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A new formulation to shape the concept of bounds in effective dielectric tensors for superlattices with two directions of periodicity

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Abstract

This paper introduces a new theoretical formulation based on a composition method and a statistical discretization approach by matrical block. Anisotropic properties and boundary conditions are considered, introducing the analytical bounds expressions of the effective dielectric constants in the limit of the long-wavelength regime for an idealized superlattice (SL) possessing two directions of periodicity (2D-SL). Such a SL can be described as a multilayer array of alternating cells, $(N \times M)$ rectangular dielectric bars, allowing the structure to be shaped as a function of the dielectric constants of each of the anisotropic constituents. It is worth noting that in the simplified case of a 2D-SL made of only two different isotropic materials showing off the same periodicity in both directions, our general matrix formulation, due to the alternative composition laws, leads to the well-established results called, respectively, 'Wiener's and Lichtenecker's bounds' regarding the dielectric constant. This new formalism refashions the concept of bounds of effective dielectric tensors and the notion of form birefringence applied to 2D-SL, with relevant $(N \times M)$ rectangular anisotropic columns for arbitrary symmetries in the low-frequency model.

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1. Introduction and problem definition

Historically, the effective properties (dielectric constant, magnetic permeability, thermal or electrical conductivity, diffusivity) ascribed to composite materials have proved to be of great interest [1–3]. These studies address the issues in classical physics of effective properties of heterogeneous composite media. These materials are considered heterogeneous when the scale of heterogeneity is much greater than the atomic scale, but much less than the relevant macroscale. Sometimes, the macroscopic response of such materials is not anywhere in between the reponses of the pure homogeneous constituents. Several methods have been developed (for example, by Lichtenecker [4, 5], by Hashin and Shtrikman [6] based on a variational principle [7], by Bergman [3], and others) to cope with a convenient approach considering the bounds of the effective dielectric constants. Most often, the main types of methods directed to obtaining approximate bounds of dielectric constants are namely statistical discretization methods or integral formulations.

Considering particular heterostructures' topology, such heterogeneous materials can take the form of periodic generalized superlattices (SLs) with periodicity along some directions [8]. A generalized nD-SL (n is the number of directions presenting periodicity) can be considered as an arrangement of alternate regions of various materials with respective dimensions. We consider the limit of small-sized SL's regions where any field change remains negligible over each respective region (static field approximation). Then, as the optical wavelength is much larger than the different periods of the SL (long-wavelength regime), the nD-SL can behave as a homogeneous medium, whose physical properties are determined by the so-called effective parameters. Moreover, when the energy of light is small compared to the gap of materials, we can neglect the modification of the absorption spectra near the gap due to the quantum confinement effects. The effective parameters are usually inferred from relevant particular averages on the parameters of the constituents. As an example, 1D-SL ($n = 1$) can be considered as stacks made up of alternating layers of different constituents. In such a specific 1D-SL optics case, an anisotropy property of the permittivity tensor, called form birefringence [9, 10], occurs in sundry multiple 1D-SL, although neither of them is anisotropic. The significant development of integrated optoelectronic heterostructure components, based on the form birefringence and made up of semiconductors such as GaAs, AlAs and their alloys, depends increasingly on new modelling tools. As numerous integrated optic devices rely upon the form birefringence (optical waveguides [11, 12], coherence modulators [13, 14], TE–TM conversion filters [15, 16], and so on), a new general analytical frame of the form birefringence in nD-SL provides an interesting guide for their study. In the case of heterostructure 1D-SL composed of layers of arbitrary symmetry, the effective tensors of dielectric constants [17–19], elastic constants [17, 20, 21], photoelastic constants [17] and electro-optic constants [19, 22] have been calculated so as to predict the behaviour. Regarding 2D-SL, such a topology can be attributed with an array of alternating ($N \times M$) dielectric bar-like slabs.

The model proposed herein presents a suitable discretization method by matrical block and deals with a SL with two directions of periodicity (2D-SL), brought down to an array of alternating cells, ($N \times M$) rectangular dielectric columns; symbols M and N represent the number of different anisotropic materials, respectively, along the x_3-direction and the x_1-direction: x_1 and x_3 represent the two directions perpendicular to the x_2-direction of columns' cells (figure 1). Then, a general matrix formulation, based on an alternative composition method, is shaped to define the general analytical bounds expressions of the effective dielectric constants, such topologic structures being made of anisotropic columns of arbitrary symmetry. Considering a general 2D-SL in an orthogonal coordinate system (x_i, $i = 1$–3), the schematic diagram of a 2D-SL featuring NM different constituents in the space is depicted in figure 1. According to figure 2, the symbols u and c describe the lines and columns of the 2D-SL, respectively. The quantities $L_{[c]}^{x_1} = \sum_{u=1}^{N} l_{[c]}^{u\_x_1}$ (with the adopted notation $[c]$ equivalent to the condition $\{\forall c$ fixed integer, $c \in [1\text{–}M]\}$ and the notation u_x_1 ascribed to the information uth line in the x_1-direction) and $L_{[u]}^{x_3} = \sum_{c=1}^{M} l_{[u]}^{c\_x_3}$ (with $[u]$ equivalent to the condition $\{\forall u$ fixed integer, $u \in [1\text{–}N]\}$ and c_x_3 attributed to the cth column in the x_3-direction) represent the periods of such general structures ($N \neq M$) along the x_1- and x_3-directions, respectively. The

