

IMPROVED FORMULATION OF SCATTERING MATRICES FOR SEMI-ANALYTICAL METHODS THAT IS CONSISTENT WITH CONVENTION

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Abstract—The literature describing scattering matrices for semi-analytical methods almost exclusively contains inefficient formulations and formulations that deviate from long-standing convention in terms of how the scattering parameters are defined. This paper presents a novel and highly improved formulation of scattering matrices that is consistent with convention, more efficient to implement, and more versatile than what has been otherwise presented in the literature. Semi-analytical methods represent a device as a stack of layers that are uniform in the longitudinal direction. Scattering matrices are calculated for each layer and are combined into a single overall scattering matrix that describes propagation through the entire device. Free space gaps with zero thickness are inserted between the layers and the scattering matrices are made to relate fields which exist outside of the layers, but directly on their boundaries. This framework produces symmetric scattering matrices so only two parameters need to be calculated and stored instead of four. It also enables the scattering matrices to be arbitrarily interchanged and reused to describe longitudinally periodic devices more efficiently. Numerical results are presented that show speed and efficiency can be increased by more than an order of magnitude using the improved formulation.

1. INTRODUCTION

Semi-analytical methods are highly efficient methods for solving partial differential equations where part of the problem is solved numerically and the other part analytically. These methods are highly efficient when the analytical direction is very large or complicated. They have

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proven to be a very powerful tool in CEM and offer incredibly efficient analysis of layered devices and structures with longitudinal periodicity. Semi-analytical methods represent devices as a stack of layers. Each of these layers may have arbitrary complexity in the transverse plane, but must be uniform in the longitudinal direction. Typically the x and y axes are made to be the transverse directions while the z axis is made to be the longitudinal direction. Devices with curved geometries are represented by many thin layers using a staircase approximation. Analysis starts by analyzing the cross section of each unique layer to numerically calculate the set of electromagnetic eigen-modes that exists in each layer. The eigen-vectors from this computation contain the amplitude functions of the eigen-modes. The eigen-values are the propagation constants of the eigen-modes which describe how they propagate in the longitudinal direction. After calculation, the eigen-modes can be analytically propagated forward and backward through each layer. Because the longitudinal direction is analytical, the layers can be of any length with no computational burden. Boundary conditions at the interfaces between the layers are enforced by equating tangential field components on either side. In this manner, propagation through the entire device is modeled rigorously.

Figure 1 shows four examples of devices that are efficiently modeled by semi-analytical methods. Figure 1(a) is a microstrip transmission line divided into three layers that are each uniform in the vertical direction. Thin metal features combined with large physical dimensions are ideally suited for efficient analysis by a semi-analytical method. Figure 1(b) is a rib waveguide grating. Often these are composed of hundreds of grating periods, but are very efficiently modeled using a semi-analytical method. Figure 1(c) shows a diffraction grating. These often contain small features in the grating, but with large dimensions in the thicknesses of the layers. This configuration is also ideally suited for analysis by a semi-analytical method. Figures 1(d) and (e) show an electromagnetic band gap (EBG) material that is ten unit cells thick. Each unit cell is further divided into 20 layers using the staircase approximation. The overall device is therefore composed of 200 layers, but only 10 are unique. Semi-analytical methods offer highly efficient analysis of structures like this.

Two popular semi-analytical techniques are the method of lines (MOL) [1, 2] and rigorous coupled-wave analysis (RCWA) [3, 4]. The MOL usually applies the finite-difference method to analyze the layer cross sections, but other techniques like finite-elements can also be used. It is well suited for analyzing metallic structures, multilayer waveguides and longitudinally inhomogeneous waveguide

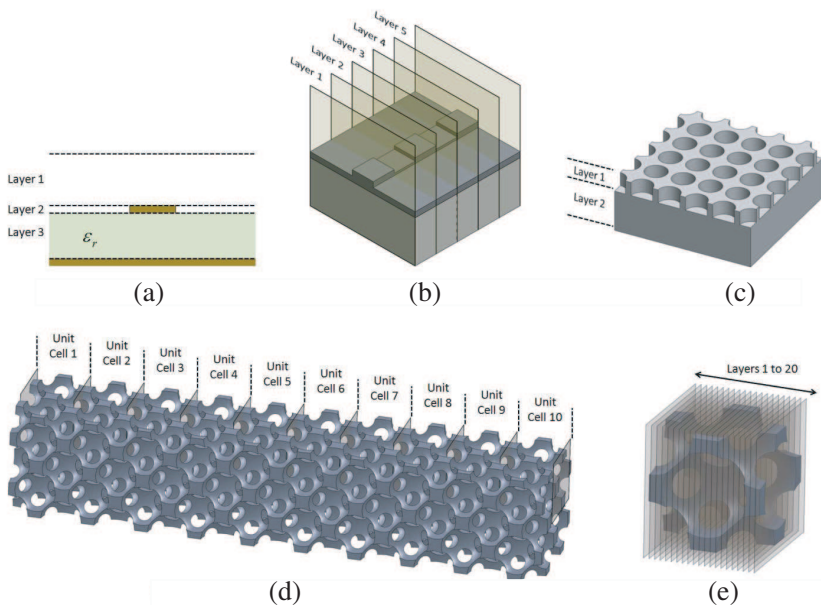


Figure 1. Examples of electromagnetic devices efficiently modeled by semi-analytical methods. (a) Microstrip transmission line. (b) Waveguide grating. (c) Diffraction grating. (d) Electromagnetic band gap material. (e) Layers in the EBG unit cell.

devices. RCWA is the MOL performed in Fourier-space and has become the dominant method for analyzing diffraction from periodic dielectric structures. Instead of using finite-differences, however, the transverse coordinates are discretized using a Fourier transform leading to a plane wave expansion inside each of the layers.

The boundary condition problem that results from semi-analytical methods can be numerically large, particularly when a device is composed of many layers. It is most efficient to use an algorithm that solves the boundary conditions one layer at a time instead of solving all layers simultaneously. To do this, CEM borrowed matrix techniques from transmission line and network theory including transfer matrices [5–7], scattering matrices [8–13], hybrid matrices [14], and impedance matrices [15, 16]. Scattering matrices have emerged as the dominate technique despite speed and efficiency benefits of the other techniques [4, 14, 16].

