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THE EFFECTIVE CONSTITUTIVE PARAMETERS AT INTERFACE OF DIFFERENT MEDIA

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Abstract—This paper presents a new approach to estimate effective constitutive parameters for a cell across an interface between two bi-anisotropic media. The work is different from those studying effective properties of bi-anisotropic mixtures in that the boundary conditions of field components are taken into consideration. The degenerated cases, including interfaces of two bi-isotropic, anisotropic and isotropic media, are discussed respectively in detail. Simulation for anisotropic media shows significant improvements can be expected from the adoption of the new approach.

Appendix A.

Acknowledgment

References

1. INTRODUCTION

One important step in the process of analyzing an electromagnetic band gap (EBG) structure using plane wave expansion (PWE) method is to solve an operator eigen equation like one in [1]:

$$\left(\nabla + j\vec{k}\right) \times \frac{1}{\varepsilon_r(\vec{r})} \left(\nabla + j\vec{k}\right) \times \sum_{\vec{G}} \vec{H}_{\vec{G}} e^{-j\vec{G}\cdot\vec{r}} = \frac{\omega^2}{c^2} \sum_{\vec{G}} \vec{H}_{\vec{G}} e^{-j\vec{G}\cdot\vec{r}} \quad (1)$$

where $\vec{G}$ are reciprocal lattice vectors and $\vec{k}$ is a given wave vector. An iterative eigen solver is attractive since the equivalent matrix of Eq. (1) is a sparse one [1]. The solver will require a procedure where a new vector (in the sense of linear algebra) is produced by operating the operator onto an old vector. According to Eq. (1) , this procedure will include the following steps: a given vector

$$\left([H_x, H_y, H_z]_{\vec{G}_1}, [H_x, H_y, H_z]_{\vec{G}_2}, [H_x, H_y, H_z]_{\vec{G}_3}, \ldots, [H_x, H_y, H_z]_{\vec{G}_N}\right)^T$$

is first modified by a curl operation, then three fast Fourier transforms are performed to transform the xyz components of this vector into the spatial domain. The resultant vector is further divided by medium parameters ε at respective spatial points, inverse fast-Fourier-transformed to the spectral domain, modified by another curl operation and at last

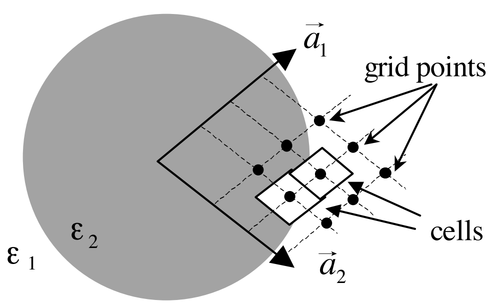

Figure 1. Spatial discretization: cells across an interface.

output as a new vector. Since the calculation of $\vec{E}(\vec{r}) = \vec{D}(\vec{r})/\varepsilon(\vec{r})$ is done only at discrete grid points, this procedure is only reasonable for those grid points whose affiliated cell is filled with a homogeneous medium. For cells running across an interface of different media, a different profile of the interface is chosen which is different from the original one (see Fig. 1) and thus errors will be introduced due to the inaccurate representation of the interface profile. In order to reduce these errors, an effective permittivity instead of the true one at a grid point should be used.

2. NOTATIONS

(1) A tilde "∼" over a field component denotes the unique (i.e., effective) value of this non-continuous component accross the interface within a cell.

(2) A superscript "*ave*" denotes the direct volume-averaging value of a medium parameter over the cell:

$$Q^{\text{ave}} = \frac{1}{V_{\text{cell}}} \int\limits_{\text{cell}} Q(\vec{r})dV = \sum_{i=1}^{2} Q_i \frac{V_i}{V_{\text{cell}}} \tag{2}$$

where V_1 and V_2 are the volumes of individual medium in a cell and V_{cell} the volume of the cell. Note that Q can be any expression of media parameters. It may be ε and ε^{-1}. It may also be $\overline{\overline{\varepsilon}}$, $\overline{\overline{\varepsilon}}^{-1}$, $\begin{pmatrix} \overline{\overline{\varepsilon}} & \overline{\overline{\xi}} \\ \overline{\overline{\zeta}} & \overline{\overline{\mu}} \end{pmatrix}$ or $\begin{pmatrix} \overline{\overline{\varepsilon}} & \overline{\overline{\xi}} \\ \overline{\overline{\zeta}} & \overline{\overline{\mu}} \end{pmatrix}^{-1}$.

