New method for evaluating the dc effective conductivities of composites with periodic structure

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A new approach to composites with periodic structure is proposed. With the integral equations derived here, one can evaluate the conductivity tensor of a composite with an array of inclusions of any shape and of low symmetry, as well as composites with anisotropic conductivity. The validity of the method is confirmed by comparisons between calculations and experiments and previous theories.

I. INTRODUCTION

The problem of evaluating the effective conductivity of a composite material has a long history, dating back to J. C. Maxwell (1873),[1] and has attracted the attention of physicists and mathematicians over the past century. There are two main schemes for attacking this problem. One considers that the second phase is randomly distributed in the first, the other, pioneered by Rayleigh,[2] assumes that the second phase consists of identical inclusions located at a periodic lattice. Maxwell derived a formula for spherical inclusions[1] and Fricke obtained a formula for spheroids.[3] These formulas are only valid for very dilute dispersion of inclusions.

When the obstacles are no longer very small in comparison to the distance between them, the effects of fields around each particle on each other must further be taken into account. Rayleigh was the first to offer a solution to the composite consisting of a cubic array of spheres.[2] His solution was later corrected by Runge[4] and improved by Meredith and Tobias.[5] After much effort invested in this field, the most complete solutions to the cubic arrays of spheres were provided respectively by McPhedran and McKenzie,[6] and Suen, Wong, and Young[7] about ten years ago.

Now the interesting task is to develop a method by which one can obtain complete solutions to arrays of arbitrarily shaped inclusions and low symmetry. Owing to the difficulty in matching boundary conditions across arbitrary interfaces, there is little hope of applying traditional method to arrays of inclusions other than spheres. The concept of a transformation field, invented by Eshelby in solving the equations of elasticity,[8] and improved by Nemat-Nasser and Taya,[8] has the advantage of matching boundary conditions across the interfaces automatically. In this work we derive the integral equations determining electric fields in a composite by the trick of introducing transformation fields into electromagnetism. Effects of inclusion shape manifest themselves only in the integral region. Calculating an integral over a sphere is no more difficult than calculating it over other regions, say, a cube, so the difficulties associated with inclusion shape are removed in principle.

We have calculated the effective conductivities for many composites of orthorhombic shape. For two-dimensional cases of rectangular inclusions our theoretical results agree excellently with recent experimental measurements, and in cases of spherical inclusions our method is equivalent to the approaches developed by McPhedran and McKenzie, and Suen, Wong, and Young. Fortunately the method is rather flexible in usage, for it can also be generalized to deal with composites with local anisotropic conductivity.

II. FORMULATION

Consider an infinitely extended conductive medium which consists of two components of different conductivities and has a periodic structure, and its cell is shown in Fig. 1. Local conductivities of domain Ω_1 and domain Ω_2 are $\sigma^1_{\alpha\beta}$ and $\alpha^2_{\alpha\beta}$, respectively, and the volume of the cell

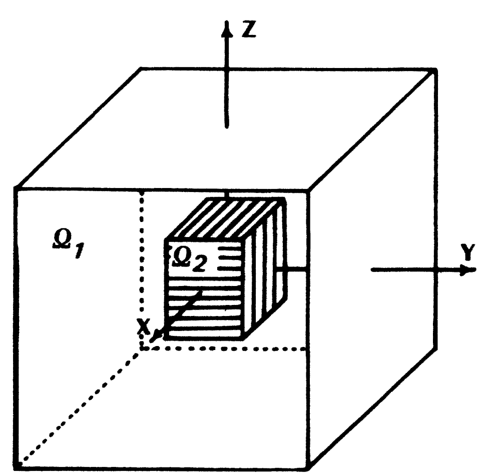

FIG. 1. Geometry of the primitive cell.

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is $D=\Omega_1+\Omega_2$. We employ the usual subscript notation for Greek letters, that is, the Greek subscripts 1, 2, and 3 represent the x, y, and z directions, respectively, and a repeated Greek subscript is summed over all values 1, 2, and 3.