A scattering matrix enables a complex structure to be represented as a “black box.” It relates waves incident on the box to the waves

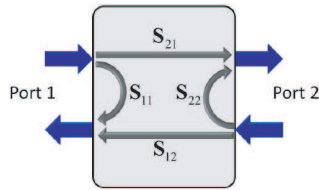


Figure 2. Conventional definition of the scattering parameters.

scattered by the box in either direction. In fact, the electromagnetic properties of any linear structure can be summarized in a scattering matrix. The scattering matrix and physical interpretation of the parameters are illustrated in Figure 2. The \mathbf{S}_{11} parameter quantifies how much of the wave applied to Port 1 reflects from Port 1. \mathbf{S}_{21} quantifies how much of that same applied wave transmits through the device to Port 2. \mathbf{S}_{12} quantifies how much of a wave applied to Port 2 will transmit through to Port 1. Finally, \mathbf{S}_{22} quantifies how much of the second applied wave reflects from Port 2. This can be generalized so that \mathbf{S}_{mn} represents how much of a wave applied to Port n exits from Port m . In this manner it is commonly understood that \mathbf{S}_{11} represents reflection and \mathbf{S}_{21} represents transmission. For symmetric devices, it is expected that $\mathbf{S}_{11} = \mathbf{S}_{22}$ and $\mathbf{S}_{21} = \mathbf{S}_{12}$.

Scattering matrices in electromagnetics became popular in the 1960s when Hewlett Packard introduced the first microwave network analyzers capable of swept amplitude and phase measurements [17]. In addition, several key papers were published around this time popularizing the concept [8, 10]. Today, scattering parameters are so common that the terms “ \mathbf{S}_{11} ” and “ \mathbf{S}_{21} ” are often used synonymously for “reflection” and “transmission.” Despite this strong and long-standing convention, the CEM community is adopting inefficient and unconventional formalisms for scattering matrices for use in semi-analytical methods [7, 16, 18–33]. The majority of the literature on this topic appears in optics journals, where the benefits of semi-analytical methods are more pronounced and the use of scattering parameters in experiments is less common. This, however, is not a universal convention used in optics; see Ref. [34]. Most of these papers define \mathbf{S}_{11} and \mathbf{S}_{22} as transmission quantities and \mathbf{S}_{12} and \mathbf{S}_{21} as reflection quantities. This practice is confusing, deviates sharply from convention, and it is no longer reliable to interpret the indices of the scattering parameters to understand what is being quantified. Further, the scattering matrices being adopted for semi-analytical methods are numerically inefficient and their order cannot be arbitrarily interchanged. This feature can be very useful to efficiently

model longitudinally inhomogeneous structures. The unconventional scattering matrices also relate fields outside of the layer on one side to fields inside the layer on the other side. This leads to scattering matrices that are inherently asymmetric regardless of what materials are placed outside of the layer.

This paper formulates a highly improved version of scattering matrices for semi-analytical methods that also adopts the proper convention for the definition of the scattering parameters. The new formulation is stable and accurate for both 2D and 3D simulations. When the layers are composed of materials that obey reciprocity, implementation is more efficient because the scattering matrices are symmetric. In this case, fewer calculations have to be performed and fewer parameters have to be stored in memory. Implementation is more versatile because the order of the layers can be arbitrarily interchanged to describe complex and longitudinally periodic devices. Discussion starts by establishing the numerical framework for scattering matrices in semi-analytical methods and unifying the MOL and RCWA. Based on this framework, formulas to calculate scattering matrices for the individual layers are derived along with the procedures to combine multiple scattering matrices into a single scattering matrix. Equations used to calculate transmitted and reflected fields are presented along with an equation for performing dispersion analysis of longitudinally periodic structures. Lastly, a numerical example is presented to illustrate the utility and efficiency of the improved scattering matrix formulation.

2. SEMI-ANALYTICAL FRAMEWORK

Formulation of a rigorous semi-analytical method begins with Maxwell's equations describing the fields inside a single uniform layer of the device. The magnitudes of the electric and magnetic fields are related through the material impedance η . For numerical robustness, it is good practice to normalize the field quantities so they are of the same order of magnitude. To do this here, the magnetic field will be normalized according to $\vec{\tilde{H}} = -j\eta_0\vec{H}$ where $j = \sqrt{-1}$ and η_0 is the impedance of free space. Maxwell's equations with the normalized magnetic field are written as

$$\nabla \times \vec{E} = k_0\mu_r\vec{\tilde{H}} \quad (1)$$

$$\nabla \times \vec{\tilde{H}} = k_0\varepsilon_r\vec{E} \quad (2)$$

The term k_0 is the free space wave number and is equal to $2\pi/\lambda_0$, where λ_0 is the free space wavelength. The terms μ_r and ε_r are functions that

describe the relative permeability and relative permittivity in the cross section of the layer. Eqs. (1) and (2) are vector equations that can be expanded into a set of six coupled partial differential equations. After eliminating the longitudinal field components E_z and \tilde{H}_z using back substitution, the remaining four equations are discretized in the x - y plane and cast into the following matrix form.

$$\frac{\partial}{\partial z} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} = k_0 \mathbf{P} \begin{bmatrix} \tilde{\mathbf{h}}_x \\ \tilde{\mathbf{h}}_y \end{bmatrix} \quad (3)$$

$$\frac{\partial}{\partial z} \begin{bmatrix} \tilde{\mathbf{h}}_x \\ \tilde{\mathbf{h}}_y \end{bmatrix} = k_0 \mathbf{Q} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} \quad (4)$$

For the MOL, \mathbf{e}_x , \mathbf{e}_y , $\tilde{\mathbf{h}}_x$ and $\tilde{\mathbf{h}}_y$ are column vectors containing the field components at discrete points across the transverse plane at points described by the Yee grid [35, 36]. For materials described by diagonal tensors, the matrices \mathbf{P} and \mathbf{Q} are computed according to

$$\mathbf{P}_{\text{MOL}} = \begin{bmatrix} -\mathbf{D}_x^e \varepsilon_{zz}^{-1} \mathbf{D}_x^h & (\mu_{yy} + \mathbf{D}_x^e \varepsilon_{zz}^{-1} \mathbf{D}_x^h) \\ -(\boldsymbol{\mu}_{xx} + \mathbf{D}_y^e \varepsilon_{zz}^{-1} \mathbf{D}_y^h) & \mathbf{D}_y^e \varepsilon_{zz}^{-1} \mathbf{D}_y^h \end{bmatrix} \quad (5)$$

$$\mathbf{Q}_{\text{MOL}} = \begin{bmatrix} -\mathbf{D}_x^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_y^e & (\varepsilon_{yy} + \mathbf{D}_x^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_x^e) \\ -(\varepsilon_{xx} + \mathbf{D}_y^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_y^e) & \mathbf{D}_y^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_x^e \end{bmatrix} \quad (6)$$

The matrices \mathbf{D}_x^e and \mathbf{D}_y^e are banded matrices that calculate spatial derivatives of the electric fields across the grid [37]. The matrices \mathbf{D}_x^h and \mathbf{D}_y^h are also banded matrices, but calculate spatial derivatives of the magnetic fields across the grid. These matrices are related through $\mathbf{D}_x^e = -(\mathbf{D}_x^h)^H$ and $\mathbf{D}_y^e = -(\mathbf{D}_y^h)^H$ where the superscript H indicates a complex transpose, or Hermitian operation. The terms ε_{xx} , ε_{yy} , ε_{zz} , $\boldsymbol{\mu}_{xx}$, $\boldsymbol{\mu}_{yy}$ and $\boldsymbol{\mu}_{zz}$ are diagonal matrices that perform point-by-point multiplications on the field terms. The dielectric function $\varepsilon_{xx}(x, y)$, for example, is reshaped into to a linear array and placed along the diagonal of a sparse matrix to construct ε_{xx} .