(3) Double over-bar denotes a dyadic. A dyadic can be expanded in any orthonormal basis $(\vec{u}_1, \vec{u}_2, \vec{u}_3)$ as: $\overline{\overline{A}} = \sum_{i=1}^{3} \sum_{j=1}^{3} A_{ij}\vec{u}_i\vec{u}_j$. Its matrix element $A_{ij} = \vec{u}_i \cdot \overline{\overline{A}} \cdot \vec{u}_j$ depends on the chosen vector basis. The relation between a dyadic and its characteristic matrix can also be expressed in the form:

$$\overline{\overline{A}} = (\vec{u}_1, \vec{u}_2, \vec{u}_3)_{1\times 3}[A]_{3\times 3}(\vec{u}_1, \vec{u}_2, \vec{u}_3)^T_{3\times 1} \tag{3}$$

$$[A]_{3\times 3} = (\vec{u}_1, \vec{u}_2, \vec{u}_3)^T_{3\times 1} \cdot \overline{\overline{A}}_{1\times 1} \cdot (\vec{u}_1, \vec{u}_2, \vec{u}_3)_{1\times 3} \tag{4}$$

(4) Superscript "EFF" denotes the indirect averaging value (i.e., an algebraic expression of other direct volume-averaging media parameters) over the cell.

(5) Assume that the interface within a cell is a plane whose normal $\hat{n}$ is given, the basis of the local coordinates system can be chosen as the basis of the spherical coordinates system: $\hat{n} = \hat{r}, \hat{t} = \hat{\theta}, \hat{\tau} = \hat{\phi}$.

(6) The transform matrix $[T]$ of two coordinates systems, the bases of which are $(\hat{t}, \hat{\tau}, \hat{n})$ and $(\hat{x}, \hat{y}, \hat{z})$ respectively, is defined as:

$$(\hat{t}\ \hat{\tau}\ \hat{n})_{1\times 3} = (\hat{x}\ \hat{y}\ \hat{z})_{1\times 3}[T]_{3\times 3} \text{ with } [T]^T[T] = [T]^{-1}[T] = [I]. \quad (5)$$

3. EFFECTIVE MEDIA PARAMETERS FOR ISOTROPIC MEDIA

For a cell filling with two different isotropic media, different components of fields (normal or tangential) should be treated in different ways. This results in the following well-known relations:

$$\begin{cases} \tilde{D}_{t,\tau} = \varepsilon^{\text{ave}} E_{t,\tau} \\ \tilde{E}_n = \left(\varepsilon^{-1}\right)^{\text{ave}} D_n \end{cases} \tag{6}$$

The dyadic form of Eq. (6) is

$$\vec{D} = \overline{\overline{\varepsilon}}^{\text{EFF}} \cdot \vec{E} \tag{7}$$

where $\vec{D} = \tilde{D}_t\hat{t} + \tilde{D}_\tau\hat{\tau} + D\hat{n}$, $\vec{E} = E_t\hat{t} + E_\tau\hat{\tau} + \tilde{E}_n\hat{n}$ and

$$\overline{\overline{\varepsilon}}^{\text{EFF}} = \varepsilon^{\text{ave}}\left(\overline{\overline{I}} - \hat{n}\hat{n}\right) + \left(\left(\varepsilon^{-1}\right)^{\text{ave}}\right)^{-1}\hat{n}\hat{n} \tag{8}$$

where $\overline{\overline{I}} = \hat{t}\hat{t} + \hat{\tau}\hat{\tau} + \hat{n}\hat{n}$ is a unit dyadic.

4. EFFECTIVE MEDIA PARAMETERS FOR COMPLEX MEDIA, OLD APPROACH

A formula to compute the effective parameters for isotropic and anisotropic media is suggested [1], following the same fashion as Eq. (8):

$$\begin{aligned} \overline{\overline{\varepsilon}}^{\text{EFF}} &= \frac{1}{2}\left(\overline{\overline{\varepsilon}}^{\text{ave}} \cdot \left(\overline{\overline{I}} - \hat{n}\hat{n}\right) + \left(\overline{\overline{I}} - \hat{n}\hat{n}\right) \cdot \overline{\overline{\varepsilon}}^{\text{ave}}\right) \\ &\quad + \frac{1}{2}\left(\left(\left(\overline{\overline{\varepsilon}}^{-1}\right)^{\text{ave}}\right)^{-1} \cdot \hat{n}\hat{n} + \hat{n}\hat{n} \cdot \left(\left(\overline{\overline{\varepsilon}}^{-1}\right)^{\text{ave}}\right)^{-1}\right). \end{aligned} \tag{9}$$

