VIETNAM ACADEMY OF SCIENCE AND TECHNOLOGY

Vietnam Journal of MECHANICS

Volume 35 Number 3

ISSN 0866-7136

VN INDEX 12.666

3
2013

35th Anniversary

Vietnam Journal of Mechanics, VAST, Vol. 35, No. 3 (2013), pp. 203 – 213

ESTIMATING EFFECTIVE CONDUCTIVITY OF UNIDIRECTIONAL TRANSVERSELY ISOTROPIC COMPOSITES

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Abstract. Three-point correlation bounds are constructed on effective conductivity of unidirectional composites, which are isotropic in the transverse plane. The bounds contain, in addition to the properties and volume proportions of the component materials, three-point correlation parameters describing the micro-geometry of a composite, and are tighter those obtained in [1]. The bounds, applied to some disordered and periodic composites, keep inside the numerical homogenization results obtained by Fast Fourier method.

Keywords: Effective conductivity, three-point correlation, numerical homogenization.

1. INTRODUCTION

Effective (thermal, electrical,...) conductivity of multicomponent materials depends on their often complicated irregular micro-structure, hence is hard to be determined exactly. Variational approach has been developed to construct upper and lower bounds in the effective conductivity of composites [1-13]. The bounds contain the properties and volume fractions of the components and possibly correlation information about the micro-geometries of the composites. On the other side, numerical homogenization methods have been developed to estimate effective properties of particular composites, mostly, the two-component ones [11-14]. An effective method to deal with the homogenization problem is the Fast-Fourier one [14-16]. Le and Pham [1] developed a variational approach to estimate effective conductivity of transversely isotropic composites. In this work we modify the approach of Pham [7] to derive bounds tighter than those obtained in [1]. The tight bounds are applied to some random and periodic composites and presented together with the Fast-Fourier homogenization results.

2. TRANSVERSELY ISOTROPIC COMPOSITES AND BOUNDS

Consider transversely isotropic composites, whose phase boundaries are cylindrical surfaces, with generators (in x_3-direction) orthogonal to the plane of isotropy (x_1, x_2). The composite is composed of transversely isotropic components sharing the common plane of isotropy, with longitudinal conductivities $C_\alpha^{\|}$, transverse conductivities $C_\alpha^{\perp}$, and volume fraction v_α $(\alpha = 1, \dots, n)$. The longitudinal effective conductivity $C_{\|}^{eff}$ has been determined, irrespective of particular transverse micro-geometry, as

$$C_{\|}^{eff} = \sum_{\alpha=1}^{n} v_\alpha C_\alpha^{\|} \tag{1}$$

However, for the transverse effective conductivity $C_{\perp}^{eff}$, we have to rely on the minimum energy definition on the representation area element V in the transverse plane

$$C_{\perp}^{eff} \mathbf{E}^0 \cdot \mathbf{E}^0 = \inf_{\langle \mathbf{E} \rangle = \mathbf{E}^0} \int_V C\mathbf{E} \cdot \mathbf{E} d\mathbf{x} \tag{2}$$

where $\mathbf{E}$ is the thermal gradient field, $\mathbf{E}^0$ is a constant vector, $\langle \bullet \rangle$ means the volume average on V, $\langle \bullet \rangle = \frac{1}{V} \int_V \bullet d\mathbf{x}$

$$C(x) = \sum_{\alpha=1}^{n} C_\alpha I_\alpha(x) \tag{3}$$

$$\mathcal{I}_\alpha(x) = \begin{cases} 1 & x \in V_\alpha \\ 0 & x \notin V_\alpha \end{cases} \tag{4}$$

and for simplicity of notations, we adopt $C_\alpha = C_\alpha^{\perp}$. To find an upper bound on $C_{\perp}^{eff}$ from (2), we substitute into them the trial gradient field

$$E_i = E_i^0 + \sum_{\alpha=1}^{n} a_\alpha E_j^\alpha \varphi_{,ij}^\alpha \quad \text{with} \quad i, j = 1, 2 \tag{5}$$

satisfying restriction (for $\mathbf{E}$ to satisfy restriction $\langle \mathbf{E} \rangle = \mathbf{E}^0$)