For RCWA, \mathbf{e}_x , \mathbf{e}_y , $\tilde{\mathbf{h}}_x$ and $\tilde{\mathbf{h}}_y$ are column vectors containing the amplitudes of the spatial harmonics of the field expansion. For materials described by diagonal tensors, the matrices \mathbf{P} and \mathbf{Q} are computed according to

$$\mathbf{P}_{\text{RCWA}} = \begin{bmatrix} -\mathbf{K}_x [\varepsilon_{zz}^*]^{-1} \mathbf{K}_y & ([\boldsymbol{\mu}_{yy}^*] - \mathbf{K}_x [\varepsilon_{zz}^*]^{-1} \mathbf{K}_x) \\ -([\boldsymbol{\mu}_{xx}^*] - \mathbf{K}_y [\varepsilon_{zz}^*]^{-1} \mathbf{K}_y) & \mathbf{K}_y [\varepsilon_{zz}^*]^{-1} \mathbf{K}_x \end{bmatrix} \quad (7)$$

$$\mathbf{Q}_{\text{RCWA}} = \begin{bmatrix} -\mathbf{K}_x [\boldsymbol{\mu}_{zz}^*]^{-1} \mathbf{K}_y & ([\varepsilon_{yy}^*] - \mathbf{K}_x [\boldsymbol{\mu}_{zz}^*]^{-1} \mathbf{K}_x) \\ -([\varepsilon_{xx}^*] - \mathbf{K}_y [\boldsymbol{\mu}_{zz}^*]^{-1} \mathbf{K}_y) & \mathbf{K}_y [\boldsymbol{\mu}_{zz}^*]^{-1} \mathbf{K}_x \end{bmatrix} \quad (8)$$

The matrices \mathbf{K}_x and \mathbf{K}_y are diagonal matrices containing the wave vector components of the plane wave expansion. The matrices $[\epsilon_{xx}^*]$, $[\epsilon_{yy}^*]$, $[\epsilon_{zz}^*]$, $[\mu_{xx}^*]$, $[\mu_{yy}^*]$, and $[\mu_{zz}^*]$ are full matrices that perform two-dimensional convolutions in Fourier-space. For one-dimensional gratings the convolution matrices will have Toeplitz symmetry. To improve convergence of the algorithm, fast Fourier factorization rules should be incorporated into the \mathbf{P} and \mathbf{Q} matrices [38–41].

Given Eqs. (3) and (4), a matrix wave equation can be derived for the electric field quantities. This is accomplished by differentiating Eq. (3) with respect to z and then eliminating the magnetic field by substituting Eq. (4) into the new expression. After normalizing the z coordinate according to $z' = k_0 z$, the matrix wave equation is

$$\frac{\partial^2}{\partial z'^2} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} - \mathbf{\Omega}^2 \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \quad (9)$$

$$\mathbf{\Omega}^2 = \mathbf{PQ} \quad (10)$$

After calculating the eigen-vectors \mathbf{W} and the eigen-values λ^2 of the matrix $\mathbf{\Omega}^2$, the general solution to Eq. (9) can be written as

$$\psi(z') = \begin{bmatrix} \mathbf{e}_x(z') \\ \mathbf{e}_y(z') \\ \tilde{\mathbf{h}}_x(z') \\ \tilde{\mathbf{h}}_y(z') \end{bmatrix} = \begin{bmatrix} \mathbf{W} & \mathbf{W} \\ -\mathbf{V} & \mathbf{V} \end{bmatrix} \begin{bmatrix} e^{-\lambda z'} & \mathbf{0} \\ \mathbf{0} & e^{\lambda z'} \end{bmatrix} \begin{bmatrix} \mathbf{c}^+ \\ \mathbf{c}^- \end{bmatrix} \quad (11)$$

$$\mathbf{V} = \mathbf{QW}\lambda^{-1} \quad (12)$$

In this equation, \mathbf{W} describes the eigen-modes of the electric fields and \mathbf{V} describes the eigen-modes of the magnetic fields. The exponential terms $e^{-\lambda z'}$ and $e^{\lambda z'}$ describe forward and backward propagation through the layer respectively. The column vectors \mathbf{c}^+ and \mathbf{c}^- are amplitude coefficients of the eigen-modes in the forward and backward directions respectively.

3. REFORMULATION OF SCATTERING MATRICES

Equation (11) can be used to calculate the field throughout a layer that is uniform in the z -direction. All real devices are composed of multiple layers and eigen-modes must be calculated separately for each layer. The eigen-vectors are the amplitude functions of the modes while the eigen-values are the propagation constants. With this information, the field can be analytically propagated through each of

the layers. To connect the layers, boundary conditions are enforced by equating the tangential components of the fields on either side of the interfaces. In this manner, propagation through the entire device can be described rigorously. To solve the boundary condition problem efficiently, scattering matrices have arisen as the most popular method and solve the boundary condition problem one layer at a time instead of all layers simultaneously. To be consistent with convention, we define the scattering matrix for the i th layer as

$$\begin{bmatrix} \mathbf{c}'_1^- \\ \mathbf{c}'_2^+ \end{bmatrix} = \begin{bmatrix} \mathbf{S}_{11}^{(i)} & \mathbf{S}_{12}^{(i)} \\ \mathbf{S}_{21}^{(i)} & \mathbf{S}_{22}^{(i)} \end{bmatrix} \begin{bmatrix} \mathbf{c}'_1^+ \\ \mathbf{c}'_2^- \end{bmatrix} \quad (13)$$

When the materials comprising the layer have no loss or gain, energy must be conserved. This makes the scattering matrix \mathbf{S} unitary where it obeys $\mathbf{S}^* \mathbf{S} = \mathbf{S} \mathbf{S}^*$ and $\mathbf{S}^* = \mathbf{S}^{-1}$.