For the most general bi-anisotropic media, a similar formula to calculate the effective constitutive parameters over a cell is suggested [3]:

$$\begin{aligned} \begin{pmatrix} \overline{\overline{\varepsilon}} & \overline{\overline{\xi}} \\ \overline{\overline{\zeta}} & \overline{\overline{\mu}} \end{pmatrix}^{\text{EFF}} &= \begin{pmatrix} \overline{\overline{\varepsilon}} & \overline{\overline{\xi}} \\ \overline{\overline{\zeta}} & \overline{\overline{\mu}} \end{pmatrix}^{\text{ave}} \cdot \begin{pmatrix} \overline{\overline{I}} - \hat{n}\hat{n} & 0 \\ 0 & \overline{\overline{I}} - \hat{n}\hat{n} \end{pmatrix} \\ &\quad + \left(\left(\begin{pmatrix} \overline{\overline{\varepsilon}} & \overline{\overline{\xi}} \\ \overline{\overline{\zeta}} & \overline{\overline{\mu}} \end{pmatrix}^{-1}\right)^{\text{ave}}\right)^{-1} \cdot \begin{pmatrix} \hat{n}\hat{n} & 0 \\ 0 & \hat{n}\hat{n} \end{pmatrix}. \end{aligned} \tag{10}$$

If one examines Eq. (9) or (10) carefully, he will find out that they are not as rigorous as Eq. (8). The weakness is caused by the dyadic nature of the media parameters. In Eq. (8), the result of $(\overline{\overline{I}}-\hat{n}\hat{n})\cdot\vec{E}$ is the tangential component of $\vec{E}$ and $\varepsilon(\overline{\overline{I}}-\hat{n}\hat{n})\cdot\vec{E}$ results in the tangential component of $\vec{D}$. In Eq. (9) or (10), however, the term $\overline{\overline{\varepsilon}}^{ave}\cdot(\overline{\overline{I}}-\hat{n}\hat{n})\cdot\vec{E}$ does not always yield the tangential component of $\vec{D}$. Although the term $(\overline{\overline{I}}-\hat{n}\hat{n})\cdot\overline{\overline{\varepsilon}}^{ave}\cdot\vec{E}$ in Eq. (9) represents the tangential component of $\vec{D}$, it utilizes the whole $\vec{E}$ instead of the tangential component of it.

The situation can be partly improved by starting the work in the following way:

$$\left\{\begin{array}{rcl}\left(\overline{\overline{I}}-\hat{n}\hat{n}\right)\cdot\vec{D} & = & \left(\overline{\overline{I}}-\hat{n}\hat{n}\right)\cdot\overline{\overline{\varepsilon}}\cdot\left(\overline{\overline{I}}-\hat{n}\hat{n}\right)\cdot\vec{E}\\ \hat{n}\hat{n}\cdot\vec{D} & = & \hat{n}\hat{n}\cdot\overline{\overline{\varepsilon}}\cdot\hat{n}\hat{n}\cdot\vec{E}\end{array}\right. \tag{11}$$

Now tangential $\vec{D}$ is related to tangential $\vec{E}$ by $(\overline{\overline{I}}-\hat{n}\hat{n})\cdot\overline{\overline{\varepsilon}}$ and normal $\vec{D}$ is related to normal $\vec{E}$ by $\hat{n}\hat{n}\cdot\overline{\overline{\varepsilon}}$. The resulted effective dyadic permittivity will be:

$$\overline{\overline{\varepsilon}}^{EFF}=\left[\left(\overline{\overline{I}}-\hat{n}\hat{n}\right)\cdot\overline{\overline{\varepsilon}}\right]^{ave}\cdot\left(\overline{\overline{I}}-\hat{n}\hat{n}\right)+\left(\left[\left(\hat{n}\hat{n}\cdot\overline{\overline{\varepsilon}}\right)^{-1}\right]^{ave}\right)^{-1}\cdot\hat{n}\hat{n}. \tag{12}$$

