Modular method for calculation of transmission and reflection in multilayered structures

Mazilu, M ; Miller, Alan; Donchev, V T

Published in:
Applied Optics

DOI:
10.1364/AO.40.006670

Publication date:
2001

Document Version
Publisher's PDF, also known as Version of record

Link to publication in Heriot-Watt University Research Portal

Citation for published version (APA):
Modular method for calculation of transmission and reflection in multilayered structures

Michael Mazilu, Alan Miller, and Vesselin T. Donchev

We describe a new modular method for the calculation of wave propagation in stratified media based on the direct use of reflection and transmission coefficients. Within this reflection from the left, transmission, and reflection from the right (LTR) method we define addition and multiplication operators that enable the theoretical construction of any multilayered structures from substructures. This modular concept allows for the design and analysis of complex multilayer structures for optical devices. © 2001 Optical Society of America

1. Introduction
Multilayers are becoming increasingly important in photonics. Antireflection coatings are standard components in optical systems, whereas dielectric multilayers are commonly used in lasers to provide high damage threshold mirrors. Multilayer semiconductor fabrication techniques are now employed to produce distributed Bragg reflectors (DBR) for a number of optoelectronic devices including vertical-cavity surface-emitting lasers.1 Incorporation of nonlinear layers within semiconductor DBRs2 leads to ultrashort pulse generation in mode-locked lasers, and chirped DBR structures have been used to produce some of the world’s shortest pulses.3 This success is based on detailed engineering of the multilayer structure to control the phase of the pulse. All this requires a convenient design tool that can take into account the complexity of these structures. Further, the design tool must be capable of incorporating fabrication imperfections including interface roughness.4

Here, we consider the one-dimensional propagation of plane waves through multilayered structures. The continuity conditions at each layer interface imply the definition of the reflection and transmission coefficients for a monochromatic plane wave that propagates through the interface. A monolayer consists of two such interfaces. Because of the multiple reflections between the two interfaces the total reflection and transmission coefficients of such a monolayer is not simply multiplication of the transmission and reflection coefficients.

Standard techniques for calculating reflectivity and transmission of multilayer structures are the matrix and the recursive methods. Here we develop an alternative procedure based on a modular concept, which we describe as reflection from the left, transmission, and reflection from the right or the LTR method. We generalize and simplify the recursive method by defining an LTR element that consists of three coefficients. This LTR method is convenient for the analysis and design of complex structures including interface roughness. The LTR element completely defines the optical properties of a multilayered structure. Further, we define a composition law that calculates the global LTR element of any two LTR elements combined. Thus any multilayered structure can be treated within this framework by combining the different LTRs of the substructures that constitute the complete multilayered structure. To simplify the calculations of periodic structures within the LTR framework we define a multiplication operator. This operator allows the direct calculation of the LTR for m periods of a structure when the LTR is known for one period. Finally, we demonstrate the usefulness of the method by applying it to the cases of a DBR structure and a fractal filter.
2. Background

In the following we introduce two standard techniques used to calculate the reflection and transmission coefficients of multilayered structures. For simplicity, here we consider only normal incidence, but both methods can be adapted to work at nonnormal incidence as well as for s and p polarization.

In the matrix method, each layer is characterized by a \(2 \times 2\) matrix\(^5\)\(^-\)\(^7\)

\[
M_j = \begin{pmatrix}
\cos(k_0 n_j z_j) & \frac{i}{n_j} \sin(k_0 n_j z_j) \\
-\frac{i}{n_j} \sin(k_0 n_j z_j) & \cos(k_0 n_j z_j)
\end{pmatrix},
\]

(1)

where \(n_j\) and \(z_j\) are the complex refractive index and the thickness of layer \(j\), respectively. The monochromatic wave is represented by a wave vector, \(k_0 = 2\pi/\lambda\). The total multilayered system is given by the matrix product of all the characteristic matrices

\[
M = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = M_1 M_2 \ldots M_{n-1}.
\]

(2)

Further, the reflection and transmission coefficients \((r\) and \(t)\) are calculated by use of

\[
\left(1 + \frac{r}{n_0 (1 - r)}\right) = M \begin{pmatrix} t \\ n_m t \end{pmatrix},
\]

