, \rho_{j_1 j_2}^{\text{is}}) \delta \left( \rho_{j_1 j_2} - \tilde{r}_j \right)
\]
\[
\tilde{\mathcal{Q}}_\alpha(\rho) = s_\alpha \sum_{n=-K}^K \tilde{G}^{\text{inc}}(\rho, \rho_{j_1 j_2}^{\text{is}}) \delta \left( \rho_{j_1 j_2} - \tilde{r}_j \right).
\]

This relationship permits \( \tilde{F}^{\text{sca}}(\rho) \) to be expressed as
\[
\tilde{F}^{\text{sca}}(\rho) = \sum_{n=-K}^K \tilde{G}^{\text{inc}}(\rho, \rho_{j_1 j_2}^{\text{is}}) \tilde{P}_n.
\]

With constitutive parameters \( (\kappa_b, \theta_b) \) when \( \alpha = 2 \), the preceding statements can be cast as
\[
\tilde{F}^{\text{inc}}(\rho) + \sum_{j=1}^{N_r} \tilde{F}^{\text{sca,j}}(\rho) = 0 \quad \text{if} \quad \rho \in \tilde{S}_j, i = 1, \ldots, N_r
\]
\[
\tilde{G}^{\text{inc,j}}(\rho) = 0 \quad \text{if} \quad \rho \in \tilde{S}_j, j = 1, \ldots, N_r.
\]

This relationship permits \( \tilde{F}^{\text{sca,j}}(\rho) \) to be expressed as
\[
\tilde{F}^{\text{sca,j}}(\rho) = \sum_{n=-K}^K \tilde{G}^{\text{inc}}(\rho, \rho_{j_1 j_2}^{\text{is}}) \tilde{P}_n.
\]
interactions between sufficiently separated replaced cylinders. Moreover, as shown in [2], such sparse matrix equations can be solved rapidly using multifrontal methods [4].

IV. FAST CALCULATION OF ALL EC GFs

No closed-form expressions exist for the EC GF \( \hat{G}_{n}^{P}(\rho_{ij}^{l'}) \). Fortunately, its numerical calculation is aided by two facts. First, because the EC is periodic, \( \hat{G}_{n}^{P}(\rho_{ij}^{l'}) \) does not depend on the exact location of irregular cylindrical element \( j \). Second, \( \hat{G}_{n}^{P}(\rho_{ij}^{l'}) \) decays exponentially with distance. As a consequence, \( \hat{G}_{n}^{P}(\rho_{ij}^{l'}) \) can be evaluated using the generalized free-space MST scheme by considering a sufficiently large finite EC of \( N_{c} = (2N_{b} + 1)^{2} \) cylindrical elements, which is assumed to be centered about the spatial origin \( \rho = 0 \) and which is excited by the EC. Likewise, define \( \hat{G}_{n}^{Q}(\rho_{ij}^{l'}) \) as the EC GF for a Huygens source with distributed components \( P_{ij}^{l'}(\rho) = (1/2\pi \tilde{r}_{j})e^{i\rho \phi} \delta(\rho - \tilde{r}_{j})\hat{z} \) and \( Q_{ij}^{l'}(\rho) = 0\hat{\phi} \) radiating in the defectless EC. Likewise, define \( \hat{G}_{n}^{Q}(\rho_{ij}^{l'}) \) as the EC GF for a Huygens source with distributed components \( P_{ij}^{l'}(\rho) = 0\hat{z} \) and \( Q_{ij}^{l'}(\rho) = (1/2\pi \tilde{r}_{j})e^{i\rho \phi} \delta(\rho - \tilde{r}_{j})\hat{\phi} \) radiating in the defectless EC. Then, it follows that

\[
\hat{G}_{n}^{P}(\rho, \tilde{r}_{j}) = \hat{G}_{n}^{Q}(\rho_{ij}^{l'}, \tilde{r}_{j}) + \sum_{p=0}^{K} Y_{pn}^{Q} G_{n}^{Q}(\rho_{ij}^{l'}, \tilde{r}_{j}).
\]  

(38)

According to (38), a dense linear system (23) of equations has to be solved for every different radius \( \tilde{r}_{j} \). However, it will be shown here that it is sufficient to calculate only \( \hat{G}_{n}^{P}(\rho, r) \) and \( \hat{G}_{n}^{Q}(\rho, r) \).