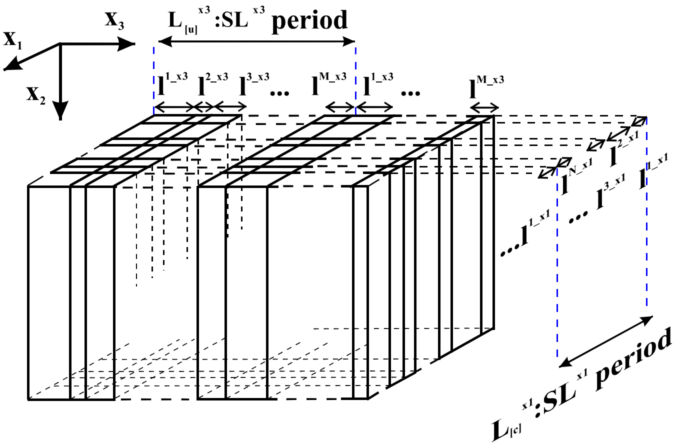

Figure 1. Layout of a generic superlattice (2D-SL) featuring ($N \times M$) different constituents along two directions of periodicity. $L_{[c]}^{x_1}$ and $L_{[u]}^{x_3}$ represent the respective periods of such structures along the x_1- and x_3-directions.

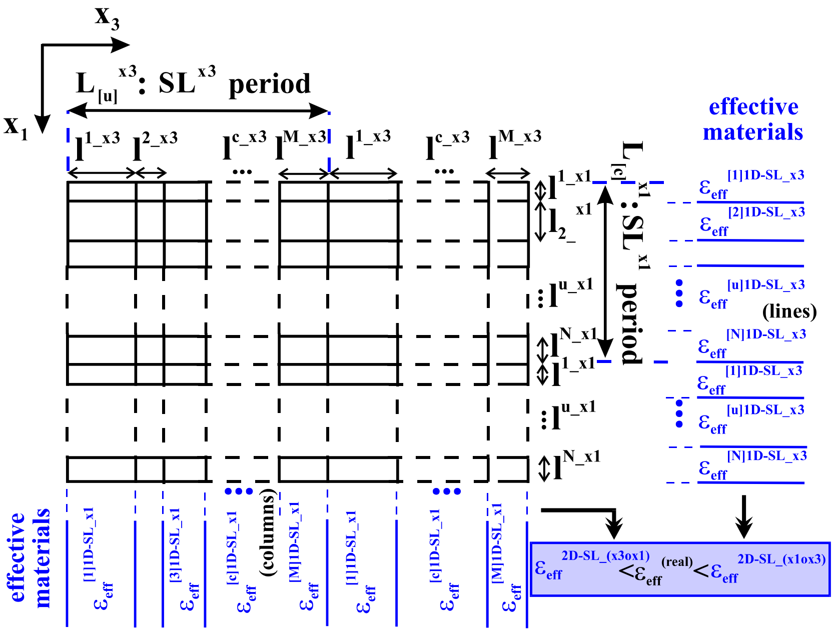

Figure 2. Schematic diagram of a 2D-SL featuring ($N \times M$) different constituents in the (x_1, x_3)-plane. $L_{[c]}^{x_1} = \sum_{u=1}^{N} l_{[c]}^{u\_x_1}$ and $L_{[u]}^{x_3} = \sum_{c=1}^{M} l_{[u]}^{c\_x_3}$ represent the periods of such general structures ($N \neq M$) along the x_1- and x_3-directions, respectively ($c \equiv$ columns and $u \equiv$ lines). The expressions ($l_{[c]}^{u\_x_1} \times l_{[u]}^{c\_x_3}$) stand for the fraction of the (u, c)th constituent in the (x_1, x_3)-plane with [u] and [c].

related fractions, respectively, of the cth column along the x_3-direction and the uth line along the x_1-direction of each constituent, are defined hereafter as $f_{[u]c\_x_3} = \frac{l_{[u]}^{c\_x_3}}{L_{[u]}^{x_3}}$ and $f_{[c]u\_x_1} = \frac{l_{[c]}^{u\_x_1}}{L_{[c]}^{x_1}}$, with $l_{[c]}^{u\_x_1}$ the dimension of the uth line along the x_1-direction and $l_{[u]}^{c\_x_3}$ the dimension of the cth column along the x_3-direction.

2. Expression of the effective dielectric tensor bounds for 2D-SL of arbitrary symmetry

We do not consider here the pyroelectric and piezoelectric classes of materials [23], that is we do not have to expand the displacement field D to linear terms in strain[3]. Then, the basic relation between the displacement field D and the electric field E through the dielectric tensors ε can be simplified as

$$D^V = \varepsilon^V E^V, \tag{1}$$

with V equivalent to the notation 2D-SL_($x_1 \circ x_3$) and 2D-SL_($x_3 \circ x_1$) for the effective material 2D-SL, $[u]$1D-SL_x_3 and $[c]$1D-SL_x_1 for the effective 1D-SL, and $[u]c\_x_3$ and $[c]u\_x_1$, respectively, for the cth material of each u-line ($u = 1$–N) and the uth material of each c-column ($c = 1$–M), according to the notation given in figure 2. The symbol $\circ$ represents the symbol of composition law.