(3)

where we consider different refractive indices \((n_0\) and \(n_m)\) on either side of the multilayered system. These coefficients read

\[
r = \frac{a_{21} + a_{11} n_0 - a_{22} n_m + a_{12} n_0 n_m}{a_{21} + a_{11} n_0 + a_{22} n_m + a_{12} n_0 n_m},
\]

\[
t = \frac{2 n_0}{a_{21} + a_{11} n_0 + a_{22} n_m + a_{12} n_0 n_m}.
\]

(4)

(5)

The reflectance and transmittance can be deduced from \(r\) and \(t\) and correspond to \(|r|^2\) and \(n_m |t|^2/n_0\).

An important property of matrix \(M\) is that its determinant is unity. This property can be used for a periodic multilayered system. Indeed, the characteristic matrix of \(m\) periods of such a system is given by \(M^m\), which can be evaluated by use of the Chebyshev polynomials of the second kind.\(^8\)

The characteristic matrix method permits us to calculate the transmission and reflection coefficients of a multilayered system by solving the linear system of Eq. (3), i.e., by use of Eqs. (4) and (5). To add a new layer to the system one must merely multiply \(M\) by the characteristic matrix of the new layer. The transmission and reflection coefficients of the new structure can be deduced again from the new total characteristic matrix by use of Eqs. (4) and (5). If the monochromatic wave is incident from the opposite direction, it is sufficient to exchange the diagonal elements of matrix \(M\) (Ref. 5) and to recalculate the coefficients \(r\) and \(t\).

The reflection and transmission coefficients for waves incident from both directions are calculated directly in the recursive method.\(^9\)\(^,\)\(^10\) This method is based on the definition of the Fresnel amplitude transmission and reflection coefficients for the interface between layers \(j\) and \(j + 1\):

\[
r_{j,j+1} = \frac{n_j - n_{j+1}}{n_j + n_{j+1}},
\]

\[
t_{j,j+1} = \frac{2 n_j}{n_j + n_{j+1}},
\]

\[
r_{j+1,j} = -r_{j,j+1},
\]

\[
t_{j+1,j} = 1 - t_{j,j+1}^2.
\]

(6)

(7)

(8)

(9)

A layer is composed of two such interfaces. All the interfaces in a multilayer structure can be taken into account step by step. Indeed, taking into account the first \(j + 1\) layers yields these coefficients\(^11\):

\[
r_{0,j+1} = \frac{r_{0,j} + r_{j,j+1} \exp(2i k_0 n_j z_j)}{r_{0,j} r_{j,j+1} + \exp(2i k_0 n_j z_j)},
\]

\[
r_{j+1,0} = \frac{r_{j+1,j} + r_{j,0} \exp(2i k_0 n_j z_j)}{r_{j+1,j} r_{j,0} + \exp(2i k_0 n_j z_j)},
\]

\[
t_{0,j+1} = \frac{t_{0,j} \exp(ik_0 n_j z_j)}{r_{0,j} r_{j,j+1} + \exp(2i k_0 n_j z_j)},
\]

\[
t_{j+1,0} = \frac{t_{j+1,j} \exp(ik_0 n_j z_j)}{r_{j+1,j} r_{j,0} + \exp(2i k_0 n_j z_j)},
\]

(10)

(11)

(12)

(13)

where the coefficients \(r_{0,j}\), \(r_{j,0}\), \(t_{0,j}\), and \(t_{j,0}\) correspond to interface effects of the first \(j\) layers.

The advantage of this method is that a structure can be built sequentially layer by layer. On the other hand this method cannot easily treat periodic multilayered structures. Further, a single monolayer is not defined as an independent element having some characteristic properties as in the case of the matrix method where each layer is defined by its characteristic matrix. In the following, we solve this problem by introducing an algebra that combines the advantages of the recurrent method with those of the matrix method.