Figure 3 illustrates the generalized mathematical framework of the improved scattering matrix for the i th layer. This construction is different than what is found in the literature in that it is consistent with convention and relates fields that exist outside of the layer on both sides. In this framework, the materials outside of the layer can be anything and can even be different on either side. The scattering parameters $\mathbf{S}_{11}^{(i)}$, $\mathbf{S}_{12}^{(i)}$, $\mathbf{S}_{21}^{(i)}$, and $\mathbf{S}_{22}^{(i)}$ are square matrices that quantify how energy scatters among the different eigen-modes. The column vectors \mathbf{c}'_1^+ , \mathbf{c}'_1^- , \mathbf{c}'_2^+ , and \mathbf{c}'_2^- contain the mode coefficients of the field immediately outside of the i th layer in both forward and backward directions. Their subscripts indicate which side of the layer is being described while the signs in their superscripts indicate the direction of propagation. Finally, it should be noted how the mode coefficients relate to position along the z axis. From Eq. (11), it can be seen that the mode coefficients completely describe the field when the local z coordinate is zero. Away from this point it is necessary to consider propagation quantified by the exponential terms in Eq. (11). We are free to choose where $z = 0$ in each layer without loss of generality because the values of the mode coefficients have not yet been calculated. In order to place the external fields exactly on the boundaries of the layer, we define the local z coordinates in the external regions to be zero at the interfaces. The mode coefficients of the external fields contain apostrophes to highlight they are quantities which reside outside of the layer. They are positioned in Figure 3 consistent with where they completely define the field without needing the complex exponential terms.

To derive expressions for the scattering parameters for the i th layer, we start by writing two expressions that enforce the boundary

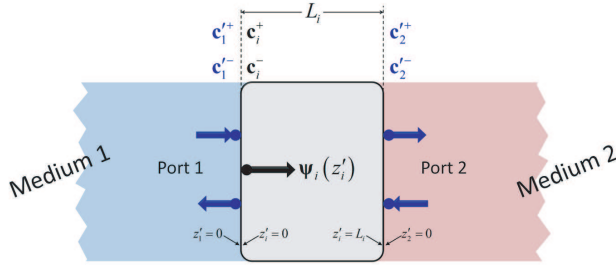


Figure 3. Mathematical framework for the scattering matrix of the i th layer.

conditions at the first and second interfaces. Respectively, these are

$$\begin{bmatrix} \mathbf{W}_1 & \mathbf{W}_1 \\ \mathbf{V}_1 & -\mathbf{V}_1 \end{bmatrix} \begin{bmatrix} \mathbf{c}'_1^+ \\ \mathbf{c}'_1^- \end{bmatrix} = \begin{bmatrix} \mathbf{W}_i & \mathbf{W}_i \\ \mathbf{V}_i & -\mathbf{V}_i \end{bmatrix} \begin{bmatrix} \mathbf{c}_i^+ \\ \mathbf{c}_i^- \end{bmatrix} \quad (14)$$

$$\begin{bmatrix} \mathbf{W}_i & \mathbf{W}_i \\ \mathbf{V}_i & -\mathbf{V}_i \end{bmatrix} \begin{bmatrix} e^{-\lambda_i k_0 L_i} & \mathbf{0} \\ \mathbf{0} & e^{\lambda_i k_0 L_i} \end{bmatrix} \begin{bmatrix} \mathbf{c}_i^+ \\ \mathbf{c}_i^- \end{bmatrix} = \begin{bmatrix} \mathbf{W}_2 & \mathbf{W}_2 \\ \mathbf{V}_2 & -\mathbf{V}_2 \end{bmatrix} \begin{bmatrix} \mathbf{c}'_2^+ \\ \mathbf{c}'_2^- \end{bmatrix} \quad (15)$$

Next, Eq. (14) is combined with Eq. (15) and the terms are rearranged to put the expression in the form of Eq. (13). When this done, the scattering matrix elements are found to be

$$\begin{aligned} \mathbf{S}_{11}^{(i)} &= (\mathbf{A}_{i1} - \mathbf{X}_i \mathbf{B}_{i2} \mathbf{A}_{i2}^{-1} \mathbf{X}_i \mathbf{B}_{i1})^{-1} (\mathbf{X}_i \mathbf{B}_{i2} \mathbf{A}_{i2}^{-1} \mathbf{X}_i \mathbf{A}_{i1} - \mathbf{B}_{i1}) \\ \mathbf{S}_{12}^{(i)} &= (\mathbf{A}_{i1} - \mathbf{X}_i \mathbf{B}_{i2} \mathbf{A}_{i2}^{-1} \mathbf{X}_i \mathbf{B}_{i1})^{-1} \mathbf{X}_i (\mathbf{A}_{i2} - \mathbf{B}_{i2} \mathbf{A}_{i2}^{-1} \mathbf{B}_{i2}) \\ \mathbf{S}_{21}^{(i)} &= (\mathbf{A}_{i2} - \mathbf{X}_i \mathbf{B}_{i1} \mathbf{A}_{i1}^{-1} \mathbf{X}_i \mathbf{B}_{i2})^{-1} \mathbf{X}_i (\mathbf{A}_{i1} - \mathbf{B}_{i1} \mathbf{A}_{i1}^{-1} \mathbf{B}_{i1}) \\ \mathbf{S}_{22}^{(i)} &= (\mathbf{A}_{i2} - \mathbf{X}_i \mathbf{B}_{i1} \mathbf{A}_{i1}^{-1} \mathbf{X}_i \mathbf{B}_{i2})^{-1} (\mathbf{X}_i \mathbf{B}_{i1} \mathbf{A}_{i1}^{-1} \mathbf{X}_i \mathbf{A}_{i2} - \mathbf{B}_{i2}) \end{aligned} \quad (16)$$

$$\begin{aligned} \mathbf{A}_{ij} &= \mathbf{W}_i^{-1} \mathbf{W}_j + \mathbf{V}_i^{-1} \mathbf{V}_j \\ \mathbf{B}_{ij} &= \mathbf{W}_i^{-1} \mathbf{W}_j - \mathbf{V}_i^{-1} \mathbf{V}_j \end{aligned} \quad (17)$$

$$\mathbf{X}_i = e^{-\lambda_i k_0 L_i} \quad (18)$$

It is important to note that the scattering parameters are not only a function of the materials inside the layer, but also the materials on either side of the layer. This makes intuitive sense since the external materials must be known in order to quantify reflection and transmission. It does, however, prevent the scattering matrices from having the ability to be arbitrarily interchanged. Conceptually, this problem is overcome by the novel approach of separating all of the layers composing the device with gaps composed of free space [33]. As

long as these gaps are given zero thickness, they will have no effect on the performance of the device. In other words, two layers separated by a zero thickness gap is physically the same thing as two adjacent layers without any separation. Numerically, this is accomplished by letting medium 1 and medium 2 in Figure 3 be free space. In this setting, the scattering matrices can be arbitrarily interchanged because each layer is surrounded by free space and all of the scattering matrices are relating mode coefficients of fields that exist in the same medium. Given the eigen-modes \mathbf{W}_0 and \mathbf{V}_0 for free space, we have $\mathbf{W}_0 = \mathbf{W}_1 = \mathbf{W}_2$ and $\mathbf{V}_0 = \mathbf{V}_1 = \mathbf{V}_2$ so Eqs. (16) and (17) reduce to