Let \( F_{mn}^{P}(l_{1}, l_{2}) \) denote the element of the excitation vector \( F \) in (23) by using the \( n \)th harmonic testing function \( T_{n}^{P}(\rho) \) on the incident fields produced by the Huygens sources on the cylindrical surface with radius \( r \) centered about \( \rho_{i}^{l_{1}l_{2}} \). For the calculation of \( \hat{G}_{n}^{P}(\rho, \tilde{r}_{j}) \), the excitation can be expressed as

\[
P_{n}^{P}(\rho_{ij}^{l'}, \tilde{r}_{j}) = \frac{jk_b}{4} \left[ H_{n}^{(2)}(k_b \tilde{r}_{j}) J_{n}^{r}(k_b \rho_{i}^{l_{1}l_{2}}) - J_{n}^{r}(k_b \tilde{r}_{j}) H_{n}^{(2)}(k_b \rho_{i}^{l_{1}l_{2}}) \right] e^{j(n-m)\phi_{i}^{l_{1}l_{2}}},
\]

if \( l_{1} = l_{2} = 0 \) and \( m = n \)

\[
= 0,
\]

if \( l_{1} = l_{2} = 0 \) and \( m \neq n \)

\[
\text{otherwise}.
\]

(39)

A combination of (38), (42), and (46) shows that all EC GFs are known once \( \hat{G}_{n}^{P}(\rho, r) \) and \( \hat{G}_{n}^{Q}(\rho, r) \) are calculated.
V. EXAMPLES

The examples presented here demonstrate the performance and accuracy of the generalized EC GF MST when applied to the analysis of a wide variety of EC devices including the following:

- devices comprising circular elements with radii and/or constitutive parameters different from those of the background EC (e.g., a third-order Chebyshev bandpass filter or a channel drop filter);
- devices comprising elements that do not snap to the background EC’s lattice (e.g., a power divider);
- devices embedded in a triangular lattice EC that supports TE\(_z\) fields (e.g., a channel drop filter or a bended waveguide);
- devices that are electromagnetically large (e.g., a multiplexer–demultiplexer);
- devices comprising noncircular elements (e.g., EC waveguide filters loaded with elliptical or starlike cylinders);
- devices comprising plasmonic cylinders (e.g., a plasmonic/dielectric EC waveguide filter).

All calculations are carried out on a 2.4-GHz PC. The multifrontal package used to solve system (37) is UMFPACK Version 4.3 [10].

A. EC-Based Third-Order Bandpass Filter

Consider the compact third-order resonant filter depicted in Fig. 4 [11]. The filter is embedded in a square (Cartesian) EC comprising homogeneous dielectric circular cylinders with constitutive parameters \((\varepsilon_\text{c}, \mu_\text{c}) = (11.56\varepsilon_0, \mu_0)\) and radius \(r = 0.2a\) that reside in a free-space background, viz. \((\varepsilon_\text{b}, \mu_\text{b}) = (\varepsilon_0, \mu_0)\). The filter comprises three identical abutting resonators in a waveguide created by removing one row of regular EC cylinders, thereby introducing a row of type-I irregular cylinders. Each resonator comprises a symmetric constellation of nine type-II irregular cylinders that differ from those of the background EC only in terms of their radii (Fig. 4). The filter’s TM\(_z\) transmission spectrum computed using the generalized EC and free-space GF MST is shown in Fig. 5. When using the generalized EC GF MST with \(K = 1\) and \(N_b = 20\) requires only 317 unknowns to describe equivalent currents on all irregular (type I + II) cylinders, 5.4 s to construct EC GFs for type-I and type-II irregular cylinders, 0.05 s to construct modal excitations and boundary conditions, and 0.05 s to fill the sparse interaction matrix and solve the resulting system of equations. Hence, the total time to analyze the filter is only 5.5 s—these CPU times are, just like all that follow, for one frequency. In contrast, application of the free-space GF MST requires 3213 unknowns to describe equivalent currents on all regular and type-II irregular cylinders and 238 s to fill and solve the resulting system of equations, the bulk of which is consumed by the matrix solution process. Clearly, the generalized EC GF MST is far more efficient at analyzing this structure than its classical counterpart.