However, Eq. (11) is still not perfect since there are two other possibilities:

$$\left\{\begin{array}{rcl}\hat{n}\hat{n}\cdot\vec{D} & = & \hat{n}\hat{n}\cdot\overline{\overline{\varepsilon}}\cdot\left(\overline{\overline{I}}-\hat{n}\hat{n}\right)\cdot\vec{E}\\ \left(\overline{\overline{I}}-\hat{n}\hat{n}\right)\cdot\vec{D} & = & \left(\overline{\overline{I}}-\hat{n}\hat{n}\right)\cdot\overline{\overline{\varepsilon}}\cdot\hat{n}\hat{n}\cdot\vec{E}\end{array}\right. \tag{13}$$

That is the tangential $\vec{E}$ will induce normal $\vec{D}$ and normal $\vec{E}$ will induce tangential $\vec{D}$. The former is simple since both normal $\vec{D}$ and tangential $\vec{E}$ remain constant over the cell. The latter is rather difficult to cope with since both normal $\vec{E}$ and tangential $\vec{D}$ are not constant over the cell. Not to say how to integrate both Eq. (11) and (13) together to produce a reasonable effective dyadic permittivity.

5. EFFECTIVE MEDIA PARAMETERS FOR COMPLEX MEDIA, NEW APPROACH

Since the amount of continuous components is equal to that of non-continuous components for either a $\vec{D}\vec{E}$ pair or a $\vec{D}\vec{B}\vec{E}\vec{H}$ quadriad, the new approach starts by expressing the non-continuous components in terms of continuous ones, doing averaging and then re-expressing the flux density in terms of field strength or vice versa.

5.1. General Procedure

For two bi-anisotropic media, the constitutive relations are:

$$\begin{pmatrix} \vec{D} \\ \vec{B} \end{pmatrix} = \begin{pmatrix} \overline{\overline{\varepsilon}} & \overline{\overline{\xi}} \\ \overline{\overline{\zeta}} & \overline{\overline{\mu}} \end{pmatrix}_i \cdot \begin{pmatrix} \vec{E} \\ \vec{H} \end{pmatrix}, \qquad i = 1, 2. \tag{14}$$

In the $t\tau n$ system, the matrix form of Eq. (14) is:

$$\begin{aligned} \begin{pmatrix} (D_t & D_\tau & D_n)^T \\ (B_t & B_\tau & B_n)^T \end{pmatrix} &= \begin{pmatrix} [\varepsilon_T] & [\xi_T] \\ [\zeta_T] & [\mu_T] \end{pmatrix}_i \begin{pmatrix} (E_t & E_\tau & E_n)^T \\ (H_t & H_\tau & H_n)^T \end{pmatrix}, \\ i &= 1, 2 \end{aligned} \tag{15}$$

where 3 by 3 matrices $[\varepsilon_T]_i$, $[\xi_T]_i$, $[\zeta_T]_i$ and $[\mu_T]_i$ are defined as:

$$[Q_T]_i = [T]^T [Q]_i [T], \qquad Q = \varepsilon, \xi, \zeta, \mu.$$

Blocks $[\varepsilon]_i$, $[\xi]_i$, $[\zeta]_i$ and $[\mu]_i$ are coefficient matrices (in the xyz system) of dyadic in Eq. (14). They are defined in the following way:

$$[Q]_{3\times 3} = (\hat{x} \quad \hat{y} \quad \hat{z})^T_{3\times 1} \cdot \overline{\overline{Q}}_{1\times 1} \cdot (\hat{x} \quad \hat{y} \quad \hat{z})_{1\times 3}, \; Q = \varepsilon, \xi, \zeta, \mu$$

and they are coordinates-system dependent.