3. LTR Method

The principal idea of this new method is to characterize each optical element or ensemble of elements of a stratified medium by its transmission and reflection coefficients. First, we count the number of parameters that characterize one multilayered structure. In the case of the characteristic matrix method a \(2 \times 2\) matrix describes one monolayer or a system of monolayers, which means four parameters are needed for the characterization of such a system. The determinant of this matrix is always equal to one, thus the four parameters identified are not independent but have to fulfill a condition. This re-
duces the number of parameters needed for the characterization of a multilayered structure to three. Indeed there are three different reflection and transmission coefficients for a given multilayered structure. The field reflection coefficients for an incident wave that propagates from the right, $R$, or from the left, $L$, are generally not the same. This accounts for two parameters. On the other hand, the transmission coefficient is the same for any stratified medium when coming from the right or from the left. Thus, the field transmission coefficient $T$ is the required third parameter. In the following we use these three complex amplitude coefficients to define the optical effects of multilayers. When defining these coefficients we use a unitary refractive index as reference (vacuum).

### A. Single Interface

The first example of an LTR element is the definition of a single interface between vacuum and a medium of index $n$. There are two possibilities for such an interface. One corresponds to the wave input from the vacuum and the other with the wave input from the medium.

The LTR element for the first case is

$$S_{01}(n) = \begin{pmatrix} \frac{L}{T} \\ \frac{R}{T} \end{pmatrix} = \begin{pmatrix} r \\ t_{01} \end{pmatrix}, \quad (14)$$

where $t_{01} = 2/(1 + n)$ and $r = (1 - n)/(1 + n)$.

The LTR element for the second case, corresponding to the wave input from the medium, is given by

$$S_{10}(n) = \begin{pmatrix} r \\ t_{10} \end{pmatrix}, \quad (15)$$

where $t_{10} = 2n/(1 + n)$.

This is the only case which we consider that is not symmetric with respect to the transmission coefficient.

### B. Propagation

Another important and simple LTR element corresponds to the propagation through a homogeneous medium with a constant refractive index $n$:

$$P(n, k_0, z) = \begin{pmatrix} 0 \\ p \end{pmatrix}, \quad (16)$$

where $z$ is the propagation distance and $p = \exp(ik_0nz)$.

### C. Single Layer

As an example of these new definitions we consider the LTR element for a monolayer $L$ of refractive index $n$ and width $z$:

$$L(n, k_0, z) = \begin{pmatrix} \frac{L}{T} \\ \frac{R}{T} \end{pmatrix} = \begin{pmatrix} r \\ 1 - p^2 \\ 1 - p^2r^2 \\ 1 - p^2r^2 \end{pmatrix} \begin{pmatrix} t_{10} \\ 1 - r^2 \\ 1 - r^2 \\ 1 - r^2 \end{pmatrix}, \quad (17)$$

with

$$r = \frac{1 - n}{1 + n}, \quad p = \exp(ik_0nz). \quad (18)$$

In this example we describe a monolayer surrounded by a vacuum of refractive index 1. This points to a further difference between our LTR method and the two methods introduced above. Indeed a monolayer is intrinsically described by an LTR element that does not depend on the neighboring layers, which is not the case for the above-mentioned methods. To achieve this, all the layers are characterized with respect to the vacuum, even when they are embedded in a multilayered structure.

### D. Addition Operator

The LTR element $L(n, k_0, z)$ defined by Eq. (17) constitutes the fundamental element of a multilayered structure. To calculate the reflection and transmission coefficients of a sequence of elements $L(n_i, k_0, z_i)$, we need to define a combination law for any two LTR elements. Using the definitions for $L$, $T$, $R$ and the recurrent method, one can define a new LTR element that describes the effect of combining two fundamental elements:

$$\begin{pmatrix} L \\ T \\ R \end{pmatrix} = \begin{pmatrix} L_1 + \frac{L_2T_1}{1 - R_1T_2} \\ T_1 + \frac{T_2L_1}{1 - R_1T_2} \\ R_1 + \frac{R_2L_1}{1 - R_1T_2} \end{pmatrix} = \begin{pmatrix} L_1 \\ T_1 \\ R_1 \end{pmatrix} \odot \begin{pmatrix} L_2 \\ T_2 \\ R_2 \end{pmatrix}$$

The composition of the two LTR elements corresponds to a basic summation formula and is equivalent to calculation of the propagation coefficients of an infinitely narrow vacuum gap limited on the left by an interface characterized by the coefficients $(L_1, T_1, R_1)$ and on the right by $(L_2, T_2, R_2)$. We have thus defined a new element $(L, T, R)$ equivalent to the fundamental element that describes all the optical properties of the combination.