Applying an electric field $\mathbf{E}^0$ along some direction if the medium is homogeneous with a constant conductivity $\sigma^1_{\alpha\beta}$, the current density $\mathbf{j}^0$, and the electric $\mathbf{E}^0$ must be constants through the medium, and we have the relation

$$j^0_\alpha=\sigma^1_{\alpha\beta}E^0_\beta \ . \tag{1}$$

If the conductivities in domain Ω_1 and domain Ω_2 become different, the current density and electric field will be changed to $\mathbf{j}^t$ and $\mathbf{E}^t$, and we have

$$\begin{aligned} j^t_\alpha(\mathbf{x})&=\sigma^1_{\alpha\beta}E^t_\beta(\mathbf{x})=\sigma^1_{\alpha\beta}[E^0_\beta+\delta E^1_\beta(\mathbf{x})] \quad \text{in } \Omega_1 \ , \\ j^t_\alpha(\mathbf{x})&=\sigma^2_{\alpha\beta}E^t_\beta(\mathbf{x})=\sigma^2_{\alpha\beta}[E^0_\beta+\delta E^2_\beta(\mathbf{x})] \quad \text{in } \Omega_2 \ , \end{aligned} \tag{2}$$

where δE^2_β and δE^1_β describe the change of the electric field inside and outside an inclusion when the homogeneous conductivity $\sigma^1_{\alpha\beta}$ is changed to $\sigma^2_{\alpha\beta}$ in Ω_2. The following boundary condition should hold:

$$j^t_\alpha(\mathbf{x})=j^t_\alpha(\mathbf{x}) \quad \text{on boundary of } \Omega_2 \ . \tag{3}$$

We define

$$\delta E_\beta(\mathbf{x})=\begin{cases}\delta E^1_\beta(\mathbf{x}) & \text{in } \Omega_1 \\ \delta E^2_\beta(\mathbf{x}) & \text{in } \Omega_2 \ ,\end{cases} \tag{4}$$

and introduce a transformation field $\mathbf{E}^*$ as

$$\begin{aligned} &\mathbf{E}^*(\mathbf{x})=0 \quad \text{in } \Omega_1 \ , \\ &\sigma^1_{\alpha\beta}[E^0_\beta+\delta E_\beta(\mathbf{x})-E^*_\beta(\mathbf{x})]=\sigma^2_{\alpha\beta}[E^0_\beta+\delta E_\beta(\mathbf{x})] \quad \text{in } \Omega_2 \ . \end{aligned} \tag{5}$$

Then we can rewrite Eq. (2) as

$$j^t_\alpha(\mathbf{x})=\sigma^1_{\alpha\beta}[E^0_\beta+\delta E_\beta(\mathbf{x})-E^*_\beta(\mathbf{x})] \quad \text{in } D=\Omega_1+\Omega_2 \ . \tag{6}$$

In the case of steady state, $\mathbf{j}^t(\mathbf{x})$ should satisfy the following equation:

$$\partial_\alpha j^t_\alpha(\mathbf{x})=0 \ . \tag{7}$$

Because $\mathbf{E}^0$ and $\sigma^1_{\alpha\beta}$ are constants, we can obtain

$$\partial_\alpha\sigma^1_{\alpha\beta}[\delta E_\beta(\mathbf{x})-E^*_\beta(\mathbf{x})]=0 \ . \tag{8}$$

Introducing the electric potential $\delta\varphi(\mathbf{x})$, we have

$$\delta E_\alpha(\mathbf{x})=-\partial_\alpha\delta\varphi(\mathbf{x}) \ . \tag{9}$$

The geometric periodicity implies the periodicities of $\delta\mathbf{E}(\mathbf{x})$, $\mathbf{E}^*(\mathbf{x})$, and $\delta\varphi(\mathbf{x})$ and all of them can be expressed in the Fourier series as

$$\delta\varphi(\mathbf{x})=\sum_n\delta\varphi(\xi_n)e^{i\xi_n\cdot\mathbf{x}} \ , \tag{10}$$

$$\mathbf{E}^*(\mathbf{x})=\sum_n\mathbf{E}^*(\xi_n)e^{i\xi_n\cdot\mathbf{x}} \ , \tag{11}$$

$$\delta\varphi(\xi_n)=V^{-1}\int_D\delta\varphi(\mathbf{x})e^{-i\xi_n\cdot\mathbf{x}}d\mathbf{x} \ , \tag{12}$$

$$\mathbf{E}^*(\xi_n)=V^{-1}\int_D\mathbf{E}^*(\mathbf{x})e^{-i\xi_n\cdot\mathbf{x}}d\mathbf{x} \ , \tag{13}$$

where $\{\xi_n\}$ are the reciprocal vectors, and V is the volume of the cell. From (9) and (10), it follows

$$\delta E_\alpha(\mathbf{x})=-i\sum_n\xi_{n\alpha}\delta\varphi(\xi_n)e^{i\xi_n\cdot\mathbf{x}}, \quad \alpha=1,2,3 \ . \tag{14}$$