$$\begin{aligned} \mathbf{S}_{11}^{(i)} = \mathbf{S}_{22}^{(i)} &= (\mathbf{A}_i - \mathbf{X}_i \mathbf{B}_i \mathbf{A}_i^{-1} \mathbf{X}_i \mathbf{B}_i)^{-1} (\mathbf{X}_i \mathbf{B}_i \mathbf{A}_i^{-1} \mathbf{X}_i \mathbf{A}_i - \mathbf{B}_i) \\ \mathbf{S}_{12}^{(i)} = \mathbf{S}_{21}^{(i)} &= (\mathbf{A}_i - \mathbf{X}_i \mathbf{B}_i \mathbf{A}_i^{-1} \mathbf{X}_i \mathbf{B}_i)^{-1} \mathbf{X}_i (\mathbf{A}_i - \mathbf{B}_i \mathbf{A}_i^{-1} \mathbf{B}_i) \end{aligned} \quad (19)$$

$$\begin{aligned} \mathbf{A}_i &= \mathbf{W}_i^{-1} \mathbf{W}_0 + \mathbf{V}_i^{-1} \mathbf{V}_0 \\ \mathbf{B}_i &= \mathbf{W}_i^{-1} \mathbf{W}_0 - \mathbf{V}_i^{-1} \mathbf{V}_0 \end{aligned} \quad (20)$$

When each layer is surrounded by free space and composed of materials that themselves obey reciprocity, the result scattering matrices become symmetric. For this reason, only two of the four scattering parameters have to be calculated for each layer. This reduces memory requirements and makes computation faster and more efficient.

4. MULTILAYER DEVICES

4.1. Redheffer Star Product

To model a device composed of multiple layers, it is necessary to combine multiple scattering matrices into a single scattering matrix. It is important to note that the combined scattering matrix typically does not have any symmetry so it becomes necessary to store all four scattering parameters in the combined matrices. Two scattering matrices can be combined as illustrated in Figure 4 using the Redheffer star product [16, 26, 42]. It is derived by writing Eq. (13) for two adjacent layers, combining the two equations to eliminate the common mode coefficients, and then rearranging terms to relate the mode coefficients of the outermost ports.

Given a scattering matrix $\mathbf{S}^{(A)}$ that is to be followed by a scattering matrix $\mathbf{S}^{(B)}$, the combined scattering matrix can be calculated using the star product $\mathbf{S}^{(AB)} = \mathbf{S}^{(A)} \otimes \mathbf{S}^{(B)}$ as follows.

$$\begin{bmatrix} \mathbf{S}_{11}^{(AB)} & \mathbf{S}_{12}^{(AB)} \\ \mathbf{S}_{21}^{(AB)} & \mathbf{S}_{22}^{(AB)} \end{bmatrix} = \begin{bmatrix} \mathbf{S}_{11}^{(A)} & \mathbf{S}_{12}^{(A)} \\ \mathbf{S}_{21}^{(A)} & \mathbf{S}_{22}^{(A)} \end{bmatrix} \otimes \begin{bmatrix} \mathbf{S}_{11}^{(B)} & \mathbf{S}_{12}^{(B)} \\ \mathbf{S}_{21}^{(B)} & \mathbf{S}_{22}^{(B)} \end{bmatrix} \quad (21)$$

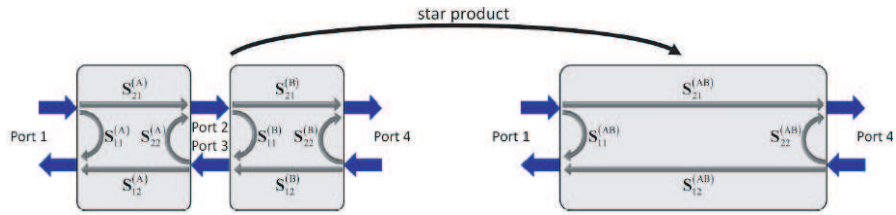


Figure 4. Concept of combining scattering matrices with the star product.

$$\begin{aligned}
 \mathbf{S}_{11}^{(AB)} &= \mathbf{S}_{11}^{(A)} + \mathbf{S}_{12}^{(A)} \left[\mathbf{I} - \mathbf{S}_{11}^{(B)} \mathbf{S}_{22}^{(A)} \right]^{-1} \mathbf{S}_{11}^{(B)} \mathbf{S}_{21}^{(A)} \\
 \mathbf{S}_{12}^{(AB)} &= \mathbf{S}_{12}^{(A)} \left[\mathbf{I} - \mathbf{S}_{11}^{(B)} \mathbf{S}_{22}^{(A)} \right]^{-1} \mathbf{S}_{12}^{(B)} \\
 \mathbf{S}_{21}^{(AB)} &= \mathbf{S}_{21}^{(B)} \left[\mathbf{I} - \mathbf{S}_{22}^{(A)} \mathbf{S}_{11}^{(B)} \right]^{-1} \mathbf{S}_{21}^{(A)} \\
 \mathbf{S}_{22}^{(AB)} &= \mathbf{S}_{22}^{(B)} + \mathbf{S}_{21}^{(B)} \left[\mathbf{I} - \mathbf{S}_{22}^{(A)} \mathbf{S}_{11}^{(B)} \right]^{-1} \mathbf{S}_{22}^{(A)} \mathbf{S}_{12}^{(B)}
 \end{aligned} \tag{22}$$

4.2. Doubling Algorithm for Scattering Matrices

For devices that are periodic in the longitudinal direction, the improved scattering matrix formulation enables a very simple, fast and efficient algorithm to model devices composed of many hundreds or thousands of periods [2]. First, the scattering matrix for one unit cell is constructed, which may be the combination of any number of scattering matrices. Second, it is combined with itself using the star product to obtain a scattering matrix that describes two unit cells in cascade. The new scattering matrix is combined with itself to obtain a scattering matrix that describes four unit cells. This process is continued until an overall scattering matrix is calculated that describes the desired number of unit cells in powers of two. Figure 5 illustrates the doubling procedure.