$$\sum_{\alpha=1}^{n} v_\alpha a_\alpha = 0 \tag{6}$$

and obtain

$$C_{\perp}^{eff} \mathbf{E}^0 \cdot \mathbf{E}^0 \leq W_{\mathbf{E}} \tag{7}$$

where

$$W_{\mathbf{E}} = \int_V C\mathbf{E} \cdot \mathbf{E} d\mathbf{x} = \left(\mathbf{E}^0 \cdot \mathbf{E}^0\right) \Big[C_V + \sum_{\alpha=1}^{n} v_\alpha C_\alpha \big(a_\alpha + \frac{1}{4} a_\alpha^2\big) + \sum_{\alpha,\beta,\gamma=1}^{n} A_\gamma^{\alpha\beta} a_\alpha a_\beta C_\gamma \Big] \tag{8}$$

where C_V is Voigt arithmetic average:

$$C_V = \sum_{\alpha=1}^{n} v_\alpha C_\alpha \tag{9}$$

$$A_\alpha^{\beta\gamma} = \int\limits_{V_\alpha} \varphi_{ij}^{\beta\alpha}\varphi_{ij}^{\gamma\alpha} d\mathbf{x} \qquad \varphi_{ij}^{\beta\alpha} = \varphi_{,ij}^{\beta} - \frac{1}{V_\alpha}\int\limits_{V_\alpha} \varphi_{,ij}^{\beta} d\mathbf{x} \tag{10}$$

$$\varphi^\alpha(\mathbf{x}) = -\int\limits_{V_\alpha} \frac{1}{2\pi} \ln \frac{1}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y}; \quad \nabla^2\varphi^\alpha(\mathbf{x}) = \delta_{\alpha\beta}, \quad \mathbf{x} \in V_\beta \tag{11}$$

Convenient summation carried out on repeating Latin indices from 1 to 2, $\delta_{\alpha\beta}$ is the Kronecker delta; Latin indices after the common designate differentiation with respective Cartesian coordinates.

We minimize the expression (8) over the variables a_α restricted by Eq. (6), with inclusion of Lagrange multiplier to get ($\alpha = 1, \ldots, n$)

$$\frac{1}{2} v_\alpha C_\alpha + \frac{1}{4} v_\alpha C_\alpha a_\alpha + \frac{1}{2} \sum_{\beta,\gamma=1}^{n} A_\gamma^{\alpha\beta} C_\gamma a_\beta - \lambda v_\alpha = 0, \tag{12}$$

Summing Eq. (12), multiplied by C_α^{-1}, on α from 1 to n and taking into account Eq. (6), one get

$$\frac{1}{2} + \frac{1}{2} \sum_{\alpha,\beta,\gamma=1}^{n} C_\alpha^{-1} A_\gamma^{\alpha\beta} C_\gamma a_\beta = \lambda C_R^{-1} \tag{13}$$

where

$$C_R^{-1} = \sum_{\alpha=1}^{n} v_\alpha C_\alpha^{-1} \tag{14}$$

Substituting λ from (13) into (12) leads to the equation

$$\mathbf{v}_c + \boldsymbol{\mathcal{A}}_c \cdot \mathbf{a} = \mathbf{0} \tag{15}$$

which has solution

$$\mathbf{a} = -\boldsymbol{\mathcal{A}}_c^{-1} \cdot \mathbf{v}_c \tag{16}$$

where we have introduced the vectors $\mathbf{a}, \mathbf{v}_c$ and matrix $\boldsymbol{\mathcal{A}}_k$ in n-space

$$\mathbf{a} = \{a_1, \ldots, a_n\}^T; \quad \mathbf{v}_c = \left\{\frac{1}{2} v_1(C_1 - C_R), \ldots, \frac{1}{2} v_n(C_n - C_R)\right\}^T \tag{17}$$

$$\boldsymbol{\mathcal{A}}_c = \{\boldsymbol{\mathcal{A}}_{\alpha\beta}^c\} \quad \alpha, \beta = 1, \ldots, n$$

$$\boldsymbol{\mathcal{A}}_{\alpha\beta}^c = \frac{1}{4} v_\alpha C_\alpha \delta_{\alpha\beta} + \frac{1}{2} \sum_{\gamma=1}^{n} \left(A_\gamma^{\alpha\beta} - v_\alpha C_R \sum_{\delta=1}^{n} C_\delta^{-1} A_\gamma^{\delta\beta} \right) C_\gamma \tag{18}$$