The permittivity tensors ε^V can be described with a (3 × 3) matrix [24] and the electric fields D^V and E^V by (3 × 1) vectors. The boundary conditions regarding the continuity of the tangential components of E and the normal component of D yield the following matrix relation (1D-SL_x_3 that represents all the $[u]$-SLs along the x_3-direction, $c = 1$–M):

$$E^{[u]\text{1D-SL\_}x_3} = \sum_{c=1}^{M} \xi^{[u]c\_x_3} E^{[u]c\_x_3} \qquad \text{with} \qquad \xi^{[u]c\_x_3} = \begin{bmatrix} 1/M & 0 & 0 \\ 0 & 1/M & 0 \\ 0 & 0 & f_{[u]c\_x_3} \end{bmatrix} \tag{2}$$

and

$$D^{[u]\text{1D-SL\_}x_3} = \sum_{c=1}^{M} \tau^{[u]c\_x_3} D^{[u]c\_x_3}$$

with (3)

$$\tau^{[u]c\_x_3} = \begin{bmatrix} f_{[u]c\_x_3} & 0 & 0 \\ 0 & f_{[u]c\_x_3} & 0 \\ 0 & 0 & 1/M \end{bmatrix} = \left(\frac{f_{[u]c\_x_3}}{M}\right) \cdot (\xi^{[u]c\_x_3})^{-1},$$

with

$$\Theta^{[l]1\_x_3} E^{[l]1\_x_3} = \cdots = \Theta^{[u]c\_x_3} E^{[u]c\_x_3} = \cdots = \Theta^{[l]M\_x_3} E^{[l]M\_x_3}$$

and (4)

$$\Theta^{[u]c\_x_3} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \varepsilon_{13}^{[u]c\_x_3} & \varepsilon_{23}^{[u]c\_x_3} & \varepsilon_{33}^{[u]c\_x_3} \end{bmatrix}.$$

In such a configuration, relations (2) and (3) according to the fraction term $f_{[u]c\_x_3}$ in the matrices $\xi^{[u]c\_x_3}$ and $\tau^{[u]c\_x_3}$ represent the electrical fields' (E and D) variations across one period $L_{[u]}^{x_3}$ of the 1D-SL^{x_3} as a result of the addition of the proportional corresponding variations' fields across the M adjacent layers (figure 1). The first and second lines of $\Theta^{[u]c\_x_3}$ account for the continuity of the tangential components of E, whereas the third line features the continuity of the normal component of D as $D_3 = \varepsilon_{3j} E_j = \varepsilon_{j3} E_j$ due to the Hermitian symmetry of the ε permittivity in the case of idealized purely anisotropic dielectric materials

[3] For piezoelectric and pyroelectric materials, when the electric displacement field D and stress are functions of independent variables, the field vector D can be expanded in linear terms in electric field E and strain T as the general relation $D = D_0 + \varepsilon E + eT$, with ε and e the isothermal dielectric and piezoelectric tensors, respectively. The constant term D_0 in the expansion depends on temperature and leads to pyroelectric effects.

(that is by considering nonconducting and nonmagnetic materials) which present negligible energy losses or no absorption[4].

The constitutive relation (1) expressed for all the SLs (1D-SL_x_3), according to equations (2) and (3), yields $\sum_{c=1}^{M} \tau^{[u]c\_x_3} D^{[u]c\_x_3} = \varepsilon_{\rm eff}^{[u]1{\rm D\text{-}SL}} [\sum_{c=1}^{M} \xi^{[u]c\_x_3} E^{[u]c\_x_3}]$. Then, equation (4) entailing $E^{[u]c\_x_3} = (\Theta^{[u]c\_x_3})^{-1} \Theta^{[l]1\_x_3} E^{[l]1\_x_3}$, with the basic relation (1) for each SL^{x_3}'s layer, yields the following system of N general matrix expressions of all the effective dielectric tensors of the N line-1D-SL_x_3 ([u], figure 2):

$$\left\{\underline{\varepsilon}_{\rm eff}^{[u]1{\rm D\text{-}SL}\_x_3}\right\} = \left[\sum_{c=1}^{M} \tau^{[u]c\_x_3} \varepsilon^{[u]c\_x_3} \left(\Theta^{[u]c\_x_3}\right)^{-1} \Theta^{1\_x_3}\right] \left[\sum_{c=1}^{M} \xi^{[u]c\_x_3} \left(\Theta^{[u]c\_x_3}\right)^{-1} \Theta^{1\_x_3}\right]^{-1}. \tag{5}$$

The matrix relation (5) refers to the notion of effective permittivity tensors of 1D-SL which have been calculated and transformed by different ways into Vegard rules [17, 18]. Then, it is possible to proceed with this method (figure 2, right) along the other x_1-direction while considering the 2D-SL as an effective material made of N effective line-1D-SL_x_3 defined by the system of N equations (5). Such an approach allows us to shape a relevant analytical matrix expression of the effective dielectric constants for the idealized 2D-SL_($x_1 \circ x_3$) for $u = 1$–N:

$$\underline{\underline{\varepsilon}}_{\rm eff}^{2{\rm D\text{-}SL}\_(x_1 \circ x_3)} = \left[\sum_{u=1}^{N} \tau^{u\_x_1} \left\{\underline{\varepsilon}_{\rm eff}^{[u]1{\rm D\text{-}SL}\_x_3}\right\} \left(\Theta_{\rm eff}^{u\_x_1}\right)^{-1} \Theta_{\rm eff}^{l\_x_1}\right] \left[\sum_{u=1}^{N} \xi^{u\_x_1} \left(\Theta_{\rm eff}^{u\_x_1}\right)^{-1} \Theta_{\rm eff}^{l\_x_1}\right]^{-1}, \tag{6}$$