As a first example of the composition law, we consider three elements combined to give a single layer. The three elements correspond to the propagation in
Eq. (16) between two interfaces, Eqs. (14) and (15). Indeed, we have

$$S_{01}(n) \oplus P(n, k_0, z) \oplus S_{10}(n) = L(n, k_0, z).$$  \hspace{1cm} (20)

Another important example of the composition law is the case of two consecutive layers with identical propagation of a wave from a medium of refractive index

where

Indeed, we must consider two cases because of the asymmetry introduced by the two different single interfaces. Indeed, when the wave is incident from the left we have

$$S_{10}(n_L) \oplus (\mathcal{L}, \mathcal{F}, \mathcal{R}) \oplus S_{01}(n_R),$$  \hspace{1cm} (22)

whereas when the wave is incident from the right we have

$$S_{01}(n_L) \oplus (\mathcal{L}, \mathcal{F}, \mathcal{R}) \oplus S_{10}(n_R).$$  \hspace{1cm} (23)

To understand the difference between these two cases, it is useful to read the first expression from left to right and the second from right to left. The first takes into account a wave that propagates from a medium of refractive index $n_L$ to vacuum then through an LTR element, which is defined with respect to vacuum on both sides, and finally it traverses an interface from vacuum to a medium of refractive index $n_R$. The second case corresponds to the propagation of a wave from a medium of refractive index $n_R$ to vacuum then through the LTR element followed by the propagation from vacuum to a medium with refractive index $n_L$.

To define a group using the additive composition in Eq. (19), we must define a neutral LTR element that does not change anything when combined with any other LTR element. In our case this corresponds to an infinitely narrow vacuum layer:

$$N = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix},$$  \hspace{1cm} (24)

which has no reflectivity from either side and a transmission coefficient of one. Further, we can show that there is always an inverse LTR element for each given LTR. This inverse element is defined by

$$\begin{pmatrix} \mathcal{L} \\ \mathcal{F} \\ \mathcal{R} \end{pmatrix} = \begin{pmatrix} -\mathcal{L} / Q \\ -\mathcal{F} / Q \\ -\mathcal{R} / Q \end{pmatrix},$$  \hspace{1cm} (25)

where the minus sign in front of the LTR element indicates the inverse and $Q = \mathcal{F}^2 - \mathcal{L} \mathcal{R}$. The inverse LTR element is not defined when $Q = 0$, which corresponds to an interesting case. Indeed, when a structure is simultaneously illuminated from the right (with the field amplitude $E_1$) and from the left ($E_2$), we have

$$F_1 = \mathcal{F} E_1 + \mathcal{L} E_2,$$  \hspace{1cm} (26)

$$F_2 = \mathcal{R} E_1 + \mathcal{F} E_2,$$  \hspace{1cm} (27)

where $F_1$ and $F_2$ are the left and the right total output fields (see Fig. 1). This corresponds to a linear system of equations linking the incident field amplitudes with the amplitudes of the field that leaves the multilayered structure. When the condition $Q = \mathcal{F}^2 - \mathcal{L} \mathcal{R} = 0$ is fulfilled, a family of input fields $E_1$ and $E_2$ exists such that no light comes out of the structure. One can say that the transmitted wave from the left destructively interferes with the reflected wave from the right and vice versa.

It is possible to build a multilayer structure having $Q = 0$ if the layers are absorbing. This means the structure does not reflect and completely absorbs all the light at one wavelength. As an example we can consider a five-layer design: ABCBA, where the A and C layers are Al (0.82 + 5.99i index, 6.44- and 201.64-nm thickness, respectively) and the B layers are Al$_2$O$_3$ (1.62 index, 123.64-nm thickness). The coefficient $Q$ is zero for this structure at 546-nm wavelength.