Substituting Eqs. (10)–(14) into (8), we can obtain

$$\delta\varphi(\xi_n)=i\sigma^1_{\alpha\beta}E^*_\alpha(\xi_n)\xi_{n\beta}/\sigma^1_{\gamma\delta}\xi_{n\delta}\xi_{n\gamma} \ . \tag{15}$$

From (14), it follows

$$\delta E_\alpha=\sum_n(\xi_{n\alpha}\sigma^1_{\beta\gamma}\xi_{n\beta}/\sigma^1_{\delta\eta}\xi_{n\delta}\xi_{n\eta})E^*_\gamma(\xi_n)e^{i\xi_n\cdot\mathbf{x}} \ , \quad \alpha=1,2,3 \ . \tag{16}$$

Finally, substituting (16) into (8), one deduces the following integral equations for the unknown transformation field $\mathbf{E}^*$:

$$\sigma^1_{\beta\alpha}E^*_\alpha(\mathbf{x})=(\sigma^1_{\beta\alpha}-\sigma^2_{\beta\alpha})E^0_\alpha+V^{-1}(\sigma^1_{\beta\alpha}-\sigma^2_{\beta\alpha})\sum_n\xi_{n\alpha}\sigma^1_{\gamma\delta}\xi_{n\gamma}\int_{\Omega_2}E^*_\delta(\mathbf{x}')e^{i\xi_n\cdot(\mathbf{x}-\mathbf{x}')}d\mathbf{x}'/\sigma^1_{\eta\xi}\xi_{n\eta}\xi_{n\xi}, \quad \beta=1,2,3 \ . \tag{17}$$

The effective conductivity tensor of a composite can be defined by the expression

$$\sigma^*_{\alpha\beta}\langle E^t_\beta\rangle=\langle j^t_\alpha\rangle, \quad \alpha=1,2,3 \tag{18}$$

where $\langle\ \rangle$ denotes the average value for corresponding operator, i.e.,

$$\langle\mathbf{A}\rangle=V^{-1}\int_D\mathbf{A}\,d\mathbf{x} \ . \tag{19}$$

Owing to the periodicity of $\delta\varphi$, we can show

$$\langle\mathbf{E}^t\rangle=\langle\mathbf{E}^0\rangle+\langle\delta\mathbf{E}\rangle=\mathbf{E}^0 \ , \tag{20}$$

$$\begin{aligned}\langle j^t_\alpha\rangle&=\sigma^1_{\alpha\beta}\langle E^0_\beta+\delta E_\beta-E^*_\beta\rangle \\ &=\sigma^1_{\alpha\beta}E^0_\beta-\sigma^1_{\alpha\beta}\langle E^*_\beta\rangle \ ,\end{aligned} \tag{21}$$

and (18) is changed to

$$\sigma^*_{\alpha\beta}E^0_\beta=\sigma^1_{\alpha\beta}E^0_\beta-\sigma^1_{\alpha\beta}\langle E^*_\beta\rangle, \quad \alpha=1,2,3 \ . \tag{22}$$

Now we can determine the effective conductivity tensor of a composite by solving the integral equation (17) for $\mathbf{E}^*(\mathbf{x})$ and substituting it into (22).