Eqs. (8), (12), (16) lead to

$$W_{\mathbf{E}} = \mathbf{E}^0 \cdot \mathbf{E}^0 \left(C_v + \frac{1}{2} \sum_{\alpha=1}^{n} v_\alpha C_\alpha a_\alpha \right) = \mathbf{E}^0 \cdot \mathbf{E}^0 \left(C_v - \mathbf{v}_c' \cdot \boldsymbol{\mathcal{A}}_c^{-1} \cdot \mathbf{v}_c \right) \tag{19}$$

where

$$\mathbf{v}_c' = \left\{ \frac{1}{2} v_1 C_1, \ldots, \frac{1}{2} v_n C_n \right\}^T \tag{20}$$

Thus (2) and (19) yield the upper bound on the effective transverse conductivity of unidirectional n-component composites

$$C_{\perp}^{eff} \leq C_A^U\Big(\{C_\alpha\},\{v_\alpha\},\{A_\alpha^{\beta\gamma}\}\Big) = C_v - \mathbf{v}_c' \cdot \boldsymbol{\mathcal{A}}_c^{-1} \cdot \mathbf{v}_c \tag{21}$$

To construct the lower bound, we start from the dual minimum complementary energy principle

$$\big(C_{\perp}^{eff}\big)^{-1}\mathbf{J}^0 \cdot \mathbf{J}^0 = \inf_{\langle \mathbf{J}\rangle = \mathbf{J}^0} \int_V C^{-1}\mathbf{J}\cdot\mathbf{J}d\mathbf{x} \tag{22}$$

where the (thermal) flux $\mathbf{J}$ should satisfy the equilibrium equation

$$\nabla \cdot \mathbf{J} = \mathbf{0} \quad \text{and} \quad \mathbf{J}^0 = \text{const}$$

To find a lower bound on $C_{\perp}^{eff}$ from (2), we substitute into them the equilibrated trial field

$$J_i = J_i^0 + \sum_{\alpha=1}^{n} a_\alpha J_j^0\big(\varphi_{,ij}^{\alpha} - \delta_{ij}\mathcal{I}_\alpha\big) \quad \text{with} \quad i,\, j = 1{,}2 \tag{23}$$

satisfying restriction (6), and obtain

$$(C_{\perp}^{eff})^{-1}\mathbf{J}^0 \cdot \mathbf{J}^0 \leq \mathbf{W}_J \tag{24}$$

where

$$\begin{aligned} W_{\mathbf{J}} &= \int_V C\mathbf{J}\cdot\mathbf{J}d\mathbf{x} \qquad (25)\\ &= \mathbf{J}^0\cdot\mathbf{J}^0\Big[C_R^{-1} - \sum_{\alpha=1}^{n} v_\alpha C_\alpha^{-1} a_\alpha + \frac{1}{4}\sum_{\alpha=1}^{n} v_\alpha C_\alpha^{-1} a_\alpha^2 + \frac{1}{2}\sum_{\alpha,\beta,\gamma=1}^{n} A_\gamma^{\beta\alpha} a_\alpha a_\beta C_\gamma^{-1}\Big] \end{aligned}$$

We minimize expression (25) restricted by (6), using Lagrange multiplier λ, to get

$$-\frac{1}{2}v_\alpha C_\alpha^{-1} + \frac{1}{4}v_\alpha C_\alpha^{-1} a_\alpha + \frac{1}{2}\sum_{\beta,\gamma=1}^{n} A_\gamma^{\alpha\beta} C_\gamma^{-1} a_\beta - \lambda v_\alpha = 0 \tag{26}$$

Summing Eq. (26), multiplied by C_α, on α from 1 to n and taking into account Eq. (6), one get

$$-\frac{1}{2} + \frac{1}{2}\sum_{\alpha,\beta,\gamma=1}^{n} C_\alpha A_\gamma^{\alpha\beta} C_\gamma^{-1} a_\beta = \lambda C_V \tag{27}$$