When combining an LTR element with its inverse
element (if it exists), one finds the neutral element as expected:
\[
\begin{bmatrix}
L \\
\mathcal{T} \\
R
\end{bmatrix}
\oplus
\begin{bmatrix}
L \\
\mathcal{T} \\
R
\end{bmatrix} =
\begin{bmatrix}
0 \\
1 \\
0
\end{bmatrix}.
\] (28)

As an example, let us consider the case of a nonabsorbing dielectric layer of refractive index 1.5 and 300-nm width. At a wavelength of 600 nm the inverse to this structure corresponds to a layer with the same refractive index and 100-nm width. Adding these two layers together gives no reflection at 600 nm and has a transmission coefficient of 1.

In conclusion, the set of LTR elements forms a group with respect to the composition law in Eq. (19). This group is non-Abelian because it does not commute (i.e., the result depends on the order of the composition).

E. Multiplication Operator

In the case of a periodic structure, we are interested in calculating the optical effects of a sequence of \(m\) identical layered substructures. Each substructure can comprise a number of multilayers characterized by a single LTR element. The optical response can be determined by a composition of \(m\) LTR elements. This defines a multiplication law in the LTR group

\[
\begin{bmatrix}
L \\
\mathcal{T} \\
R
\end{bmatrix}
\oplus
\begin{bmatrix}
L \\
\mathcal{T} \\
R
\end{bmatrix}
\oplus \ldots \oplus
\begin{bmatrix}
L \\
\mathcal{T} \\
R
\end{bmatrix} =
\begin{bmatrix}
L \\
\mathcal{T} \\
R
\end{bmatrix}.
\] (29)

To define this operator, it is useful to introduce parameters \(a\) and \(b\) as functions of \(L\), \(\mathcal{T}\), and \(R\). Indeed, inspired by the composition of two monolayer LTR elements with the same indices as defined by Eq. (21), we define \(a\) and \(b\) to satisfy the following equation:

\[
\begin{bmatrix}
L \\
\mathcal{T} \\
R
\end{bmatrix} =
\begin{bmatrix}
La - b^2 \\
L(\mathcal{T} - a^2b^2) \\
Ra - b^2
\end{bmatrix}.
\] (30)

Comparing the definitions of parameters \(a\) and \(b\) with Eq. (21), we note that parameter \(b\) corresponds to propagation term \(p\).

The relation in Eq. (21) implies the following equations for parameters \(a\) and \(b\):

\[0 = a - \mathcal{T}b + \mathcal{T}^2 - RL,\] (31)

\[0 = \mathcal{T}b^2 - (1 - RL + \mathcal{T}^2)b + \mathcal{T}.\] (32)

Equations (31) and (32) give two solutions for Eq. (30):

\[b_{1,2} = \frac{1 - RL + \mathcal{T}^2 \pm [(1 - RL + \mathcal{T}^2)^2 - 4\mathcal{T}^2]^{1/2}}{2\mathcal{T}},\] (33)

\[a_{1,2} = \mathcal{T}b_{1,2} - \mathcal{T}^2 + RL.\] (34)

We note that the two solutions \(b_{1,2}\) are reciprocals of each other, \(b_1 = 1/b_2\). They correspond to the two possible signs of the phase in the propagation term in Eq. (18), which is defined by the positive \(z\) direction.

Further, if the transmission coefficient \(\mathcal{T} = 0\), only one solution exists, \(a = RL\) and \(b = 0\).

Using either solution for parameters \(a\) and \(b\), the multiplication operator is given by

\[
m\begin{bmatrix}
L \\
\mathcal{T} \\
R
\end{bmatrix} =
\begin{bmatrix}
La - b^{2m} \\
L(\mathcal{T} - a^2b^{2m}) \\
Ra - b^{2m}
\end{bmatrix}.\] (35)

This definition implies other interesting properties. Multiplication by zero gives the neutral element for the composition law, whereas multiplication by minus one gives the inverse element as follows:

\[
0
\begin{bmatrix}
L \\
\mathcal{T} \\
R
\end{bmatrix} =
\begin{bmatrix}
0 \\
1 \\
0
\end{bmatrix},\] (36)

\[-1
\begin{bmatrix}
L \\
\mathcal{T} \\
R
\end{bmatrix} =
\begin{bmatrix}
-L/Q \\
T/Q \\
-R/Q
\end{bmatrix}.\] (37)

Another benefit of this definition of the multiplication operator is its direct applicability to multiplication by noninteger numbers. If the initial LTR element is a general multilayer stack, the multiplication automatically replaces this element with a homogeneous monolayer of equal width having an effective refractive index. The multiplication operator simply changes the width of this effective layer by the multiplication factor.