III. COMPARISONS WITH EXPERIMENTS AND PREVIOUS THEORIES

If we consider only composites with local isotropic conductivity, the integral equations (17) and algebraic equation (22) reduce, respectively, to

$$V^{-1}\sum_n (\xi_{n\alpha}\xi_{n\beta}/\xi_n^2)\int_{\Omega_2} E_\beta^*(\mathbf{x}')e^{i\xi_n\cdot(\mathbf{x}-\mathbf{x}')}d\mathbf{x}' = -E_\alpha^0+\sigma_1 E_\alpha^*(\mathbf{x})/(\sigma_1-\sigma_2),\quad \alpha=1,2,3 \text{ in } \Omega_2\,, \tag{23}$$

$$\sigma_{\alpha\beta}^* E_\beta^0=\sigma_1 E_\alpha^0-\sigma_1\langle E_\alpha^*\rangle,\quad \alpha=1,2,3 \tag{24}$$

where σ_1 and σ_2 are the isotropic conductivities in Ω_1 and Ω_2, respectively.

In order to compare with experiments and previous theories, in this section we consider the composites which have symmetries of the orthogonal system. In these cases, the effective conductivity tensor must be a diagonal matrix, that is, only the coefficients, σ_{xx}^*, σ_{yy}^*, and σ_{zz}^*, are nonzero. We can determine the effective conductivity σ_{zz}^* by applying an external electric field E_z^0 along the z axis, and do the same for σ_{xx}^* and σ_{yy}^*.

$\mathbf{E}^*(\mathbf{x})$ can be expanded as a polynomial series:

$$E_\alpha^*(\mathbf{x})=\sum_{i,j,k} C_\alpha^{ijk}(x/l_x)^i(y/l_y)^j(z/l_z)^k\,, \tag{25}$$

where l_x, l_y, and l_z are the edge lengths of the cell. Because of the symmetry of the cell, we have $k=2n$ for $\alpha=3$, and $k=2n+1$ for $\alpha=1,2$. Using the usual procedure, we can transform the integral equation (23) into a matrix equation:

$$-E_\alpha^0 A^{ijk}=\sum_{p,q,r}\left[V^{-1}\sum_n G^{ijk}(\xi_n)\xi_{n\alpha}\xi_{n\beta}C_\beta^{pqr}G^{pqr}(-\xi_n)/\xi_n^2 - A^{i+p,j+q,k+r}C_\alpha^{pqr}\sigma_1/(\sigma_1-\sigma_2)\right],$$
$$G^{ijk}(\xi_n)=\int_{\Omega_2}(x/l_y)^i(y/l_y)^j(z/l_z)^k e^{i\xi_n\cdot\mathbf{x}}d\mathbf{x}\,, \tag{26}$$
$$A^{ijk}=\int_{\Omega_2}(x/l_x)^i(y/l_y)^j(z/l_z)^k d\mathbf{x}\,.$$

Let T denote the total exponent of a term in series (25), and the maximum T in the truncation of the series denotes the order of an approximation. Symmetries of the problem lead directly to a proof that the C_α^{ijk} with odd T are zero.

At lowest order of the approximation, we have a neat formula for the effective conductivity

$$\sigma_{zz}^*=1+V_{\Omega_2}A^{000}\Big/\left[\sum_n G^{000}(\xi_n)G^{000}(-\xi_n)\xi_{nz}^2/\xi_n^2 - VA^{000}\sigma_1/(\sigma_1-\sigma_2)\right], \tag{27}$$

where V_{Ω_2} is the volume of domain Ω_2. It coincides with Maxwell's formula[1] in cases of spherical inclusions and Fricke's in cases of spheroids,[3] over the range of inclusion concentration in which these two formulas are valid.

In cases of spherical geometry, all $G^{ijk}(\xi_n)$ can be calculated analytically; the formulas of them are given in the Appendix. Because φ dependence of the fields has been taken into account, even at the third-order approximation, the results are better than Rayleigh's,[2] and Meredith and Tobias's.[5] Comparisons between previous results[9] and ours are given schematically in Fig. 2.

Recently, associated with the research of critical exponents for electrical conductivity, experiments on effective conductivities of two-dimensional composites with rectangular inclusions were performed.[10] It offers a good test for the validity of our treatment. The calculations have been tabulated in Table I for first-, third-, and fifth-order approximation and compared with experi-