After exchanging D_n with E_n and B_n with H_n in Eq. (15) (see Appendix A), one gets:

$$\begin{aligned} \begin{pmatrix} (D_t & D_\tau & E_n)^T \\ (B_t & B_\tau & H_n)^T \end{pmatrix} &= \begin{pmatrix} [\varepsilon_{T'}] & [\xi_{T'}] \\ [\zeta_{T'}] & [\mu_{T'}] \end{pmatrix}_i \begin{pmatrix} (E_t & E_\tau & D_n)^T \\ (H_t & H_\tau & B_n)^T \end{pmatrix}, \\ i &= 1, 2 \end{aligned} \tag{16}$$

Now volume-averaging procedure can be applied to all the elements of $[\varepsilon_{T'}]_i$, $[\xi_{T'}]_i$, $[\zeta_{T'}]_i$ and $[\mu_{T'}]_i$ in Eq. (16). Non-continuous components D_t, D_τ, E_n, B_t B_τ and H_n in Eq. (16) can be evaluated in the following way:

$$\begin{pmatrix} (\tilde{D}_t & \tilde{D}_\tau & \tilde{E}_n)^T \\ (\tilde{B}_t & \tilde{B}_\tau & \tilde{H}_n)^T \end{pmatrix} = \begin{pmatrix} [\varepsilon^{\text{ave}}_{T'}] & [\xi^{\text{ave}}_{T'}] \\ [\zeta^{\text{ave}}_{T'}] & [\mu^{\text{ave}}_{T'}] \end{pmatrix} \begin{pmatrix} (E_t & E_\tau & D_n)^T \\ (H_t & H_\tau & B_n)^T \end{pmatrix}. \tag{17}$$

Exchanging $\tilde{E}_n$ with D_n and $\tilde{H}_n$ with B_n in Eq. (17) yields:

$$\begin{pmatrix} (\tilde{D}_t & \tilde{D}_\tau & D_n)^T \\ (\tilde{B}_t & \tilde{B}_\tau & B_n)^T \end{pmatrix} = \begin{pmatrix} [\varepsilon^{\text{EFF}}_{T}] & [\xi^{\text{EFF}}_{T}] \\ [\zeta^{\text{EFF}}_{T}] & [\mu^{\text{EFF}}_{T}] \end{pmatrix} \begin{pmatrix} (E_t & E_\tau & \tilde{E}_n)^T \\ (H_t & H_\tau & \tilde{H}_n)^T \end{pmatrix}. \tag{18}$$

The matrix forms of effective constitutive parameters in the xyz system can be obtained in the following way:

$$\left[Q^{\mathrm{EFF}}\right] = [T]\left[Q_T^{\mathrm{EFF}}\right][T]^T, \qquad Q = \varepsilon, \xi, \zeta, \mu. \tag{19}$$

The respective dyadic forms can be obtained formally in the following way:

$$\overline{\overline{Q}}^{\mathrm{EFF}} = (\hat{t}\ \hat{\tau}\ \hat{n})\left[Q_T^{\mathrm{EFF}}\right](\hat{t}\ \hat{\tau}\ \hat{n})^T, \qquad Q = \varepsilon, \xi, \zeta, \mu. \tag{20}$$

From the procedure above one can see that this new approach is as rigorous as that in isotropic case (Eq. 8).

5.2. Effective Medium Parameters for Bi-Isotropic Media

For bi-isotropic medium, the constitutive relations are formulated as:

$$\begin{pmatrix} \vec{D} \\ \vec{B} \end{pmatrix} = \begin{pmatrix} \varepsilon & \xi \\ \zeta & \mu \end{pmatrix}_i \begin{pmatrix} \vec{E} \\ \vec{H} \end{pmatrix}, \qquad i = 1, 2 \tag{21}$$

Blocks $[\varepsilon_{T'}]_i$, $[\xi_{T'}]_i$, $[\zeta_{T'}]_i$ and $[\mu_{T'}]_i$ in (16) can be easily derived as

$$\begin{pmatrix} [\varepsilon_{T'}] & [\xi_{T'}] \\ [\zeta_{T'}] & [\mu_{T'}] \end{pmatrix}_i = \begin{pmatrix} \begin{pmatrix} \varepsilon & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & -\overline{\mu} \end{pmatrix} & \begin{pmatrix} \xi & 0 & 0 \\ 0 & \xi & 0 \\ 0 & 0 & -\overline{\xi} \end{pmatrix} \\ \begin{pmatrix} \zeta & 0 & 0 \\ 0 & \zeta & 0 \\ 0 & 0 & -\overline{\zeta} \end{pmatrix} & \begin{pmatrix} \mu & 0 & 0 \\ 0 & \mu & 0 \\ 0 & 0 & \overline{\varepsilon} \end{pmatrix} \end{pmatrix}_i, \quad i = 1, 2 \tag{22}$$

where $\overline{Q}_i = Q_i/(\varepsilon_i\mu_i - \xi_i\zeta_i)$, $Q = \varepsilon, \xi, \zeta, \mu$.