Another possible use of multiplication with a non-integer parameter is the backward calculation of the reflectivity coefficient of one period from a measurement of the optical properties of \(m\) periods of a multilayered structure. In this case, the measured LTR element is simply multiplied by \(1/m\). We must note here that this multiplication operator is based on parameter \(b\) to the power of \(1/m\). If \(m\) is not an integer, \(b^m\) is not uniquely defined and special care must be taken because the power function is multivalued.

4. Examples

In our first straightforward example, we illustrate the usefulness of the multiplication operator. The
reflection coefficient of a DBR structure was studied as a function of the number of periods of the structure. This number is simply the multiplication factor of the LTR element corresponding to one period. In this example we chose material A to have a refractive index of 2.5 and a width of 100 nm \((LTR)_A\) and material B to have a refractive index of 1.5 and the same width \((LTR)_B\):

\[
\begin{pmatrix}
L \\
T \\
R
\end{pmatrix}_m = \begin{pmatrix}
L \\
T \\
R
\end{pmatrix}_A \oplus \begin{pmatrix}
L \\
T \\
R
\end{pmatrix}_B.
\]

The reflectivity calculated with this expression shows the usual reflectivity of a DBR structure; see Fig. 2. As the number of periods increases, the maximum reflectivity in the stop band of the DBR increases. Additional layers or chirped elements can easily be incorporated by this method.

Another test for our method is to calculate the transmission coefficients of a complex structure in which we use the addition and multiplication operators alternately, which is the case when we consider a fractal structure. A good example of such a structure is to use the Cantor fractal\(^{12}\) to define a multilayer composed of two materials of different refractive indices. To build such a structure imagine a thick layer of material A and divide its width into six sections of equal width. Then replace every second section with layers of material B. We then take each of the three remaining material A sections and repeat the procedure.

To calculate the transmission coefficient for this Cantor fractal multilayered structure we define the total LTR using a recursive sequence of LTR elements:

\[
\begin{pmatrix}
L \\
T \\
R
\end{pmatrix}_{j+1} = 3 \left( \begin{pmatrix}
L \\
T \\
R
\end{pmatrix}_j \oplus 6 \begin{pmatrix}
L_0 \\
T_0 \\
R_0
\end{pmatrix} \right),
\]

where we chose \((LTR)_0 = L(2.5, k_0, 10 \text{ nm})\) for material A and \((LTR)_0 = L(1.5, k_0, 10 \text{ nm})\) for material B. As \(j\) goes to infinity this sequence constructs a growing pseudo-Cantor fractal with a fractal dimension of \(D = \ln(3)/\ln(6) = 0.613\). In our example we terminated the sequence after seven steps \((LTR)_7\), which makes a 2.7-mm wide structure.

Figure 3 shows the logarithmic transmission coefficient of the Cantor fractal structure. We observe that this structure does not transmit over large wavelength domains but is interrupted by some sharp transmission features. Further, the spectrum has a fractal behavior in which the same features can be observed on different wavelength scales. This example shows how easy it is to use the two operators and to reuse the coefficients calculated for substructures. The sharp features could be used for complex optical filtering.

5. Conclusion

We have introduced a formalism that allows a simple method for the calculation of reflection and transmission amplitude coefficients in multilayered structures while employing only physical parameters. This formalism consists of a combination law that enables the optical properties of two successive multilayered structures to be calculated when the optical properties of each is known individually. Further, the formalism comprises a multiplicative operator that allows the direct calculation of optical properties of a periodic structure when the optical properties are known for one period.

The special case of \(Q = 0\) shows the existence of total absorption in multilayered structures under certain conditions and examples of DBR, and fractal structures illustrate the usefulness of the LTR method. The modular approach allows the step-by-step design of complex optical components from simpler elements. Reusing the reflectivity and transmission coefficients gives physical insight and easy visualization at each step of the calculation.
References