Substituting λ from (27) into (26) leads to the equation

$$\overline{\mathbf{v}}_c + \overline{\boldsymbol{\mathcal{A}}}_c \cdot \overline{\mathbf{a}} = \mathbf{0} \tag{28}$$

which has solution

$$\overline{\mathbf{a}} = \overline{\boldsymbol{\mathcal{A}}}_c^{-1} \cdot \overline{\mathbf{v}}_c \tag{29}$$

where

$$\overline{\mathbf{a}} = \{a_1, \ldots, a_n\}^T; \quad \overline{\mathbf{v}}_c = \Big\{\frac{1}{2}v_1(C_V^{-1} - C_1^{-1}), \ldots, \frac{1}{2}v_n(C_V^{-1} - C_n^{-1})\Big\}^T$$

$$\overline{\boldsymbol{\mathcal{A}}}_c = \{\overline{\boldsymbol{\mathcal{A}}}^c_{\alpha\beta}\} \quad \alpha, \beta = 1, \ldots, n$$

$$\overline{\boldsymbol{\mathcal{A}}}^c_{\alpha\beta} = \frac{1}{4}v_\alpha C_\alpha^{-1}\delta_{\alpha\beta} + \frac{1}{2}\sum_{\gamma=1}^{n}\Big(A_\gamma^{\alpha\beta} - v_\alpha C_V^{-1}\sum_{\delta=1}^{n} C_\delta A_\gamma^{\delta\beta}\Big)C_\gamma^{-1} \tag{30}$$

Thus we have

$$W_{\mathbf{J}} = \mathbf{J}^0 \cdot \mathbf{J}^0\big(C_R^{-1} - \overline{\mathbf{v}}_c^{\prime} \cdot \overline{\boldsymbol{\mathcal{A}}}_c^{-1} \cdot \overline{\mathbf{v}}_c\big) \tag{31}$$

where

$$\overline{\mathbf{v}}_c^{\prime} = \Big\{ -\frac{1}{2}v_1 C_1^{-1}, ..., -\frac{1}{2}v_n C_n^{-1}\Big\}^T \tag{32}$$

Finally, (25) and (31) yield the lower bound

$$C_\perp^{eff} \geq C_A^L\Big(\{C_\alpha\}, \{v_\alpha\}, \{A_\alpha^{\beta\gamma}\}\Big) = (C_R^{-1} - \overline{\mathbf{v}}_c^{\prime} \cdot \overline{\boldsymbol{\mathcal{A}}}_c^{-1} \cdot \overline{\mathbf{v}}_c)^{-1} \tag{33}$$

The bounds (22), (33) contain the conductivities C_α, volume fraction v_α of the phases, and three-point correlation parameters $A_\alpha^{\beta\gamma}$ describing the micro structure of the composite. The expressions are much simpler than those obtained in [13] because of modifications in the approach.

3. APPLICATIONS

Firstly, consider three phase doubly-coated circle model, where the disks made of material-1 are embedded in the circular shells of material-2, the latter are embedded in the circular shell of material-3, and all composite circles of all possible sizes but with the same volume proportions of phases fill all the material space (Fig. 1). The three-point correlation parameters $A_\alpha^{\beta\gamma}$ of the model have been determined [8, 12]

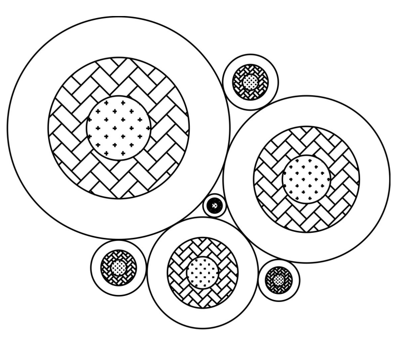


Fig. 1. Doubly-coated circles

$$A_2^{11} = A_2^{22} = -A_2^{12} = -A_2^{21} = \frac{1}{2}\frac{v_1 v_2}{(v_1+v_2)}; \quad A_3^{11} = \frac{1}{2}\frac{v_1^2 v_3}{(v_1+v_2)}$$
$$A_3^{12} = A_3^{21} = \frac{1}{2}\frac{v_1 v_2 v_3}{(v_1+v_2)}; \quad A_3^{13} = A_3^{31} = -\frac{1}{2}v_1 v_3; \quad A_3^{22} = \frac{1}{2}\frac{v_2^2 v_3}{(v_1+v_2)}$$
$$A_3^{23} = A_3^{32} = -\frac{1}{2}v_2 v_3; \quad A_3^{33} = \frac{1}{2}v_3(v_1+v_2) \tag{34}$$