with

$$\xi^{u\_x_1} = \begin{bmatrix} f_{[c]u\_x_1} & 0 & 0 \\ 0 & 1/N & 0 \\ 0 & 0 & 1/N \end{bmatrix},$$
$$\tau^{u\_x_1} = \begin{bmatrix} 1/N & 0 & 0 \\ 0 & f_{[c]u\_x_1} & 0 \\ 0 & 0 & f_{[c]u\_x_1} \end{bmatrix} = \left(\frac{f_{[c]u\_x_1}}{N}\right) \cdot (\xi^{u\_x_1})^{-1} \tag{7}$$

and

$$\Theta_{\rm eff}^{u\_x_1} = \begin{bmatrix} \underline{\varepsilon}_{{\rm eff}\,11}^{[u]1{\rm D\text{-}SL}\_x_3} & \underline{\varepsilon}_{{\rm eff}\,12}^{[u]1{\rm D\text{-}SL}\_x_3} & \underline{\varepsilon}_{{\rm eff}\,13}^{[u]1{\rm D\text{-}SL}\_x_3} \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

It is important to note that both the first line of the last matrix $\Theta_{\rm eff}^{u\_x_1}$ and expression (6) hinge on the prior system (5). One should note the crucial cast of the notation since regarding the N equations (5) and equation (6), we first have $N \neq M$. Indeed, $\Theta_{\rm eff}^{u\_x_1} \neq \Theta^{[u]c\_x_3}$, the matrices ξ, τ and ε are different regarding the two expressions (5) and (6). As an example, in equation (5), the NM number of (3×3) matrices $\Theta^{[u]c\_x_3}$ depict the continuity of the tangential components of E along both x_1- and x_2-directions, and the normal component of D along the x_3-direction (equation (4)) in the ($N \times M$) anisotropic-material-columns; on the

[4] For idealized purely anisotropic dielectric materials, the Hermitian condition on the permittivity tensors $\varepsilon_{ij} = \varepsilon_{ji}^*$ can be simplified as $\varepsilon_{ij}^{\rm sym} = \varepsilon_{ji}^{\rm sym}$ on the symmetrical part of the tensors. Materials are not considered optically active (gyrotropic), otherwise the constitutive relation should contain spatial derivatives of the field and the dielectric tensor a nonzero imaginary part antisymmetric in the coordinate indices ($\varepsilon_{ij}^{\rm antisym} = -\varepsilon_{ji}^{\rm antisym}$).

other hand, in expression (6), the N matrices $\Theta_{\rm eff}^{u\_x_1}$ feature the continuity of the tangential components of E along both x_2- and x_3-directions, and the normal component of D along the x_1-direction (equation (7)) along the N effective 1D-SL_x_3 (figure 2). One can note that the first term $\left(\sum_{u=1}^{N}\cdots\left\{\underline{\varepsilon}_{\rm eff}^{[u]\rm 1D\text{-}SL\_x_3}\right\}\cdots\right)$ of the general expression (6) directly includes the N equations (5), and this model naturally accounts for the notion of permittivity with inclusions regarding such topologic 2D-SL. Actually, such a versatile matrix expression (6) stems from a $(x_1 \circ x_3)$ composition reasoning while encompassing all the matrices defined in equations (2)–(7) related to each column and each effective line-1D-SL_x_3.

Thereby, in the same way, we can achieve the overall matrix expression of the effective dielectric constants of an idealized 2D-SL relevant to the composition $(x_3 \circ x_1)$; to this end, consider first the calculus of the M effective column-SLs (1D-SL_x_1 equivalent to all the $[c]$-SLs along the x_1-direction) constituting the 2D-SL (figure 2). This first step yields the system of M general matrix expressions of the effective dielectric tensors of the M effective column-1D-SL_x_1 ($u = 1$–N, $[c]$, figure 2):

$$\left\{\underline{\varepsilon}_{\rm eff}^{[c]\rm 1D\text{-}SL\_x_1}\right\} = \left[\sum_{u=1}^{N}\tau^{[c]u\_x_1}\varepsilon^{[c]u\_x_1}\left(\Theta^{[c]u\_x_1}\right)^{-1}\Theta^{1\_x_1}\right]\left[\sum_{u=1}^{N}\xi^{[c]u\_x_1}\left(\Theta^{[c]u\_x_1}\right)^{-1}\Theta^{1\_x_1}\right]^{-1}, \tag{8}$$

with

$$\xi^{[c]u\_x_1} = \begin{bmatrix} f_{[c]u\_x_1} & 0 & 0 \\ 0 & 1/N & 0 \\ 0 & 0 & 1/N \end{bmatrix}, \qquad \tau^{[c]u\_x_1} = \left(\frac{f_{[c]u\_x_1}}{N}\right)\cdot\left(\xi^{[c]u\_x_1}\right)^{-1}$$

and (9)

$$\Theta^{[c]u\_x_1} = \begin{bmatrix} \varepsilon_{11}^{[c]u\_x_1} & \varepsilon_{12}^{[c]u\_x_1} & \varepsilon_{13}^{[c]u\_x_1} \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