B. EC-Based Power Divider

Next, consider the T-shaped EC power divider depicted in the inset of Fig. 6 [13]. The divider is embedded in the background EC described in Section V-A. The divider is constructed by removing cylinders from the EC, i.e., all irregular cylinders
are of type-I. The divider’s TM sub-reflection and transmission spectra computed using the generalized EC and free-space GF MSTs are shown in Fig. 6; excellent agreement between both data sets is observed. The divider’s properties are far from desirable but can be improved, as was done in [13], by adjusting the constitutive parameters, radii, and/or center positions of the cylinders near the T-junction (type-II irregular cylinders). One such adjusted design, which was obtained by moving the cylinders in the marked square in Fig. 6 without changing their constitutive parameters or radii, is detailed in the inset of Fig. 7, which shows the transmission spectra of the adjusted divider calculated with the generalized EC and free-space GF MST. Again, excellent agreement between both data sets is observed. Application of the generalized EC GF MST with K = 2 and N_b = 23 requires only 523 unknowns to describe equivalent currents on irregular (type I + II) cylinders, 30 s to construct the type-I and type-II EC GFs, 0.14 s to construct modal excitations and boundary conditions, and 0.5 s to fill the sparse interaction matrix and solve the resulting system of equations. The total CPU time is 30.64 s and is significantly less than that required by the free-space GF MST, which is 134 s. The (deterministic/evolutionary) synthesis of EC devices typically calls for the evaluation of hundreds if not thousands of design candidates; the preceding example demonstrates the potential usefulness of EC GF MST methods for this purpose. Moreover, note that it is only necessary to calculate the EC GFs \( \tilde{G}^P(\rho, r) \) and \( \tilde{G}^Q(\rho, r) \) at the first iteration step. Hence, from the second iteration step on, the evaluation of a design candidate would require less than 1 s!

**C. Channel Drop Filters**

Channel drop filters are key components of many wavelength-division multiplexing communication systems [14]–[18]. Not surprisingly, in recent years, a host of EC-based channel drop filter designs has been proposed; two distinct layouts are analyzed here.

The first filter is depicted in Fig. 8 [16]. This filter is embedded in the EC described in Section V-A. All EC waveguides are formed by removing rows of cylinders. The so-called bus waveguide—through which the EC device is excited—is connected to five output waveguides by distinct resonators. Each resonator comprises five cylinders. The four outermost cylinders in each resonator belong to the background EC; the center cylinder in each resonator is irregular as it has a radius that differs from those in the EC—specific radii are detailed in Fig. 8. Fig. 9 shows the filter’s transmission spectrum calculated via the generalized EC GF MST. This spectrum agrees well with the finite-difference time-domain method result obtained in [16]. With \( K = 1 \), this example calls for 408 equivalent currents. The time to calculate the EC GF and to construct the modal excitations/boundary conditions is the same as that in Section V-A. Filling and solving the sparse linear system of equations take 0.3 s. The total time to analyze the device for one frequency therefore is only 5.75 s. Analysis of the EC device via the free-space GF MST would require more than 9000 unknowns to describe equivalent currents. Needless to say, the CPU time required to analyze the device via the free-space GF MST would be several orders of magnitude larger than that required by the EC GF MST.