The effective medium parameters in $t\tau n$ system, namely blocks $[\varepsilon_T^{\mathrm{EFF}}]$, $[\xi_T^{\mathrm{EFF}}]$, $[\zeta_T^{\mathrm{EFF}}]$, and $[\mu_T^{\mathrm{EFF}}]$ in (18) are:

$$\left[Q_T^{\mathrm{EFF}}\right] = \begin{pmatrix} Q^{\mathrm{ave}} & 0 & 0 \\ 0 & Q^{\mathrm{ave}} & 0 \\ 0 & 0 & Q_n^{\mathrm{EFF}} \end{pmatrix}, \qquad Q = \varepsilon, \xi, \zeta, \mu \tag{23}$$

where $Q_n^{\mathrm{EFF}} = \overline{Q}^{\mathrm{ave}}/(\overline{\varepsilon}^{\mathrm{ave}}\overline{\mu}^{\mathrm{ave}} - \overline{\xi}^{\mathrm{ave}}\overline{\zeta}^{\mathrm{ave}})$, $Q = \varepsilon, \xi, \zeta, \mu$.

The respective dyadic forms can be written as:

$$\overline{\overline{Q}}^{\mathrm{EFF}} = Q^{\mathrm{ave}}\left(\hat{t}\hat{t} + \hat{\tau}\hat{\tau}\right) + Q_n^{\mathrm{EFF}}\hat{n}\hat{n}, \qquad Q = \varepsilon, \xi, \zeta, \mu. \tag{24}$$

It is trivial to obtain Eq. (8) from (24) for the case where all the media are isotropic.

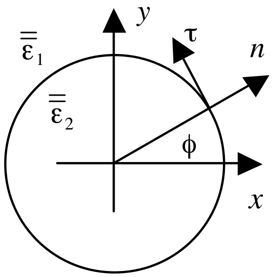

Figure 2. Local coordinates definition.

5.3. Effective Dyadic Permittivity for Anisotropic Media

For anisotropic media, only $\vec{D} \sim \vec{E}$ relation needs to be considered:

$$\vec{D} = \overline{\overline{\varepsilon}}_i \cdot \vec{E}, \qquad i = 1, 2 \tag{25}$$

To view the details of $\overline{\overline{\varepsilon}}^{\mathrm{EFF}}$, let us take a 2-D interface as an example (Fig. 2).

Let the cylinder be parallel to $\hat{z}$. Dyadic permittivities of two media are:

$$\overline{\overline{\varepsilon}}_i = \varepsilon_{11,i}\hat{x}\hat{x} + \varepsilon_{12,i}\hat{x}\hat{y} + \varepsilon_{21,i}\hat{y}\hat{x} + \varepsilon_{22,i}\hat{y}\hat{y} + \varepsilon_{33,i}\hat{z}\hat{z}, \qquad i = 1, 2,$$

and the unit vectors of the local coordinates system are

$$\begin{cases} \hat{t} = -\hat{z} \\ \hat{\tau} = -\sin\phi\hat{x} + \cos\phi\hat{y} \\ \hat{n} = \cos\phi\hat{x} + \sin\phi\hat{y} \end{cases}.$$

Then $[\varepsilon_T]_i$ (in $t\tau n$ system) in (15) can be derived as:

$$[\varepsilon_T]_i = \begin{pmatrix} \varepsilon_{T11} & 0 & 0 \\ 0 & \varepsilon_{T22} & \varepsilon_{T23} \\ 0 & \varepsilon_{T32} & \varepsilon_{T33} \end{pmatrix}_i, \qquad i = 1, 2 \tag{26}$$

where

$$\begin{aligned}
\varepsilon_{T11,i} &= \varepsilon_{33,i}, \\
\varepsilon_{T22,i} &= \varepsilon_{11,i}\sin^2\phi + \varepsilon_{22,i}\cos^2\phi - (\varepsilon_{21,i} + \varepsilon_{12,i})\sin\phi\cos\phi, \\
\varepsilon_{T33,i} &= \varepsilon_{11,i}\cos^2\phi + \varepsilon_{22,i}\sin^2\phi + (\varepsilon_{21,i} + \varepsilon_{12,i})\sin\phi\cos\phi, \\
\varepsilon_{T23,i} &= -\varepsilon_{12,i}\sin^2\phi + \varepsilon_{21,i}\cos^2\phi + (\varepsilon_{22,i} - \varepsilon_{11,i})\sin\phi\cos\phi, \\
\varepsilon_{T32,i} &= \varepsilon_{12,i}\cos^2\phi - \varepsilon_{21,i}\sin^2\phi + (\varepsilon_{22,i} - \varepsilon_{11,i})\sin\phi\cos\phi.
\end{aligned}$$