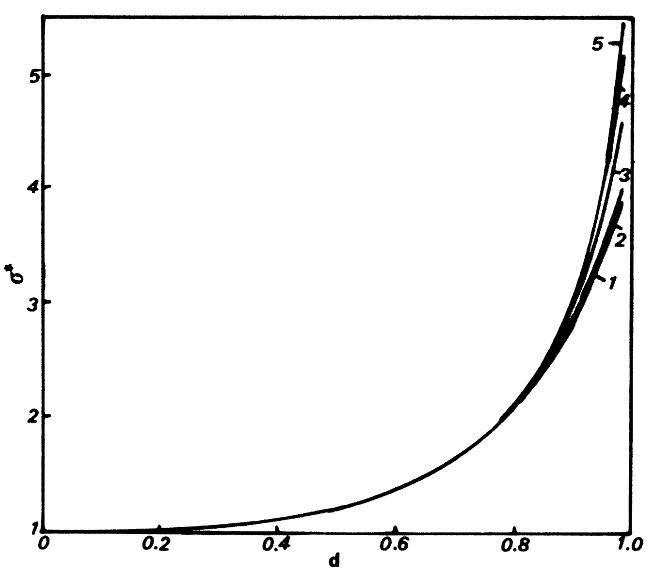

FIG. 2. Comparisons between calculations and previous theories. Domain Ω_2 is a perfectly conducting material. σ^* and d are the effective conductivity and the diameter of the inclusion. The edge length of the cell and σ_1 are used as the length unit and the conductivity unit. Curve 1 is for Maxwell's, curve 2 for our first-order approximation, curve 3 for Rayleigh's, curve 4 for Meredith and Tobias's and our third-order approximation, and curve 5 for McPhedran and McKenzie's, Suen, Wong, and Young's (as cited earlier), and Zick's (Ref. 9).

TABLE I. Effective electrical conductivities, σ^*_{xx}, of the composites with the cell shown in Fig. 3, and domain Ω_2 is an insulator. The conductivity of domain Ω_1, σ_1, is used as the conductivity unit. The experimental values are from Yuan and Tao (Ref. 11).

Size			Approximation		Experimental
a	b	First order	Third order	Fifth order	value
$\frac{1}{2}$	$\frac{1}{2}$	0.6013	0.5823	0.5807	0.5824
$\frac{1}{3}$	$\frac{1}{3}$	0.8014	0.7885	0.7870	0.7853
$\frac{1}{4}$	$\frac{1}{4}$	0.8837	0.8757	0.8744	0.8735
$\frac{1}{5}$	$\frac{1}{5}$	0.9243	0.9190	0.9197	0.9176
$\frac{1}{6}$	$\frac{1}{6}$	0.9469	0.9433	0.9413	0.9414
$\frac{1}{5}$	$\frac{2}{5}$	0.7979	0.7828	0.7785	0.7746
$\frac{1}{5}$	$\frac{3}{5}$	0.6371	0.6106	0.6035	0.5980
$\frac{1}{5}$	$\frac{4}{5}$	0.4330	0.3999	0.3919	0.3987
$\frac{2}{5}$	$\frac{1}{5}$	0.8848	0.8782	0.8781	0.8826
$\frac{3}{5}$	$\frac{1}{5}$	0.8493	0.8428	0.8427	0.8498
$\frac{4}{5}$	$\frac{1}{5}$	0.8186	0.8140	0.8138	0.8155

ments. Agreement between experiments and theoretical results is inspiring.

IV. ANISOTROPIC COMPOSITES

The integral equations enable us to calculate the effective conductivity tensor of anisotropic composites, as well as composites with local anisotropic conductivities. This is another merit of the method developed in this work. For simplicity and without loss of generality, we can only discuss two-dimensional systems.

Restrictions on C^{ijk}_α should be taken out and the matrix equation takes the form of

$$-(\sigma^1_{\beta\alpha}-\sigma^2_{\beta\alpha})E^0_\alpha A^{ijk}+\sum_{p,q,r}\sigma^1_{\beta\alpha}A^{i+p,j+q,k+r}E^0_\alpha = \sum_{p,q,r}V^{-1}(\sigma^1_{\beta\alpha}-\sigma^2_{\beta\alpha})\sum_n G^{ijk}(\xi_n)C^{pqr}_\delta G^{pqr}(-\xi_n)\xi_{n\alpha}\sigma^1_{\gamma\delta}\xi_{n\gamma}/(\sigma^1_{\eta\zeta}\xi_{n\eta}\xi_{n\zeta}) . \tag{28}$$