We can proceed with this method (figure 2, lower part) along the other x_3-direction, considering then the 2D-SL as an effective material made of M effective column-1D-SL_x_1 defined by the system of the M equations (8). By doing so, we can define ($c = 1$–M)

$$\underline{\varepsilon}_{\rm eff}^{\rm 2D\text{-}SL\_(x_3\circ x_1)} = \left[\sum_{c=1}^{M}\tau^{c\_x_3}\left\{\underline{\varepsilon}_{\rm eff}^{[c]\rm 1D\text{-}SL\_x_1}\right\}\left(\Theta_{\rm eff}^{c\_x_3}\right)^{-1}\Theta_{\rm eff}^{l\_x_3}\right]\left[\sum_{c=1}^{M}\xi^{c\_x_3}\left(\Theta_{\rm eff}^{c\_x_3}\right)^{-1}\Theta_{\rm eff}^{l\_x_3}\right]^{-1}, \tag{10}$$

with

$$\xi^{c\_x_3} = \begin{bmatrix} 1/M & 0 & 0 \\ 0 & 1/M & 0 \\ 0 & 0 & f_{[u]c\_x_3} \end{bmatrix}, \qquad \tau^{c\_x_3} = \left(\frac{f_{[u]c\_x_3}}{M}\right)\cdot\left(\xi^{c\_x_3}\right)^{-1}$$

and (11)

$$\Theta_{\rm eff}^{c\_x_3} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \underline{\varepsilon}_{{\rm eff}\,13}^{[c]\rm 1D\text{-}SL\_x_1} & \underline{\varepsilon}_{{\rm eff}\,23}^{[c]\rm 1D\text{-}SL\_x1} & \underline{\varepsilon}_{{\rm eff}\,33}^{[c]\rm 1D\text{-}SL\_x_1} \end{bmatrix}.$$

Expression (10) clearly derives from the above-mentioned $(x_3 \circ x_1)$ composition rationale, as it contains all the matrices defined previously.

General analytical expressions (6) and (10) depict the overall concept of bounds regarding the effective dielectric tensors for SLs that presents two directions of periodicity (2D-SL); they

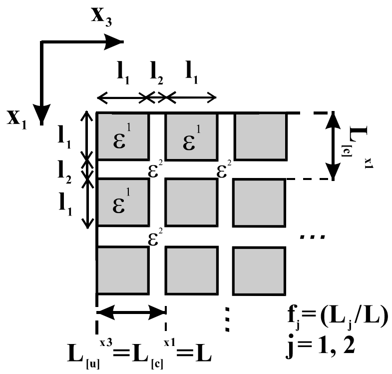

Figure 3. Schematic diagram of a 2D-SL featuring only two different constituents ($N = M = 2$) and a same period along the two directions, $L^{x1}_{[c]} = L^{x3}_{[u]} = l_1 + l_2$. The matrix ε^n and l_n account for the dielectric matrix of the constituent n and its dimension along x_1 and x_3, respectively ($n = 1$ and 2).

can be seen as a multilayer array structure of alternating ($N \times M$) rectangular dielectric cells made of anisotropic constituents of arbitrary symmetry:

$$\underline{\varepsilon}^{\text{2D-SL\_}(x_j \circ x_i)}_{\text{eff}} \leqslant \underline{\varepsilon}^{\text{2D-SL}}_{\text{eff}} \leqslant \underline{\varepsilon}^{\text{2D-SL\_}(x_i \circ x_j)}_{\text{eff}} \qquad (\text{for } i, j = 1, 3 \text{ or } 3, 1). \tag{12}$$

Eventually, the (3 × 3) matrix relation (12) is applied to each permittivity tensor component of the 2D-SL $\underline{\varepsilon}^{\text{2D-SL}}_{\text{eff}\,uv}$ which are ranging in two exhaustive bounds $\left[\underline{\varepsilon}^{\text{2D-SL\_}(x_j \circ x_i)}_{\text{eff}\,uv} - \underline{\varepsilon}^{\text{2D-SL\_}(x_i \circ x_j)}_{\text{eff}\,uv}\right]$ (for u and $v = 1$–3).

The nomenclature is pivotal as in the notation regarding relation (12) together with equations (6) and (10), many matrices Θ are different, especially $\Theta^{c\_x_3}_{\text{eff}} \neq \Theta^{u\_x_1}_{\text{eff}} \neq \Theta^{[c]u\_x_1} \neq \Theta^{[u]c\_x_3}$; moreover, matrices such as ξ, τ and ε are also different.

3. Discussion and conclusion

As an example, consider a 2D-SL made of rectangular dielectric bars involving only two different isotropic materials ($N = M = 2$). Let there be now the condition $L^{x_1} = L^{x_3} = L$ for a specific 2D-SL with the same periodicity along the x_1- and x_3-directions as represented in figure 3. In such a topologic case, many simplifications can be done on the notation. To this end, we can advantageously define two conditions about the parity of both symbols u (lines) and c (columns), in order to define the two areas of the special topology shown in figure 3 (a and $b \neq 0$ integers):

area(1): $\{[\forall u[1\text{–}N] \text{ and } c = (2a + 1)\}$, that describes the first area in figure 3

and

area(2): $\{[u = 2b,\ \forall c[1\text{–}M]] \text{ with } [u = (2a + 1),\ c = 2b]\}$

or

$$\{[c = 2b,\ \forall u[1\text{–}N]] \text{ with } [c = (2a + 1),\ u = 2b]\} \tag{13}$$

which are two ways to describe the second area in figure 3.