It is possible to generalize this procedure to calculate scattering matrices for any integer number of cascaded unit cells. This is accomplished by converting the desired number of unit cells into binary and constructing the overall scattering matrix from only the doubled scattering matrices that correspond to the required binary digits. For example, suppose a scattering matrix is needed to describe a device composed of 166 unit cells. Converting this number to binary we get 10100110. Each binary digit of ‘1’ indicates a doubled scattering matrix that is needed to model exactly 166 unit cells. Altogether, the

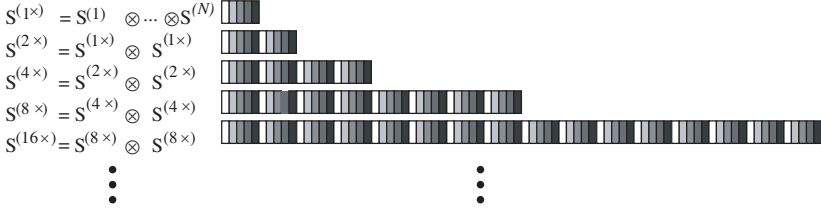


Figure 5. Doubling procedure.

combined scattering matrix is

$$\begin{aligned}
 \mathbf{S}^{(\times 166)} &= \mathbf{S}^{(\times 128)} \otimes \cancel{\mathbf{S}^{(\times 64)}} \otimes \mathbf{S}^{(\times 32)} \otimes \cancel{\mathbf{S}^{(\times 16)}} \otimes \cancel{\mathbf{S}^{(\times 8)}} \otimes \mathbf{S}^{(\times 4)} \otimes \mathbf{S}^{(\times 2)} \otimes \cancel{\mathbf{S}^{(\times 1)}} \\
 &= \mathbf{S}^{(\times 128)} \otimes \mathbf{S}^{(\times 32)} \otimes \mathbf{S}^{(\times 4)} \otimes \mathbf{S}^{(\times 2)}
 \end{aligned} \tag{23}$$

4.3. External Regions

After the entire device has been reduced to a single scattering matrix using the procedures described above, the device resides in free space by default. Sometimes it is desired to have a material other than free space outside of the device as an infinite half-space. This is common practice in photonics where a device resides on a very thick substrate. To account for this, additional scattering matrices must be incorporated that “connect” the device to the external regions. Given a scattering matrix $\mathbf{S}^{(\text{ref})}$ that connects the device to the reflection region and a scattering matrix $\mathbf{S}^{(\text{trn})}$ that connects the device to the transmission region, the final scattering matrix is calculated according to Eq. (24) using the star product.

$$\mathbf{S}^{(\text{global})} = \mathbf{S}^{(\text{ref})} \otimes \underbrace{\left[\mathbf{S}^{(1)} \otimes \mathbf{S}^{(2)} \otimes \dots \otimes \mathbf{S}^{(N)} \right]}_{\text{Device in free space}} \otimes \mathbf{S}^{(\text{trn})} \tag{24}$$

It is now necessary to derive equations to calculate the scattering matrices which connect the device to the external regions. In order to preserve the correct phase information in the global scattering matrix, the additional scattering matrices are made to describe layers with zero thickness. This is in addition to including free space gaps with zero thickness. The concept is illustrated in Figure 6. By definition, $\mathbf{S}^{(\text{ref})}$ and $\mathbf{S}^{(\text{trn})}$ are not symmetric so all four scattering parameters must be calculated and so Eqs. (16)–(18) are used to derive them.

The equations to calculate the four scattering parameters for $\mathbf{S}^{(\text{ref})}$ are derived from Eqs. (16)–(18) by letting $L = 0$, $\mathbf{W}_1 = \mathbf{W}_i = \mathbf{W}_{\text{ref}}$,

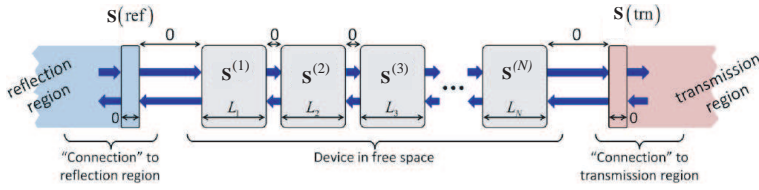


Figure 6. Construction of the global scattering matrix and connection to external regions.

$\mathbf{V}_1 = \mathbf{V}_i = \mathbf{V}_{\text{ref}}$, $\mathbf{W}_2 = \mathbf{W}_0$ and $\mathbf{V}_2 = \mathbf{V}_0$. This scattering matrix is only needed when the reflection region is composed of a material other than free space.

$$\begin{aligned}
 \mathbf{S}_{11}^{(\text{ref})} &= -\mathbf{A}_{\text{ref}}^{-1} \mathbf{B}_{\text{ref}} \\
 \mathbf{S}_{12}^{(\text{ref})} &= 2\mathbf{A}_{\text{ref}}^{-1} \\
 \mathbf{S}_{21}^{(\text{ref})} &= 0.5 (\mathbf{A}_{\text{ref}} - \mathbf{B}_{\text{ref}} \mathbf{A}_{\text{ref}}^{-1} \mathbf{B}_{\text{ref}}) \\
 \mathbf{S}_{22}^{(\text{ref})} &= \mathbf{B}_{\text{ref}} \mathbf{A}_{\text{ref}}^{-1}
 \end{aligned} \tag{25}$$

$$\begin{aligned}
 \mathbf{A}_{\text{ref}} &= \mathbf{W}_0^{-1} \mathbf{W}_{\text{ref}} + \mathbf{V}_0^{-1} \mathbf{V}_{\text{ref}} \\
 \mathbf{B}_{\text{ref}} &= \mathbf{W}_0^{-1} \mathbf{W}_{\text{ref}} - \mathbf{V}_0^{-1} \mathbf{V}_{\text{ref}}
 \end{aligned} \tag{26}$$

The equations to calculate the four scattering parameters for $\mathbf{S}^{(\text{trn})}$ are derived from Eqs. (16)–(18) by letting $L = 0$, $\mathbf{W}_1 = \mathbf{W}_0$, $\mathbf{V}_1 = \mathbf{V}_0$, $\mathbf{W}_i = \mathbf{W}_2 = \mathbf{W}_{\text{trn}}$ and $\mathbf{V}_i = \mathbf{V}_2 = \mathbf{V}_{\text{trn}}$. This scattering matrix is only needed when the transmission region is composed of a material other than free space.

$$\begin{aligned}
 \mathbf{S}_{11}^{(\text{trn})} &= \mathbf{B}_{\text{trn}} \mathbf{A}_{\text{trn}}^{-1} \\
 \mathbf{S}_{12}^{(\text{trn})} &= 0.5 (\mathbf{A}_{\text{trn}} - \mathbf{B}_{\text{trn}} \mathbf{A}_{\text{trn}}^{-1} \mathbf{B}_{\text{trn}}) \\
 \mathbf{S}_{21}^{(\text{trn})} &= 2\mathbf{A}_{\text{trn}}^{-1} \\
 \mathbf{S}_{22}^{(\text{trn})} &= -\mathbf{A}_{\text{trn}}^{-1} \mathbf{B}_{\text{trn}}
 \end{aligned} \tag{27}$$

$$\begin{aligned}
 \mathbf{A}_{\text{trn}} &= \mathbf{W}_0^{-1} \mathbf{W}_{\text{trn}} + \mathbf{V}_0^{-1} \mathbf{V}_{\text{trn}} \\
 \mathbf{B}_{\text{trn}} &= \mathbf{W}_0^{-1} \mathbf{W}_{\text{trn}} - \mathbf{V}_0^{-1} \mathbf{V}_{\text{trn}}
 \end{aligned} \tag{28}$$

4.4. Scattering Matrix Algorithm

Equation (24) and the discussion above lead to an efficient algorithm for implementing semi-analytical methods using scattering matrices.