The second filter considered is depicted in the inset of Fig. 10 [15]. This filter is embedded in a triangular lattice EC of air holes \((\epsilon_c, \mu_c) = (\epsilon_0, \mu_0)\) of radius \( r = 0.29a \) residing in a homogeneous background with constitutive parameters

![Fig. 7. Structure and transmission spectrum of the adjusted EC power divider.](image)

![Fig. 8. Structure of the five-channel drop filter. The radii of the irregular cylinders are \( r_A = 0.1a, r_B = 0.08a, r_C = 0.065a, r_D = 0.05a, \) and \( r_E = 0 \).](image)

![Fig. 9. Transmission spectrum of the five-channel drop filter.](image)
Fig. 10. Structure and transmission spectrum of the channel drop filter.

Fig. 11. Structure of the large multiplexer–demultiplexer. The radius of a regular cylinder is $r = 0.2a$. The radii of the irregular cylinders are $r_1 = 0.16a$, $r_2 = 0.18a$, $r_3 = 0.22a$, $r_4 = 0.17a$, and $r_5 = 0.14a$. The lengths of the coupling regions are $l_1 = 82a$, $l_2 = 44a$, $l_3 = 48a$, $l_4 = 70a$, and $l_5 = 30a$. ($\epsilon_b, \mu_b = (7.6176\epsilon_0, \mu_0$). The filter comprises two identical EC waveguides that couple through identical resonant cavities. The waveguides and cavities are obtained by filling holes with background material, i.e., the structure only contains type-I irregularities. The cavities each span three hole locations and are separated by two holes. Fig. 10 shows the transmission spectrum calculated with the generalized EC GF MST. Excellent agreement is observed with the spectrum calculated with the finite-difference time-domain technique given in [15]. With $K = 2$ and $N_b = 20$, the generalized EC GF MST requires only 534 unknowns to model equivalent currents on the type-I irregular cylinders, 36 s to calculate the EC GF, 0.13 s to construct modal excitations and boundary conditions, and 0.65 s to fill and solve the resulting system of equations. Hence, the total time to analyze the device is only 30.78 s.

D. Multiplexer–Demultiplexer Based on EC Waveguide Couplers

The ability of the generalized EC GF MST to efficiently analyze large EC devices is demonstrated via its application to the six-channel multiplexer–demultiplexer depicted in Fig. 11. The multiplexer–demultiplexer is embedded in the EC described in Section V-A. The device comprises several EC waveguides that are formed by removing a row of type-I cylinders. In five coupling regions, these waveguides are separated only by one row of type-II cylinders. The waveguide coupling lengths are $l_1 = 82a$, $l_2 = 44a$, $l_3 = 48a$, $l_4 = 70a$, and $l_5 = 30a$. The radii of the type-II cylinders that separate the waveguides are $r_1 = 0.16a$, $r_2 = 0.18a$, $r_3 = 0.22a$, $r_4 = 0.17a$, and $r_5 = 0.14a$. Their permittivity equals that of the EC background cylinders. Fig. 12 shows the transmission spectrum for three of the six output ports. With $K = 1$, analysis of this multiplexer–demultiplexer calls for 3349 equivalent currents. The time to calculate the EC GF and to construct the modal excitations/boundary conditions is the same as in Section V-A. Filling and solving the sparse linear system of equations takes 3 s. Hence, the total time to analyze the multiplexer–demultiplexer is only 8.4 s. For comparison, when modeled with the conventional free-space GF MST, this large multiplexer–demultiplexer would require more than 60,000 equivalent currents.

E. Waveguide Bends

The ability to efficiently guide light along bend waveguides is critical to many photonics applications. In recent years,
many different EC bend waveguide configurations have been proposed; two specific configurations are analyzed here.