Then, the significant simplification $l_{[u]}^{c\_x_3} \equiv l_{[c]}^{u\_x_1} \equiv l_j$ can be carried out entailing $f_{[u]c\_x_3} \equiv f_{[c]u\_x_1} \equiv f_j$ (figure 3), and $\varepsilon^{[u]c\_x_3} \equiv \varepsilon^{[c]u\_x_1} \equiv \varepsilon^j$, with

$$\varepsilon^j = \begin{bmatrix} \varepsilon_{11}^j & 0 & 0 \\ 0 & \varepsilon_{11}^j & 0 \\ 0 & 0 & \varepsilon_{11}^j \end{bmatrix}$$

due to the isotropic nature of both constituents, respectively, for both conditions (13) (that is into the area(j), $j = 1, 2$). As regard to equations (2), (11); (3), (11) and (4), (11), respectively, we can note that $W^{[u]c\_x_3} \equiv W^{j\_x_3}$, with $W = \xi$, τ and Θ, for area(j). Such a simplification leads to ($j = 1$ and 2)

$$\xi^{j\_x_3} = \begin{bmatrix} 1/2 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & f_j \end{bmatrix}, \qquad \tau^{j\_x_3} = \begin{bmatrix} f_j & 0 & 0 \\ 0 & f_j & 0 \\ 0 & 0 & 1/2 \end{bmatrix}$$

and (14)

$$\Theta^{j\_x_3} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \varepsilon_{11}^{j\_x_3} \end{bmatrix}.$$

In this way (figure 3), equations (7) and (9) allow us to define $X^{[c]u\_x_1} \equiv X^{j\_x_1}$ with $X = \xi$, τ and Θ, for area(j) ($j = 1, 2$):

$$\xi^{j\_x_1} = \begin{bmatrix} f_j & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 1/2 \end{bmatrix}, \qquad \tau^{j\_x_1} = \begin{bmatrix} 1/2 & 0 & 0 \\ 0 & f_j & 0 \\ 0 & 0 & f_j \end{bmatrix}$$

and (15)

$$\Theta^{j\_x_1} = \begin{bmatrix} \varepsilon_{11}^{j\_x_1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Then, according to equations (5) and (8), featuring the lines- and columns-1D-SL, we obtain

$$\left\{\underline{\varepsilon}_{\text{eff}}^{v=x_3 \text{ or } x_1}\right\} \equiv \left\{ {}^{[u]}_{[c]}\text{1D-SL}, v\equiv\left\{\begin{matrix}x_3\\x_1\end{matrix}\right\} \atop \underline{\varepsilon}_{\text{eff}} \right\} = \left[\sum_{j=1}^{2} \tau^{j\_v}\varepsilon^j\left(\Theta^{j\_v}\right)^{-1}\Theta^{1\_v}\right]\left[\sum_{j=1}^{2} \xi^{j\_v}\left(\Theta^{j\_v}\right)^{-1}\Theta^{1\_v}\right]^{-1}$$

$$= \begin{cases} \begin{pmatrix} f_1\varepsilon_{11}^1 + f_2\varepsilon_{11}^2 & 0 & 0 \\ 0 & f_1\varepsilon_{11}^1 + f_2\varepsilon_{11}^2 & 0 \\ 0 & 0 & \left(\varepsilon_{11}^1\varepsilon_{11}^2/\left(f_1\varepsilon_{11}^2 + f_2\varepsilon_{11}^1\right)\right) \end{pmatrix} & \text{for} \quad v = x_3, \\ \begin{pmatrix} \left(\varepsilon_{11}^1\varepsilon_{11}^2/\left(f_1\varepsilon_{11}^2 + f_2\varepsilon_{11}^1\right)\right) & 0 & 0 \\ 0 & f_1\varepsilon_{11}^1 + f_2\varepsilon_{11}^2 & 0 \\ 0 & 0 & f_1\varepsilon_{11}^1 + f_2\varepsilon_{11}^2 \end{pmatrix} & \text{for} \quad v = x_1. \end{cases} \tag{16}$$

It is clear that we obtain the canonical Wiener's bounds [25] for the effective permittivity as isotropic limiting cases of our formulation. Thus, for 1D-SLs involving only two different isotropic materials, the general matrix formulations (5) and (8) lead to the classical concept of permittivity called form birefringence [9–12]. Indeed, such particular 1D-SLs (equation (16)) behave as anisotropic effective materials which exhibit tetragonal $\bar{4}2m$ symmetry.

Moreover, in the simplified 2D-SL topologic example, we can simplify the notation according to the position of the second constituent (figure 3). Then, in equations (6), (7), and (10), (11), respectively, we can simplify the notation for both c and u even (=2b) as

$$\Theta_{\text{eff}}^{c\_x_3} = \Theta^{2\_x_3} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \varepsilon_{11}^2 \end{bmatrix} \qquad \text{and} \qquad \Theta_{\text{eff}}^{u\_x_1} = \Theta^{2\_x_1} = \begin{bmatrix} \varepsilon_{11}^2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

according to $\underline{\varepsilon}_{\text{eff}\,11}^{[u]1\text{D-SL}\_x_3} = \underline{\varepsilon}_{\text{eff}\,33}^{[c]1\text{D-SL}\_x_1} = \varepsilon_{11}^2$ in equations (7) and (11). Indeed, we can note that in such a simplified case, all the even lines- or columns-1D-SLs are equivalent to the second isotropic constituent of the 2D-SL (figure 3).

Moreover, for the odd lines- and columns-1D-SL (c and u odd $= (2a+1)$), according to equation (16) we have, respectively,

$$\Theta_{\text{eff}}^{u\_x_1} = \Theta_{\text{eff}}^{1\_x_1} = \begin{pmatrix} f_1\varepsilon_{11}^1 + f_2\varepsilon_{11}^2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

(equation (9)) and

$$\Theta_{\text{eff}}^{c\_x_3} = \Theta_{\text{eff}}^{1\_x_3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \left(\varepsilon_{11}^1\varepsilon_{11}^2 / \left(f_1\varepsilon_{11}^2 + f_2\varepsilon_{11}^1\right)\right) \end{pmatrix}$$

(equation (11)), as a characteristic property of the same periodicity $(\varepsilon^1|\varepsilon^2|\varepsilon^1|\varepsilon^2\ldots)$ for such 2D-SL along the x_1- and x_3-directions (figure 3).