While many variations to the algorithm exist, the most basic goes as follows. Prior to the main loop, the eigen-modes of free space \mathbf{W}_0 and \mathbf{V}_0 are calculated and the global scattering matrix $\mathbf{S}^{(\text{global})}$ is initialized by setting $\mathbf{S}_{11}^{(\text{global})} = \mathbf{S}_{22}^{(\text{global})} = \mathbf{0}$ and $\mathbf{S}_{12}^{(\text{global})} = \mathbf{S}_{21}^{(\text{global})} = \mathbf{I}$ where \mathbf{I} is the identity matrix. The main loop of the algorithm starts at the first layer by calculating its scattering matrix $\mathbf{S}^{(1)}$. It then updates the global scattering matrix using the star product as $\mathbf{S}^{(\text{global})} = \mathbf{S}^{(\text{global})} \otimes \mathbf{S}^{(1)}$. The main loop then iterates a second time by calculating the scattering matrix for the second layer $\mathbf{S}^{(2)}$ and updating the global scattering matrix as $\mathbf{S}^{(\text{global})} = \mathbf{S}^{(\text{global})} \otimes \mathbf{S}^{(2)}$. After the main loop iterates through all of the layers, the global scattering matrix describes propagation through the entire device. If the device is periodic in the longitudinal direction, the main loop should iterate through all of the layers of one unit cell. The doubling algorithm can then be applied to efficiently cascade any number of periods into a single scattering matrix. When all of this is finished, the entire device resides in free space by default. If the materials outside the device are something other than free space, the global scattering matrix must be connected to the external regions as $\mathbf{S}^{(\text{global})} = \mathbf{S}^{(\text{ref})} \otimes \mathbf{S}^{(\text{global})} \otimes \mathbf{S}^{(\text{trn})}$. Now the global scattering matrix is complete and a solution to the problem can be found.

Some variations exist that can make the algorithm even more efficient. For example, it is not necessary to surround each layer by free space. In the improved framework, it is only necessary to surround all the layers with the same external medium. The external medium can be conveniently chosen to be the transmission or reflection region. When this is done, it is no longer necessary to incorporate the “connection” scattering matrix for that region because the global scattering matrix will calculate fields in that medium by default. A second variation is to calculate the scattering matrices of the first and last layers separately using Eqs. (16)–(18). By doing this, the “connection” scattering matrices are not needed so they do not have to be calculated.

5. CALCULATING THE SOLUTION

5.1. Reflected Fields and Transmitted Fields

The global scattering matrix $\mathbf{S}^{(\text{global})}$ relates the mode coefficients of an incident wave \mathbf{c}_{inc} to the mode coefficients of the reflected \mathbf{c}_{ref} and transmitted waves \mathbf{c}_{trn} . Assuming there is no wave incident from the

transmission region, this relation is

$$\begin{bmatrix} \mathbf{c}_{\text{ref}} \\ \mathbf{c}_{\text{trn}} \end{bmatrix} = \begin{bmatrix} \mathbf{S}_{11}^{(\text{global})} & \mathbf{S}_{12}^{(\text{global})} \\ \mathbf{S}_{21}^{(\text{global})} & \mathbf{S}_{22}^{(\text{global})} \end{bmatrix} \begin{bmatrix} \mathbf{c}_{\text{inc}} \\ \mathbf{0} \end{bmatrix} \quad (29)$$

From Eq. (29), we can write two formulas to calculate the mode coefficients of the transmitted and reflected waves given the mode coefficients of the incident wave and the scattering parameters.

$$\mathbf{c}_{\text{ref}} = \mathbf{S}_{11}^{(\text{global})} \mathbf{c}_{\text{inc}} \quad (30)$$

$$\mathbf{c}_{\text{trn}} = \mathbf{S}_{21}^{(\text{global})} \mathbf{c}_{\text{inc}} \quad (31)$$

The mode coefficients are related to the fields through Eq. (11) as follows.

$$\begin{bmatrix} \mathbf{e}_x^{\text{inc}} \\ \mathbf{e}_y^{\text{inc}} \end{bmatrix} = \mathbf{W}_{\text{ref}} \mathbf{c}_{\text{inc}} \quad (32)$$

$$\begin{bmatrix} \mathbf{e}_x^{\text{ref}} \\ \mathbf{e}_y^{\text{ref}} \end{bmatrix} = \mathbf{W}_{\text{ref}} \mathbf{c}_{\text{ref}} \quad (33)$$

$$\begin{bmatrix} \mathbf{e}_x^{\text{trn}} \\ \mathbf{e}_y^{\text{trn}} \end{bmatrix} = \mathbf{W}_{\text{trn}} \mathbf{c}_{\text{trn}} \quad (34)$$

From the above equations, it is straightforward to calculate the reflected and transmitted fields given the incident field $[\mathbf{e}_x^{\text{inc}} \ \mathbf{e}_y^{\text{inc}}]^T$.

$$\begin{bmatrix} \mathbf{e}_x^{\text{ref}} \\ \mathbf{e}_y^{\text{ref}} \end{bmatrix} = \mathbf{W}_{\text{ref}} \mathbf{S}_{11}^{(\text{global})} \mathbf{W}_{\text{ref}}^{-1} \begin{bmatrix} \mathbf{e}_x^{\text{inc}} \\ \mathbf{e}_y^{\text{inc}} \end{bmatrix} \quad (35)$$

$$\begin{bmatrix} \mathbf{e}_x^{\text{trn}} \\ \mathbf{e}_y^{\text{trn}} \end{bmatrix} = \mathbf{W}_{\text{trn}} \mathbf{S}_{21}^{(\text{global})} \mathbf{W}_{\text{ref}}^{-1} \begin{bmatrix} \mathbf{e}_x^{\text{inc}} \\ \mathbf{e}_y^{\text{inc}} \end{bmatrix} \quad (36)$$

If needed, the longitudinal field components can be calculated from these results using Maxwell's divergence equations.

5.2. Dispersion Analysis

It is possible to calculate the dispersion through a longitudinally periodic device using scattering matrices. This information can be used to construct electromagnetic band diagrams [7], to homogenize periodic structures [43], or to calculate effective material properties of metamaterials [44–46]. For dispersion analysis, no source is needed.