and other $A_\alpha^{\beta\gamma} = 0$. For numerical illustrations, we take

$$C_1 = 1, \quad C_2 = 5, \quad C_3 = 20, \quad v_1 = 0.1 \to 0.9, \quad v_2 = v_3 = \frac{1}{2}\big(1 - v_1\big)$$

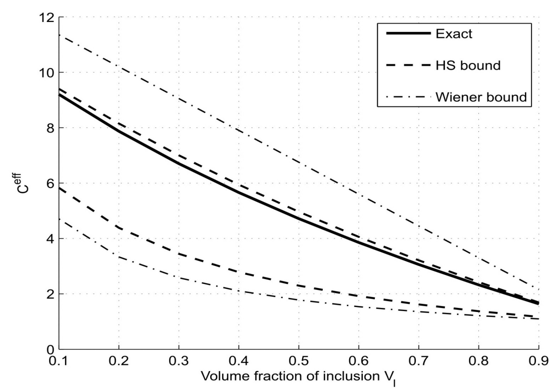


Fig. 2. Bounds and exact effective conductivity of doubly-coated circle model

The results of calculations are reported in Fig. 2. The upper bound (22) and lower bound (33) converge to give unique value of the effective transverse conductivity $C_\perp^{eff}$ (shown as Exact in Fig. 2). Wiener bounds and Hashin-Shtrikman bounds [2] are also given for comparisons. In the case $C_\alpha^{\|} = C_\alpha\big(= C_\alpha^{\perp}\big), \alpha = 1,2,3$, the effective longitudinal conductivity of the unidirectional composite $C_{\|}^{eff}$ equal to the Wiener upper bound according to (1).

For symetric cell materials (without distinct inclusion and matrix phase) [4, 9], we have $(\alpha \neq \beta \neq \gamma \neq \alpha)$

$$A_\alpha^{\beta\gamma} = v_\alpha v_\beta v_\gamma\left(2e_1 - \frac{1}{2}\right); \quad A_\alpha^{\alpha\alpha} = v_\alpha(1 - v_\alpha)\left[(1 - 2v_\alpha)e_1 + \frac{v_\alpha}{2}\right] \tag{35}$$
$$A_\alpha^{\alpha\beta} = v_\alpha v_\beta\left[(2v_\alpha - 1)e_1 - \frac{v_\alpha}{2}\right]; \quad A_\alpha^{\beta\beta} = v_\alpha v_\beta\left[\frac{1}{2}(1 - v_\beta) + (2v_\beta - 1)e_1\right]$$

where

$$0 \leq e_1 \leq \frac{1}{2} \tag{36}$$

The bounds for symetric cell materials read

$$\max_{0\le e_1\le \frac{1}{2}} C^U\left(\{C_\alpha\},\{v_\alpha\},\{A_\alpha^{\beta\gamma}\}\in(35)\right)\ge C_\perp^{eff}\ge \min_{0\le e_1\le \frac{1}{2}} C^L\left(\{C_\alpha\},\{v_\alpha\},\{A_\alpha^{\beta\gamma}\}\in(35)\right) \quad (37)$$

Numerical results of the bounds for symetric cell materials in the particular case (34) are given in Fig. 3. In Figs. 3-6 new bound means the presented one.