Then, in the case of 2D-SLs involving only two different isotropic materials (figure 3), the matrix formulation (equations (6) and (10)) of the effective permittivity tensors' bounds leads to the expression

$$\underline{\underline{\varepsilon}}_{\text{eff}}^{2\text{D-SL}\_(z\circ v)\equiv\left\{\substack{x_1\circ x_3 \\ x_3\circ x_1}\right\}} = \left[\sum_{j=1}^{2} \tau^{j\_z}\left\{\underline{\varepsilon}_{\text{eff}}^{v}\right\}\left(\Theta_{\text{eff}}^{j\_z}\right)^{-1}\Theta_{\text{eff}}^{1\_z}\right]\left[\sum_{j=1}^{2}\xi^{j\_z}\left(\Theta_{\text{eff}}^{j\_z}\right)^{-1}\Theta_{\text{eff}}^{1\_z}\right]^{-1}$$

$$= \begin{cases} \begin{pmatrix} \frac{\varepsilon_{11}^2\left(f_1\varepsilon_{11}^1+f_2\varepsilon_{11}^2\right)}{f_1\varepsilon_{11}^2+f_1f_2\varepsilon_{11}^1+(f_2)^2\varepsilon_{11}^2} & 0 & 0 \\ 0 & (f_1)^2\varepsilon_{11}^1 + f_1f_2\varepsilon_{11}^2 + f_2\varepsilon_{11}^2 & 0 \\ 0 & 0 & \frac{\varepsilon_{11}^2\left(f_1\varepsilon_{11}^1+f_1f_2\varepsilon_{11}^2+(f_2)^2\varepsilon_{11}^1\right)}{f_1\varepsilon_{11}^2+f_2\varepsilon_{11}^1} \end{pmatrix} \\ \text{for} \quad z\circ v = x_1\circ x_3, \\ \\ \begin{pmatrix} \frac{\varepsilon_{11}^2\left(f_1\varepsilon_{11}^1+f_1f_2\varepsilon_{11}^2+(f_2)^2\varepsilon_{11}^1\right)}{f_1\varepsilon_{11}^2+f_2\varepsilon_{11}^1} & 0 & 0 \\ 0 & (f_1)^2\varepsilon_{11}^1 + f_1f_2\varepsilon_{11}^2 + f_2\varepsilon_{11}^2 & 0 \\ 0 & 0 & \frac{\varepsilon_{11}^2\left(f_1\varepsilon_{11}^1+f_2\varepsilon_{11}^2\right)}{f_1\varepsilon_{11}^2+f_1f_2\varepsilon_{11}^1+(f_2)^2\varepsilon_{11}^2} \end{pmatrix} \\ \text{for} \quad z\circ v = x_3\circ x_1. \end{cases} \tag{17}$$

One should note that no indetermination occurs regarding the component of the tensor $\underline{\underline{\varepsilon}}_{\text{eff}\,22}^{2\text{D-SL}} = (f_1)^2\varepsilon_{11}^1 + f_1f_2\varepsilon_{11}^2 + f_2\varepsilon_{11}^2$ that accounts for a $(x_2\circ x_2)$ composition law. Conversely, the other ones lead to the concept of bounds since there are two different ways to shape the 2D-SL via, respectively, the $(x_1\circ x_3)$ and $(x_3\circ x_1)$ compositions laws. One can verify the validity of the three expressions according to the results $\varepsilon_{\text{eff}\,11}^{2\text{D-SL}} = \varepsilon_{\text{eff}\,22}^{2\text{D-SL}} = \varepsilon_{\text{eff}\,33}^{2\text{D-SL}} = \varepsilon_{11}^1$ when $f_1 = 1$ ($f_2 = 0$, that is considering only one bulk constituent ε^1) and $\varepsilon_{\text{eff}\,11}^{2\text{D-SL}} = \varepsilon_{\text{eff}\,22}^{2\text{D-SL}} = \varepsilon_{\text{eff}\,33}^{2\text{D-SL}} = \varepsilon_{11}^2$

when $f_2 = 1$ ($f_1 = 0$, with only one bulk constituent ε^2). These results can be expressed in the case of two isotropic materials with the notation $f_1 = f, f_2 = 1 - f$ and $\varepsilon_{11}^j = \varepsilon^j$ (for $j = 1$ and 2) on the results $\varepsilon_{\text{eff\_}x_2} = f^2\varepsilon^1 + (1 - f^2)\varepsilon^2$, and $\underline{\underline{\varepsilon}}_{\text{eff}}^{\text{2D-SL\_Lower}} \leqslant \underline{\underline{\varepsilon}}_{\text{eff}}^{\text{2D-SL}} \leqslant \underline{\underline{\varepsilon}}_{\text{eff}}^{\text{2D-SL\_Upper}}$, with $\underline{\underline{\varepsilon}}_{\text{eff}}^{\text{2D-SL\_Lower}} = \varepsilon^2 \cdot \frac{f\varepsilon^1+(1-f)\varepsilon^2}{f\varepsilon^2+f(1-f)\varepsilon^1+(1-f)^2\varepsilon^2}$ and $\underline{\underline{\varepsilon}}_{\text{eff}}^{\text{2D-SL\_Upper}} = \varepsilon^2 \cdot \frac{f\varepsilon^1+f(1-f)\varepsilon^2+(1-f)^2\varepsilon^1}{f\varepsilon^2+(1-f)\varepsilon^1}$, respectively, called the lower and upper canonical Lichtenecker's bounds on permittivity [4, 5]. Thus, it is clear that the concept of Wiener's and Lichtenecker's bounds directly stems from our general composition formulation. In this way, the approach given by relationships (6), (10) and (12) is more global as an overall matrix composition formulation of the concept of bounds fitted for effective dielectric tensors of SLs with a double periodicity composed by a multilayer array structure of alternating ($N \times M$) rectangular dielectric cells. Equations (6), (7), (10) and (11) provide comprehensive analytical formulations intended to unify the notion of effective dielectric constants for 2D-SL of arbitrary symmetry.