The matrix $[\varepsilon_{T'}^{\text{ave}}]$ (in the $t\tau n$ system) in (17) can be derived as:

$$[\varepsilon_{T'}^{\text{ave}}] = \begin{pmatrix} \varepsilon_{T'11}^{\text{ave}} & 0 & 0 \\ 0 & \varepsilon_{T'22}^{\text{ave}} & \varepsilon_{T'23}^{\text{ave}} \\ 0 & \varepsilon_{T'32}^{\text{ave}} & \varepsilon_{T'33}^{\text{ave}} \end{pmatrix} \tag{27}$$

where

$$\begin{aligned} \varepsilon_{T'11}^{\text{ave}} &= (\varepsilon_{T11})^{\text{ave}}, \\ \varepsilon_{T'22}^{\text{ave}} &= (\varepsilon_{T22} - \varepsilon_{T23}\varepsilon_{T32}/\varepsilon_{T33})^{\text{ave}}, \\ \varepsilon_{T'23}^{\text{ave}} &= (\varepsilon_{T23}/\varepsilon_{T33})^{\text{ave}}, \\ \varepsilon_{T'32}^{\text{ave}} &= -(\varepsilon_{T32}/\varepsilon_{T33})^{\text{ave}}, \\ \varepsilon_{T'33}^{\text{ave}} &= (1/\varepsilon_{T33})^{\text{ave}}. \end{aligned}$$

The dyadic form $\overline{\overline{\varepsilon}}^{\text{EFF}}$ in (20) can be derived as:

$$\overline{\overline{\varepsilon}}^{\text{EFF}} = \overline{\overline{\varepsilon}}_{T11}^{\text{EFF}}\hat{t}\hat{t} + \overline{\overline{\varepsilon}}_{T22}^{\text{EFF}}\hat{\tau}\hat{\tau} + \overline{\overline{\varepsilon}}_{T23}^{\text{EFF}}\hat{\tau}\hat{n} + \overline{\overline{\varepsilon}}_{T32}^{\text{EFF}}\hat{n}\hat{\tau} + \overline{\overline{\varepsilon}}_{T33}^{\text{EFF}}\hat{n}\hat{n} \tag{28}$$

where

$$\begin{aligned} \varepsilon_{T11}^{\text{EFF}} &= \varepsilon_{T'11}^{\text{ave}}, \\ \varepsilon_{T22}^{\text{EFF}} &= \varepsilon_{T'22}^{\text{ave}} - \varepsilon_{T'32}^{\text{ave}}\varepsilon_{T'23}^{\text{ave}}/\varepsilon_{T'33}^{\text{ave}}, \\ \varepsilon_{T23}^{\text{EFF}} &= \varepsilon_{T'23}^{\text{ave}}/\varepsilon_{T'33}^{\text{ave}}, \\ \varepsilon_{T32}^{\text{EFF}} &= -\varepsilon_{T'32}^{\text{ave}}/\varepsilon_{T'33}^{\text{ave}}, \\ \varepsilon_{T33}^{\text{EFF}} &= 1/\varepsilon_{T'33}^{\text{ave}}. \end{aligned}$$

If one works on Eq. (9), the effective dyadic looks like this:

$$\overline{\overline{\varepsilon}}_{\text{ref}}^{\text{EFF}} = (\varepsilon_{T11})^{\text{ave}}\hat{t}\hat{t} + (\varepsilon_{T22})^{\text{ave}}\hat{\tau}\hat{\tau} + (\cdots)\hat{\tau}\hat{n} + (\cdots)\hat{n}\hat{\tau} + (\cdots)\hat{n}\hat{n}. \tag{29}$$

where ε_{T11} and ε_{T22} are defined in (26). The first term in (29) is identical to $\varepsilon_{T11}^{\text{EFF}}$ in (28). The second term in (29) is different from $\varepsilon_{T22}^{\text{EFF}}$ in (28) and permuting and averaging in Eq. (9) cannot change the situation. They will become identical only when both $\varepsilon_{12,i} = \varepsilon_{21,i} = 0$ and $\varepsilon_{11,i} = \varepsilon_{22,i}$ hold. In other words, Eq. (9) is valid only when both permittivity dyadic are either isotropic or uni-axial. A similar conclusion can be drawn for Eq. (10): it is valid only when all the four dyadic $\overline{\overline{\varepsilon}}$, $\overline{\overline{\xi}}$, $\overline{\overline{\zeta}}$ and $\overline{\overline{\mu}}$ are either isotropic or uni-axial.