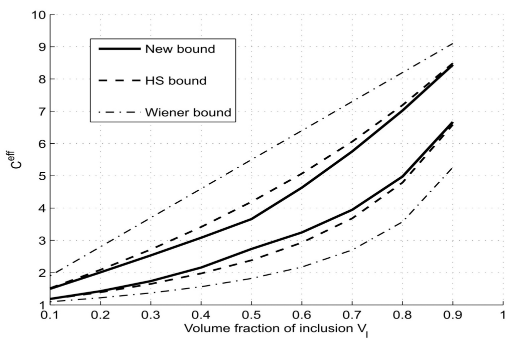
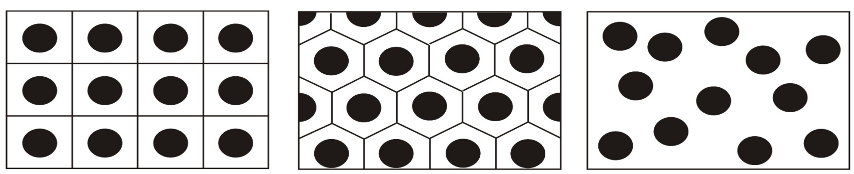
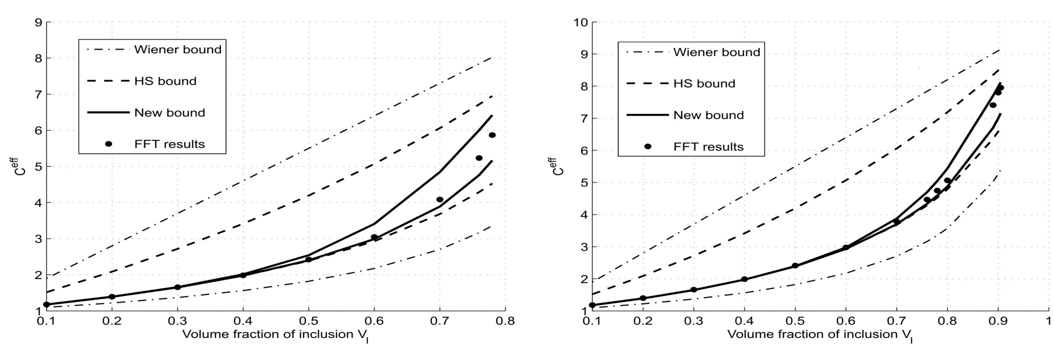


Fig. 3. Bounds for symmetric cell materials



(a) Square (b) Hexagonal (c) Random (non-overlapping)

Fig. 4. Some periodic and random two-phase models



(a) (b)

Fig. 5. (a) Square model; (b) Hexagonal model

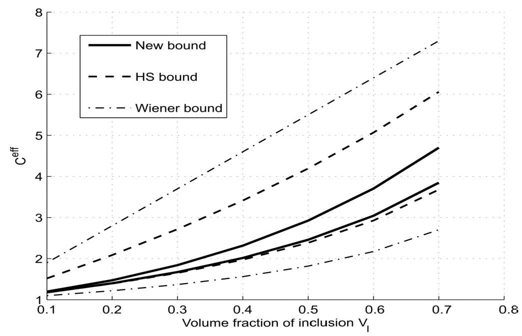


Fig. 6. Random model

Now consider some periodic and random two-phase models (Fig. 4), the correlation parameter of which has been tabulated in [11].

Assume $C_I = 10$ (inclusion), $C_M = 1$ (matrix). The bounds for the square, hexagonal and random models at $v_I = 0.1 \to 0.9$ are projected in Figs. 5(a)-5(b)-6, respectively.

The results presented in Figs. 2-3-5-6 shows the performance of the new bounds. One can see that the three-point correlation bounds (22), (33) are tighter than the second order Hashin-Shtrikman bounds.

4. FAST FOURIER TRANSFORM AND HOMOGENIZATION

The Fast Fourier Transform (FFT) has been used to compute the effective properties of periodic composites by G.Bonnet and J.C.Michel [15, 16]. Then, this method is also used to calculate the permeability of the porous media [14]. In this section, we present the Fast Fourier method for calculating the effective conductivity of periodic two-component materials.

Due to the periodic property of the microstructures, one can consider a unit cell as a representative volume element (RVE) which consisting of a matrix medium (M) and inclusion (I). Both matrix and inclusions are assumed to be homogeneous and have the behavior described by Fourier's law

$$\mathbf{J}(\mathbf{x}) = C(\mathbf{x})\mathbf{E}(\mathbf{x}) \tag{38}$$

where $C(\mathbf{x})$ is the second order local conductivity tensor governed by (3) with $\mathbf{E}(\mathbf{x})$ being the local temperature gradient

$$\mathbf{E}(\mathbf{x}) = -\nabla T(\mathbf{x}) \tag{39}$$

and $\mathbf{J}(\mathbf{x})$ being equilibrated thermal flux

$$\nabla \cdot \mathbf{J}(\mathbf{x}) = 0 \tag{40}$$

Let the unit cell be subjected to the macroscopic temperature gradient $\mathbf{E}^0$, from (38), one finds

$$\mathbf{Q} = \langle \mathbf{J}(\mathbf{x}) \rangle_V = C^{eff}\mathbf{E}^0 \tag{41}$$

in which C^{eff} is the effective thermal conductivity.