The effective conductivity tensor is no longer a diagonal matrix for an anisotropic composite, so we need a formula for σ^*_{xy}. By imposing an external electric field E^0_x, we can determine the corresponding solution, $\mathbf{E}^{*(x)}(\mathbf{x})$. Upon substituting it into (22), we have

$$\sigma^*_{xx}E^0_x=\sigma^1_{xx}E^0_x-\sigma^1_{xx}\langle E^{*(x)}_x\rangle-\sigma^1_{xy}\langle E^{*(x)}_y\rangle . \tag{29}$$

Similarly, we have

$$\sigma^*_{yy}E^0_y=\sigma^1_{yy}E^0_y-\sigma^1_{yy}\langle E^{*(y)}_y\rangle-\sigma^1_{yx}\langle E^{*(y)}_x\rangle . \tag{30}$$

If the imposed external field is $E^0_x\hat{\mathbf{i}}+E^0_y\hat{\mathbf{j}}$, then the corresponding solution of the integral equations must be $\mathbf{E}^{*(x)}(\mathbf{x})+\mathbf{E}^{*(y)}(\mathbf{x})$ in accordance with the superposition principle. Substituting it into (22), and using (30) and (31), one reaches

$$\sigma^*_{xy}E^0_y=\sigma^1_{xy}E^0_y-\sigma^1_{xx}\langle E^{*(y)}_x\rangle-\sigma^1_{xy}\langle E^{*(y)}_y\rangle \tag{31}$$

and

$$\sigma^*_{yx}E^0_x=\sigma^1_{yx}E^0_x-\sigma^1_{yy}\langle E^{*(x)}_y\rangle-\sigma^1_{yx}\langle E^{*(x)}_x\rangle . \tag{32}$$

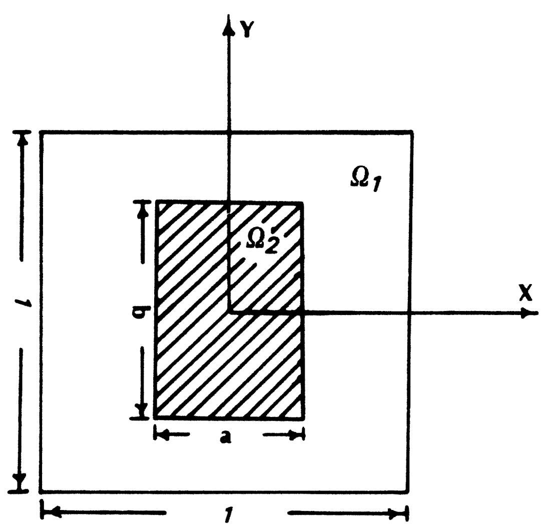

FIG. 3. The cell of a two-dimensional composite with rectangular inclusions.

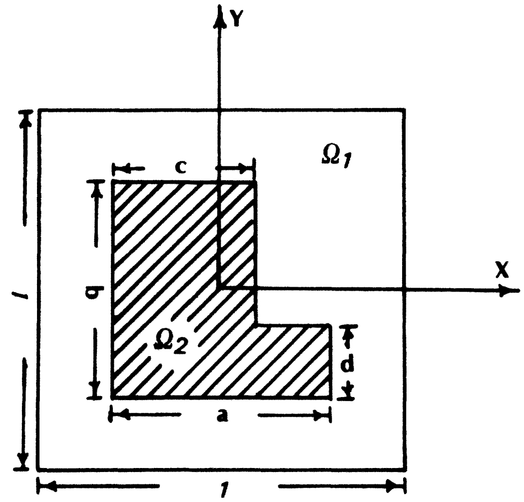

FIG. 4. The cell of a two-dimensional anisotropic composite.

Conductivity tensors of the composites, whose cells are shown in Fig. 4, are evaluated with third-order approximation, and the results are tabulated in Table II.