5.4. Numerical Example

The EBG structure is made of a triangular lattice of air cylinders embedded in an anisotropic host. The lattice constant is a and the radius of the cylinders is $r = 0.48a$. The permittivity of the host is

$$\bar{\bar{\varepsilon}}/\varepsilon_0 = 13\left(\hat{x}\hat{x} + \hat{y}\hat{y} + \hat{z}\hat{z}\right) + \varepsilon_{12} j\hat{x}\hat{y} - \varepsilon_{12} j\hat{y}\hat{x}. \tag{30}$$

Eq. (1) is solved using two software packages, one is mpb [1], the averaging scheme of which is Eq. (9) and the other is a component in wpb [3], developed by the author, the averaging scheme of which is Eq. (28). For a given ε_{12}, each software outputs 128 eigen values (16 k-points times 8 bands) and each eigen value is compared with its counterpart and the maximum difference is recorded. The result is presented in Table 1.

Table 1. Maximum difference of 128 pairs of eigen values from mpb and wpb.

ε_{12}	0.0	0.1	1.0	3.0	5.0	7.0	9.0	10.0	11.0
Maximum difference of eigen values from mpb and wpb(%)	0.98	0.98	0.98	0.98	6.10	6.23	12.07	16.42	11.37

From Table 1, one can see that when ε_{12} is small, the difference of eigen values from two approaches is trivial. A difference of about 1% is due to the different implementation of the software packages. For larger ε_{12}, the difference become larger too. This trend agrees well with the discussion in the previous section. It is obvious that the large differences are caused by the defect in the old approach.

6. CONCLUSION

A general but rigorous procedure is proposed to calculate effective medium parameters for cells running across an interface of two different media. It is rigorous because all the field components and all the media parameters are treated equally. No projection or permuting-averaging operation is involved. It is general since it can be applied to interfaces consisting of two media ranging from isotropic ones to bi-anisotropic ones.

APPENDIX A.

The way to express non-continuous components in terms of continuous ones is quite simple.

Firstly turning Eq. (15) into six homogenous equations yields:

$$\left\{\begin{array}{lcl} -[I][D]+[0][B]+[\varepsilon_T]_i[E]+[\xi_T]_i[H] & = & [0] \\ [0][D]-[I][B]+[\zeta_T]_i[E]+[\mu_T]_i[H] & = & [0] \end{array}\right., \quad i=1,2 \tag{A1}$$

where $[I]$ and $[0]$ are 3 by 3 unit matrix and zero matrix respectivley. Eq. (A1) can be also written in simple matrix form:

$$\begin{aligned}[A]_i(D_t\ D_\tau\ D_n\ B_t\ B_\tau\ B_n\ E_t\ E_\tau\ E_n\ H_t\ H_\tau\ H_n)^T \\ =(0\ 0\ 0\ 0\ 0\ 0)^T, \qquad i=1,2\end{aligned} \tag{A2}$$

where $[A]_i$ is a 6 by 12 matrix.

Secondly, exchanging the position of variable D_n with E_n, B_n with H_n yields a new coefficients matrix $[A']_i$ which satisfies:

$$\begin{aligned}[A']_i(D_t\ D_\tau\ E_n\ B_t\ B_\tau\ H_n\ E_t\ E_\tau\ D_n\ H_t\ H_\tau\ B_n)^T \\ =(0\ 0\ 0\ 0\ 0\ 0)^T, \qquad i=1,2\end{aligned} \tag{A3}$$

Thirdly, by reforming the first 6 by 6 block in $[A']_i$ to the same form as the first 6 by 6 block in $[A]_i$, variables D_t, D_τ, E_n, B_t, B_τ, and H_n in Eq. (A3). (A3) can be moved to the right hand side and the resultant equations in block matrix form look like Eq. (16).

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