The localization problem can be reduced to finding the V-periodic perturbation terms $\mathbf{e}^{per}$ and T^{per} given by the expressions

$$\mathbf{E}(\mathbf{x}) = \mathbf{E}^0 + \mathbf{e}^{per}, \quad T = \mathbf{E}^0 \cdot \mathbf{x} + T^{per}$$

By introducing a reference medium with conductivity C^0, the Eq. (40) becomes

$$\nabla \cdot \mathbf{J}(\mathbf{x}) = \nabla \cdot \left[\left(C^0 + \Delta C\right)\mathbf{E}(\mathbf{x})\right] = 0 \tag{42}$$

where

$$\Delta C(\mathbf{x}) = C(\mathbf{x}) - C^0$$

Replacing $\mathbf{E}(\mathbf{x})$ by (39), the Eq. (42) can be rewritten in the equivalent form

$$-\nabla \cdot \left[C^0 \nabla T^{per}\right] + \nabla \cdot \tau(\mathbf{x}) = 0 \tag{43}$$

where the "polarization tensor" $\tau(\mathbf{x})$ is defined by

$$\tau(\mathbf{x}) = \Delta C(\mathbf{x})[\mathbf{E}^0 + \mathbf{e}^{per}(\mathbf{x})] \tag{44}$$

Due to the V-periodicity, $\mathbf{e}^{per}$, T^{per} and τ admit the Fourier series representations

$$\mathbf{F}(\mathbf{x}) = \sum_{\xi} \widehat{\mathbf{F}}(\xi) e^{i\xi.\mathbf{x}}, \quad \widehat{\mathbf{F}}(\xi) = \left\langle \mathbf{F}(\mathbf{x}) e^{-i\xi.\mathbf{x}} \right\rangle$$

in which $\mathbf{F}$ denotes $\mathbf{e}^{per}$, T^{per}, τ and $\widehat{\mathbf{F}}$ denotes their Fourier transform $\widehat{\mathbf{e}}^{per}$, $\widehat{T}^{per}$ and $\widehat{\tau}$.

Substituting the Fourier representation of $\mathbf{e}^{per}$, T^{per}, τ into Eq. (43) yields

$$\sum_{\xi} (\xi_m C^0_{mj} \xi_j) \widehat{T}^{per}(\xi) e^{i\xi\cdot\mathbf{x}} + \sum_{\xi} i\xi_m \widehat{\tau}_m(\xi) e^{i\xi\cdot\mathbf{x}} = 0 \tag{45}$$

Therefore, the field $\widehat{T}^{per}$ and $\widehat{\mathbf{e}}^{per}$ can be expressed as

$$\widehat{T}^{per}(\xi) = -\frac{i\xi \cdot \widehat{\tau}(\xi)}{\xi \cdot C^0 \xi} \tag{46}$$

$$\widehat{\mathbf{e}}^{per}(\xi) = -i\xi \widehat{T}^{per}(\xi) = -\frac{\xi \cdot \widehat{\tau}(\xi)}{\xi \cdot C^0 \xi}\xi \tag{47}$$