First, the scattering matrix for a single unit cell $\mathbf{S}^{(\text{cell})}$ is constructed using procedures described above. This scattering matrix is related to its external mode coefficients through

$$\begin{bmatrix} \mathbf{c}'_1^- \\ \mathbf{c}'_2^+ \end{bmatrix} = \begin{bmatrix} \mathbf{S}_{11}^{(\text{cell})} & \mathbf{S}_{12}^{(\text{cell})} \\ \mathbf{S}_{21}^{(\text{cell})} & \mathbf{S}_{22}^{(\text{cell})} \end{bmatrix} \begin{bmatrix} \mathbf{c}'_1^+ \\ \mathbf{c}'_2^- \end{bmatrix} \quad (37)$$

The terms in this equation are rearranged almost to the form of a transfer matrix. That is, the new form relates the fields on either side of the unit cell instead of relating input and output waves.

$$\begin{bmatrix} \mathbf{0} & -\mathbf{S}_{12}^{(\text{cell})} \\ \mathbf{I} & -\mathbf{S}_{22}^{(\text{cell})} \end{bmatrix} \begin{bmatrix} \mathbf{c}'_2^+ \\ \mathbf{c}'_2^- \end{bmatrix} = \begin{bmatrix} \mathbf{S}_{11}^{(\text{cell})} & -\mathbf{I} \\ \mathbf{S}_{21}^{(\text{cell})} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{c}'_1^+ \\ \mathbf{c}'_1^- \end{bmatrix} \quad (38)$$

Assuming the device is infinitely periodic in the z direction with period Λ , the following periodic boundary condition must hold where β is the propagation constant of the Bloch wave.

$$\begin{bmatrix} \mathbf{c}'_2^+ \\ \mathbf{c}'_2^- \end{bmatrix} = e^{-j\beta\Lambda} \begin{bmatrix} \mathbf{c}'_1^+ \\ \mathbf{c}'_1^- \end{bmatrix} \quad (39)$$

Substituting this periodic boundary condition into Eq. (38) leads to a generalized eigen-value problem $\mathbf{A}\mathbf{x} = \lambda\mathbf{B}\mathbf{x}$ that can be solved to find solutions of β as well as the Bloch modes if they are desired.

$$\begin{bmatrix} \mathbf{0} & -\mathbf{S}_{12}^{(\text{cell})} \\ \mathbf{I} & -\mathbf{S}_{22}^{(\text{cell})} \end{bmatrix} \begin{bmatrix} \mathbf{c}'_1^+ \\ \mathbf{c}'_1^- \end{bmatrix} = e^{j\beta\Lambda} \begin{bmatrix} \mathbf{S}_{11}^{(\text{cell})} & -\mathbf{I} \\ \mathbf{S}_{21}^{(\text{cell})} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{c}'_1^+ \\ \mathbf{c}'_1^- \end{bmatrix} \quad (40)$$

6. NUMERICAL EXAMPLE

To demonstrate the utility and performance enhancement of the approach described in this paper, a three dimensional electromagnetic band gap (EBG) material was modeled using RCWA. A structure with face-centered-cubic (FCC) symmetry was chosen for this example because this has the highest symmetry of all the Bravais lattices and is of great interest to the research community. The slab and one of its ten unit cells are depicted in Figures 1(d) and (e) respectively. The unit cell was modeled as being a dielectric with $\epsilon_r = 6.0$ with air filled spheres cut away from the dielectric body so as to form FCC symmetry. The unit cell was divided into 20 uniform layers using a staircase approximation. Periodic boundary conditions were used to approximate a slab that was infinitely periodic in the transverse directions.

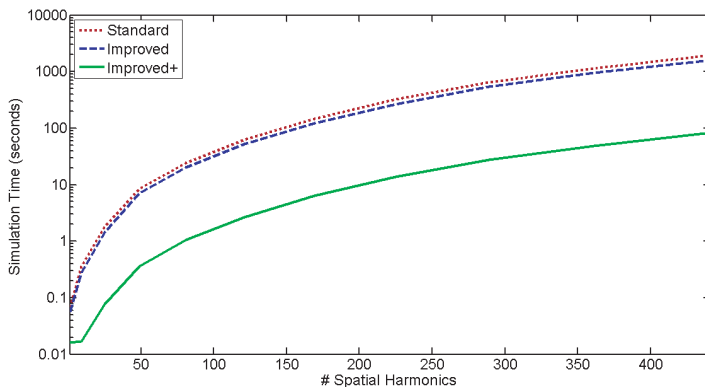


Figure 7. Simulation times for three different scattering matrix formulations.

The EBG material was modeled using three different versions of RCWA. The first version was based on the scattering matrix formulation found throughout most of the literature describing semi-analytical methods. Best effort was made to use as representative of an implementation as possible. This was chosen to be that of Ref. [21]. The second model was based on the improved scattering matrix formulation presented in this paper. The only difference between these algorithms was the manner in which the layer scattering matrices were calculated. This second version was chosen to illustrate the efficiency improvement due solely to the symmetry afforded by the improved scattering matrices. The third version was also based on the improved scattering matrix formulation, but it exploited the ability to interchange layers and perform doubling to more efficiently analyze the structure. Due to symmetry, there existed only 10 unique layers in the entire structure so even fewer calculations were necessary in this case. Other than the scattering matrix manipulations, the three versions of RCWA were kept identical. The codes were run on a single core of a computer with an Intel i5 CPU running at 2.53 GHz.

The time required to calculate the transmittance and reflectance at a single frequency was recorded for each version of the model as the number of spatial harmonics was increased from 1 to 441. This data is provided in Figure 7. The improved scattering matrix formulation performed 20% faster than the standard formulation. This was due solely to there being fewer computations when calculating the layer scattering matrices. When the other benefits of the improved scattering matrix formulation were exploited, the speed increased by more than $23\times$ over the standard formulation.

7. CONCLUSION

The computational electromagnetics community has been adopting inefficient and unconventional scattering matrix formulations for semi-analytical methods. The scattering parameters are being defined different than long-standing convention. In many formulations, \mathbf{S}_{11} is defined as a transmission quantity instead of reflection and \mathbf{S}_{21} is defined as a reflection quantity instead of transmission. To address this situation, scattering matrices in this paper were reformulated consistent with convention. In addition, each layer was separated by free space gaps with zero thickness enabling scattering matrices for each layer to be arbitrarily interchanged. The symmetry imposed by this procedure leads to symmetric scattering matrices where $\mathbf{S}_{11} = \mathbf{S}_{22}$ and $\mathbf{S}_{12} = \mathbf{S}_{21}$ for all of the layers composing the device. This makes the simulation faster, more efficient, and require less memory. By simulating transmittance and reflectance for an electromagnetic band gap material, speed was increased by 20% due solely to the improved symmetry of the scattering matrices. A 23 fold increase in simulation speed was observed when the ability to interchange layers was exploited in the algorithm.

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