First, consider the crude bend waveguide depicted in the inset of Fig. 13 [19]. The waveguide is embedded in the same triangular lattice EC considered in the second example of Section V-C. The bend waveguide is constructed exclusively by filling EC voids; hence, it comprises only type-I irregularities. The waveguide’s TE$_2$ reflection and transmission spectra, which were calculated with the generalized EC GF MST, are shown in Fig. 13. Unfortunately, the power transmission coefficient only exceeds 0.9 in frequencies ranging from $f = 0.2716(c/a)$ to $f = 0.275(c/a)$ and $f = 0.2773(c/a)$ to $f = 0.2783(c/a)$. This example required 302 unknowns to model equivalent currents on type-I irregular cylinders, 36 s to calculate the EC GF, 0.13 s to construct modal excitations and boundary conditions, and 0.15 s to fill and solve the linear system of equations.

Second, consider the optimized bend waveguide depicted in the inset of Fig. 14 [19]. The waveguide portion of the optimized structure is identical to that of the previously described crude bend waveguide; the bend regions, however, differ as type-II irregularities in the form of extra air holes with a radius of 0.14$a$ are added. The optimized waveguide’s TE$_2$ reflection and transmission spectra computed using the EC GF MST are shown in Fig. 14. The optimized waveguide achieves continuous high transmission from $f = 0.2714(c/a)$ up to $f = 0.2795(c/a)$. The (extra) computational cost associated with the analysis of this optimized design is very low. Indeed, assuming that the EC GF $G^\rho(\rho,r)$ and $G^\rho(\rho,r)$ and the modal excitations/boundary conditions computed while analyzing the nonoptimized structure remain available, analysis of the optimized design requires only 0.2 s to fill and store the sparse system of equations for the optimized design.

F. ECS Comprising Noncircular Cylindrical Elements

All previous examples concerned EC devices comprising circular cylinders for which the matrices $Y$ in (19) and (34) are known analytically. Many practical EC devices, however, comprise noncircular elements; deviations from the circular shape may be intended or due to manufacturing imperfections. The ability of the generalized EC GF MST to efficiently simulate such EC devices is demonstrated via its application to the EC waveguide filters depicted in Figs. 15 and 16. Both filters are embedded in a square (Cartesian) EC comprising homogeneous noncircular dielectric cylindrical elements with constitutive parameters $(\epsilon_c, \mu_c) = (11.56, 11.56)$ and comprise a waveguide loaded with three cylindrical elements. The two outermost are identical to those of the EC background. The center element has the same shape but is smaller. The elements in the filter shown in Fig. 15 are ellipses [20]. The major axes of the elliptical cylinders are aligned with the waveguide channel. The large (small) ellipse’s major and minor axes measure 0.4$a$(0.24$a$) and 0.28$a$(0.16$a$), respectively. The cylindrical elements in the filter shown in Fig. 15 are starlike with angle-dependent radius given by

$$r(\theta) = r_1 + r_2 \cos(m \theta), \quad \theta = 0, \ldots, 2\pi. \quad (47)$$

For the large (small) cylindrical elements, $r_1 = 0.16(r_1 = 0.08)$, $r_2 = 0.04(r_2 = 0.02)$, and $m = 10(m = 10)$. Fig. 17 shows the transmission spectrum of both EC filters calculated with the generalized EC GF MST. For both examples, the matrices $Y$ were calculated numerically with a simple volume integral-equation-based scheme [21]. Application of the generalized EC GF MST with $K = 2$ and $N_b = 20$ requires only 192 unknowns to describe the fields in the channel and uses 9.34 s to construct the type-I and type-II EC GFs, 0.14 s to construct
modal excitations and boundary conditions, and 0.03 s to fill and solve the sparse system of equations.