Owing to the fact that $\widehat{\mathbf{E}}(\xi) - \widehat{\mathbf{E}}^0(\xi) = \widehat{\mathbf{e}}^{per}(\xi)$ with

$$\widehat{\mathbf{E}}^0(\xi) = \begin{cases} E^0 & \text{for} \quad \xi = 0 \\ 0 & \text{for} \quad \xi \neq 0 \end{cases} \tag{48}$$

we obtain

$$\widehat{\mathbf{E}}(\xi) = \widehat{\mathbf{E}}^0(\xi) - \widehat{\Gamma}(\xi) : \widehat{\tau}(\xi) \tag{49}$$

where the Green operator $\widehat{\Gamma}(\xi)$ is given by

$$\widehat{\Gamma}(\xi) = \frac{\xi \otimes \xi}{\xi \cdot C^0 \xi} \tag{50}$$

The solution $\widehat{\mathbf{E}}(\xi)$ is obtained by the recurrence process

$$\begin{cases} \widehat{\mathbf{E}}^{i+1}(\xi) = -\widehat{\Gamma}(\xi).\left[(C(\xi) - C^0) * \widehat{\mathbf{E}}^i(\xi)\right] & \text{for} \quad \xi \neq 0 \\ \widehat{\mathbf{E}}^{i+1}(\xi) = E^0 & \text{for} \quad \xi = 0 \end{cases} \tag{51}$$

starting from the initial value $\widehat{\mathbf{E}}^1 = \mathbf{E}^0$.

Note that $\forall \xi \neq 0$ one has $\widehat{\Gamma} C^0 \widehat{\mathbf{E}}^i(\xi) = \widehat{\mathbf{E}}^i(\xi)$ (see [16]), the Eq. (51) can be rewritten in the form

$$\begin{cases} \widehat{\mathbf{E}}^{i+1}(\xi) = \widehat{\mathbf{E}}^i(\xi) - \widehat{\Gamma}(\xi).\left[C(\xi) * \widehat{\mathbf{E}}^i(\xi)\right] & \text{for} \quad \xi \neq 0 \\ \widehat{\mathbf{E}}^{i+1}(\xi) = E^0 & \text{for} \quad \xi = 0 \end{cases} \tag{52}$$

The numerical algorithm is given as follows

$$\begin{array}{ll} \text{Iteration } i = 1: & \mathbf{E}^1(\mathbf{x}) = \mathbf{E}^0 \\ & \mathbf{J}^1(\mathbf{x}) = C(\mathbf{x}).\mathbf{E}^1(\mathbf{x}) \\ \text{Iteration } i: & \mathbf{E}^i(\mathbf{x}) \text{ and } \mathbf{J}^i(\mathbf{x}) \text{ are known} \\ & \widehat{\mathbf{J}}^i(\xi) = \mathcal{F}(\mathbf{J}^i(\mathbf{x})) \\ & \text{convergence test} \\ & \widehat{\mathbf{E}}^{i+1}(\xi) = \widehat{\mathbf{E}}^i(\xi) - \widehat{\mathbf{\Gamma}}^0(\xi).\widehat{\mathbf{J}}^i(\xi) \\ & \mathbf{E}^{i+1}(\mathbf{x}) = \mathcal{F}^{-1}(\widehat{\mathbf{E}}^{i+1}(\xi)) \\ & \mathbf{J}^{i+1}(\mathbf{x}) = C(\mathbf{x}).\mathbf{E}^{i+1}(\mathbf{x}) \end{array}$$

The convergence of the iterative procedure is reached when

$$\frac{\parallel \widehat{\mathbf{J}}^{i+1}(\xi) - \widehat{\mathbf{J}}^i(\xi) \parallel}{\parallel \widehat{\mathbf{J}}^{i+1}(\xi) \parallel} < \epsilon \tag{53}$$

where ϵ is a prescribed value (10^{-3} in the present work).

The numerical results for the microstructures of Fig. 4 are presented in Figs. 5(a)-5(b), which fall inside all the bounds.

5. CONCLUSION

Effective behaviour of transverse-isotropic unidirectional composites is studied. Bounds on the effective transverse conductivity have been derived from minimum energy principles with the help of generalized polarization trial fields, which contain optimizing multi-parameters. The procedure improves over the previous bounds based on Hashin-Shtrikman-one-parameter polarization trial fields. They give the bounds that yield tight simple estimates for some periodic and random models, which are also simulated by FFT method in this paper.

ACKNOWLEGEMENTS

The work is supported by Vietnam Nafosted, project N. 107.02-2011.12

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Received February 20, 2013

VIETNAM ACADEMY OF SCIENCE AND TECHNOLOGY
VIETNAM JOURNAL OF MECHANICS VOLUME 35, N. 3, 2013

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