V. CONCLUSION

We have adopted the transformation field in dealing with the conduction in a composite, and derived a set of integral equations, by which one can determine the electric fields in a periodic composite with any symmetry and arbitrarily shaped inclusions, and even a composite with local anisotropic conductivity. So it also enables people to study other kinds of property of composite, say, the Hall coefficient.[12] The tensor form of the effective conductivity is used systematically, and it is suitable for systems with low symmetry. We have used a polynomial series to approximate the real solution of the integral equations. It turned out that, for composites with a simple structure, the procedure is very efficient over almost the entire range of the concentration. But for a complex structure, such as the second and third stage of Sierpinski carpet, the convergence is not good. We have developed a set of numerical methods to cope with these situations, and it gave the correct exponents for electrical conductivity.[13] In fact, the restriction on periodicity of the structure also can be removed.[13]

ACKNOWLEDGMENTS

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APPENDIX

We discuss here the integrals,

$$G^{ijk}(\xi_n)=\int_{\Omega_2}(x/l_x)^i(y/l_y)^j(z/l_z)^k e^{i\xi_n\cdot\mathbf{x}}d\mathbf{x}\ . \quad \text{(A1)}$$

For simplicity, we let edge lengths of the cell be unity. We have

$$G^{000}(\xi_n)=4\pi[\sin(\xi_n R)/\xi_n - R\cos(\xi_n R)]/\xi_n^2\ . \quad \text{(A2)}$$

If $i+j+k>0$, $G^{ijk}(\xi_n)$ can be performed analytically only when ξ_n is parallel to direction **z**. In such cases, we can obtain the analytical formulas of $G^{ijk}(\xi_n)$ for any i, j, and k, but we only write down the formulas for $i+j+k=2$:

$$G^{200}(\xi_n')=4\pi[(3/\xi_n^2-R^2)\sin(\xi_n R) - 3R\cos(\xi_n R)/\xi_n]/\xi_n^3\ , \quad \text{(A3)}$$

$$G^{020}(\xi_n')=G^{200}(\xi_n')\ , \quad \text{(A4)}$$

$$G^{002}(\xi_n^*)=4\pi[(5R^2-12/\xi_n^2)\sin(\xi_n R) + R(12/\xi_n - R^2\xi_n)\cos(\xi_n R)]/\xi_n^3\ , \quad \text{(A5)}$$

where ξ_n' means that ξ_n coincides with axis z.

In other cases one can make ξ_n lie on axis z by a transformation of the coordinate system, which has the transformation matrix

TABLE II. Effective conductivity tensors of the composites with the cell shown in Fig. 4. σ_1 is used as the conductivity unit. $\sigma_{xx}^1=0.3919$, $\sigma_{xy}^1=0.0$, $\sigma_{yy}^1=0.8138$, $l_x/l_y=1.0$, $a=0.5l_y$, $a=2c$, $b=0.5l_y$, $b=2d$.

σ_{xx}^2	σ_{xy}^2	σ_{yy}^2	σ_{xx}^*	σ_{xy}^*	σ_{yy}^*
0.5663	−0.0453	0.6821	0.4202	−0.0076	0.7867
0.8454	0.0	0.8454	0.4527	−0.0002	0.8196
1.1056	0.0	1.1056	0.4748	−0.0017	0.8613
0.8811	−0.0038	0.8811	0.4561	−0.0008	0.8260
1.0785	−0.0016	1.0785	0.4728	−0.0017	0.8574
0.5792	0.0	0.8250	0.4220	−0.0000	0.8159
1.4891	−0.1265	1.8107	0.4998	−0.0142	0.9380
0.7949	−0.0360	0.6102	0.4476	−0.0046	0.7705
1.7875	−0.2642	1.7875	0.5139	−0.0222	0.9353
1.3146	0.0	2.2993	0.4897	−0.0071	0.9726

$$S=\begin{pmatrix} \xi_{ny}/\xi_{tn}^{1/2} & -\xi_{nx}/\xi_{tn}^{1/2} & 0 \\ \xi_{nx}\xi_{nz}/(\xi_n\xi_{tn}^{1/2}) & \xi_{ny}\xi_{nz}/(\xi_n\xi_{tn}^{1/2}) & -\xi_{tn}/(\xi_n\xi_{tn}^{1/2}) \\ \xi_{nx}/\xi_n & \xi_{ny}/\xi_n & \xi_{nz}/\xi_n \end{pmatrix}, \tag{A6}$$

where $\xi_{tn}=\xi_{nx}^2+\xi_{ny}^2$. With the help of this matrix and $G^{ijk}(\xi'_n)$, one can obtain the formulas for $G^{ijk}(\xi_n)$ straightforwardly.

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