**G. ECS Comprising Plasmonic Elements**

In recent years, the development of optical devices that incorporate plasmonic materials has attracted significant attention [22]. In this section, it will be shown that a bandpass filter can be designed by loading an EC waveguide with plasmonic and dielectric cylinders. Consider the plasmonic/dielectric EC device depicted in Fig. 18. The device is embedded within the EC described in Section V-A. The EC waveguide is loaded with four plasmonic cylinders followed by six dielectric cylinders. The radius and permittivity of the plasmonic cylinders are \( r_1 = 0.2 a \) and \( \epsilon_1 = \epsilon_0 \left[ 1 - \left( \frac{f_p}{f} \right)^2 \right] \), with \( f_p = 0.662 \left( \frac{c}{a} \right) \). The permittivity of the irregular dielectric cylinders is \( \epsilon_2 = 4.9 \epsilon_0 \), respectively.

Fig. 19 shows the transmission spectrum calculated with the generalized EC GF MST. Within the frequency range shown, the four plasmonic cylinders act as a high-pass filter, while the six irregular dielectric cylinders behave as a low-pass filter. Consequently, the combined structure behaves as a bandpass filter. With \( K = 1 \) and \( N_b = 20 \), this device calls for 152 equivalent currents. The time to calculate the EC GF and to construct

**VI. CONCLUSION**

A generalized EC GF MST enabling the characterization of EC devices obtained by replacing cylindrical elements from an infinite doubly periodic and defectless EC by nonconforming ones was presented. Both EC background and nonconforming cylinders can be of arbitrary shape and composition. When combined with a volume integral-equation (or finite-elements)-based scheme to construct scattering matrices of nonconforming cylindrical elements, the generalized EC GF MST can handle a much larger class of EC devices than the original EC GF MST presented in [2]. The versatility of the generalized scheme was demonstrated via its application to several practical examples. An extension of the generalized EC GF MST to the characterization of 3-D EC slab devices, i.e., slab waveguides strategically loaded with 2-D ECs, is under study. Very recently, a 3-D version of the free-space GF MST was published [23]. It is anticipated that a combination of the latter scheme with fast matrix–vector multiplication algorithms will permit the computationally efficient calculation of 3-D EC GFs. This, in turn, will permit the extension of the generalized EC GF MST to
3-D and the subsequent computationally efficient characterization of 3-D EC slab devices.

APPENDIX

This Appendix details the relationship between the scattering matrix $S^j$ and the matrix $\mathbf{\mathcal{Y}}^j$, as used in (19) and (34), of a cylindrical element embedded in a homogeneous medium with constitutive parameters $(\varepsilon_b, \mu_b)$. Consider the cylindrical element depicted in Fig. 20. The scattering matrix $S^j$ relates scattered fields to incident fields cast in terms of Bessel/Hankel functions, i.e., if the incident and scattered fields on $S_j$ are expressed as

$$F^{\text{inc}}(\rho) = \left\{ \begin{array}{ll} -\frac{\omega b}{4} \sum_{n=-K}^{K} H_n^2(k_b r_j) P_n^j + \sqrt{\frac{\omega}{b_k}} H_n^2(k_b r_j) Q_n^j J_n(k_b r_j) e^{j n \phi_j}, & \text{if } \rho_j < r_j \\ -\frac{\omega b}{4} \sum_{n=-K}^{K} J_n(k_b r_j) P_n^j + \sqrt{\frac{\omega}{b_k}} J_n(k_b r_j) Q_n^j H_n^2(k_b r_j) e^{j n \phi_j}, & \text{if } \rho_j > r_j \end{array} \right. \quad (A.4)$$

Third, combine (16), (31), and (A.1)–(A.4) to find the relationship between the unknown $P_n^i$ and $Q_n^i$.

$$Q = -[S^j D_2 + D_4]^{-1}[S^j D_1 + D_3] P \quad (A.9)$$
or

$$\mathbf{\mathcal{Y}}^j = -[S^j D_2 + D_4]^{-1}[S^j D_1 + D_3]. \quad (A.10)$$

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