Moreover, we can verify, with the limiting case of a single (that is $M = N = 1$) homogeneous anisotropic material, the validity of this formulation. By considering only one anisotropic cell material with the fractions $f_{c=1\_x_3} = 1$ (with $c = 1$ the column fixed) and $f_{c\_x_3} = 0$ (with $\forall c \neq 1$, that is without another column), the matrix relation (5) is simplified ($c = 1$ to be considered fixed in the summation):

$$\left\{\underline{\underline{\varepsilon}}_{\text{eff}}^{\text{1D-SL\_}x_3}\right\} = \left[\tau^{1\_x_3}\, \varepsilon^{1\_x_3} (\Theta^{1\_x_3})^{-1} \Theta^{1\_x_3}\right]\left[\xi^{1\_x_3} (\Theta^{1\_x_3})^{-1} \Theta^{1\_x_3}\right]^{-1}. \tag{18}$$

The (3×3) matrix $\varepsilon^{1\_x_3}$ in equation (18) represents the permittivity tensors of the single homogeneous anisotropic material. According to equations (2) and (3) in this particular case, we can remark that

$$\tau^{1\_x_3} = \xi^{1\_x3} = \text{Id}_{3\times 3} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

($M = 1$ and $f_{c=1\_x_3} = 1$); then, simplifications lead to $\left\{\underline{\underline{\varepsilon}}_{\text{eff}}^{\text{1D-SL\_}x_3}\right\} = [\text{Id}_{3\times 3}\varepsilon^{1\_x_3} (\Theta^{1\_x_3})^{-1} \Theta^{1\_x_3}][\text{Id}_{3\times 3}(\Theta^{1\_x_3})^{-1}\Theta^{1\_x_3}]^{-1} = [\text{Id}_{3\times 3}\varepsilon^{1\_x_3}(\Theta^{1\_x_3})^{-1}\Theta^{1\_x_3}(\Theta^{1\_x_3})^{-1}\Theta^{1\_x_3}\text{Id}_{3\times 3}] = \varepsilon^{1\_x_3}$. In the same way, equation (6) leads to the relevant result $\underline{\underline{\varepsilon}}_{\text{eff}}^{\text{2D-SL\_}(x_1\circ x_3)} = \varepsilon^{1\_x_3}$. It is easy to verify that with the other alternative composition ($x_3\circ x_1$) (equations (8) and (10)) the result is the same, that is $\underline{\underline{\varepsilon}}_{\text{eff}}^{\text{2D-SL\_}(x_3\circ x_1)} = \varepsilon^{1\_x_3} = \underline{\underline{\varepsilon}}_{\text{eff}}^{\text{2D-SL\_}(x_1\circ x_3)}$. Then, in such a limiting case (single homogeneous anisotropic material), we do not have to sum into the matrix relation because only one cell is to be considered. Then, due to the localization of the cell, it is not necessary to unfold in the (x_1, x_3)-plane the alternative composition law and we find that the notion of bounds (equations (6) and (10)) is naturally degenerated into only one matrix expression $\varepsilon^{1\_x_3}$ regarding the matrix permittivity of the single anisotropic cell material.

In conclusion, the new approach, based on an alternative composition method, presented in this paper can deal with the anisotropic nature of materials, that is dielectric tensors and space fractions. This formulation, taking account of the boundary conditions, yields an interesting improvement of the concept of effective dielectric tensor bounds and the notion of form birefringence ascribed to a 2D-SL topology. As demonstrated, the notions of Wiener's and Lichtenecker's bounds directly stem from such a global formulation as isotropic limiting cases when considering the simplified case of a 2D-SL comprising two different isotropic materials with the same periodicity in both directions. Moreover, the validity of the general effective permittivity expressions (6) and (10) has been tested on the limiting case of a single homogeneous anisotropic material. The general expressions of the dielectric tensor bounds ((6) and (10)) involving, respectively, equations (5) and (8), stress that this matrix formulation is based on relevant composition laws ($x_1 \circ x_3$) and ($x_3 \circ x_1$); moreover, this formulation is based directly on the notion of inclusions due to the discretization approach by cells. Such a composition law formulation is conveniently fitted to depict more general multi-scale 2D-SLs that could encompass another 2D-SL located in given rectangular dielectric bars (that is based on the location of 2D-SLs in some columns' elements of the general structure 2D-SL). Such a formulation seems to be adapted to define information on the permittivity tensors and on particular limiting special cases of the generalized 3D unity cell model like coated inclusion by using adapted and variable discretization step on the three directions of the 3D-SLs. Moreover, it is expected that such a generalized approach will be of substantial interest to designing new integrated components in optical telecommunication based on the form birefringence.

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