Commun. Theor. Phys. 15(1991)141–148
© International Academic Publishers Vol. 15, No. 2

Thermal Conductivity of Periodic Composite Media with Spherical Inclusions[1]

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(Received June 29, 1990)

Abstract

The thermal conductivity of periodic composite media with spherical inclusions embedded in a homogeneous matrix is discussed. Using Green's function, we show that the Rayleigh identity can be generalized to deal with the thermal properties of these systems. A technique for calculating effective thermal conductivities is proposed. Systems with cubic symmetries (including simple cubic, body centered cubic and face centered cubic symmetry) are investigated in detail, and useful formulae for evaluating effective thermal conductivities are derived.

I. Introduction

The transport properties of inhomogeneous media have been of interest since nearly the time of Maxwell[1]. The reason for this interest is, of course, the enormous variety of physical systems in which inhomogeneities occur. All polycrystalline and composite media, for example, are inhomogeneous systems. Recently, evaluating properly constants of composite media based on the first-principle approaches was received much attention[2–5], because many important problems were raised in engineering field[2,6–9] and some controversies with profound theoretical background are related to it[10–12]. In this paper, we discuss the thermal conductivities of composite media. The reason for this investigation is not only the interest of thermal engineering, but also its theoretical meaning. Present approaches in this domain dealt mainly with electrical conductivities[13], dielectric constants[14] and elasticities of the composite media[15] and viscosities of suspensions[16]. The common feature in these aspects of the composite theory is that one needs to deal with continuous boundary conditions on interfaces between different phases, that is, both the flow (or its equivalence) and potential are continuous on interfaces. When we analyse the thermal conductivities of composite media, we will encounter with a more general boundary condition for composite media. The potential is no longer continuous on interfaces. It complicates the mathematical task intensely and explains why these problems have been overdued such a long time.

[1]The project supported by National Natural Science Foundation of China through grant No. 1880727 and Shanghai Science Funds.

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In Ref. [5]. We studied the thermal properties of composite media with spherical inclusions arranged in a periodic lattice. Present article is a continuation of Ref. [5]. We comprehensively approach the thermal properties of composite media with periodic structure and supply some proofs and discussions about the basis of this study. The paper is arranged as follows. In Sec. II governing equations and boundary conditions for thermal conduction of composite media are specified. In Sec. III, an identity, which forms basis of the study, is discussed. In Sec. IV the definition of the effective thermal conductivities of composite media is established and a technique for evaluating effective thermal conductivities of composite media is proposed. In Sec. V, convergence of numerical evaluation is discussed. In Sec. VI, useful formulae for the effective thermal conductivities of composite media with cubic symmetries are derived.

II. Equations and Boundary Conditions

Consider a composite medium whose matrix, with conductivity k_m, contains inclusions of conductivity k_i, and suppose that the contact resistance on surface of the inclusion is h_{im} with $h_{mi} = h_{im}$. The heat flow in matrix and in inclusion has component given by

$$q_\alpha^m = -k_m \partial_\alpha T_m \,, \quad \text{in} \quad \Omega_m \,, \tag{1}$$

$$q_\alpha^i = -k_i \partial_\alpha T_i \,, \quad \text{in} \quad \Omega_i \,, \tag{2}$$

where Ω_m and Ω_i denote, respectively, the domain occupied by the matrix and inclusion, and T_m and T_i are the temperature field in the matrix and inclusion.

In steady state, the heat flow satisfies the following equations:

$$\partial_\alpha q_\alpha^m = 0 \quad \text{in} \quad \Omega_m \,, \tag{3}$$

$$\partial_\alpha q_\alpha^i = 0 \quad \text{in} \quad \Omega_i \,. \tag{4}$$

The condition for continuity of the heat flow must be applied on surface of the inclusions:

$$\boldsymbol{n}_{im} \cdot \boldsymbol{q}^m = \boldsymbol{n}_{im} \cdot \boldsymbol{q}^i \quad \text{on} \quad \partial\Omega_i \,,$$

where $\boldsymbol{n}_{im}$ is the outward unit normal vector on surface of an inclusion. The secondary condition for composite media with contact resistance is

$$-k_i \frac{\partial T_i}{\partial n_{im}} = h_{im}(T_i - T_m) \quad \text{on} \quad \partial\Omega_i \,. \tag{5}$$

III. The Generalized Rayleigh Identity

We consider a lattice of identical spheres embedded in a homogeneous medium. We apply a homogeneous temperature gradient T_0 along the z axis. The radius of the sphere is a. Let us introduce spherical polar coordinates (r, θ, ϕ) relative to an origin placed at the center (O) of a sphere. θ is measured from the z axis and ϕ is an azimuthal angle measured from the plane of $x - z$. We characterize the field distribution within the composite medium by specifying the temperature potential $T(r, \theta, \phi)$ everywhere within it. T satisfies Laplace's equation in both regions, and so a general form suitable for its expansion about the point O is

$$T_i(r, \theta, \phi) = D_0 + \sum_{l=1}^{\infty} \sum_{m=-l}^{l} D_{lm} r^l Y_{lm}(\theta, \phi) \,, \tag{6}$$

$$T_m(r,\theta,\phi) = E_0 + \sum_{l=1}^{\infty}\sum_{m=-l}^{l}(E_{lm}r^l + F_{lm}r^{-l-1})Y_{lm}(\theta,\phi)\,. \tag{7}$$

Applying boundary conditions on surface of the central inclusion, we derive

$$E_{lm} = \frac{F_{lm}}{G_l a^{2l+1}}\,, \qquad D_{lm} = \frac{F_{lm}(2l+1)}{l(1-k+lk/Bl)a^{2l+1}}\,,$$

where

$$G_l = \frac{l-k+lk/Bl}{k+(l+1)/l+(l+1)k/Bl}\,, \qquad k = \frac{k_i}{k_m}\,,$$

and

$$Bl = \frac{h_{im}a}{k_m} \tag{8}$$

is the Biot number. According to the theory of Green's function, discontinuities of the temperature gradient and the temperature at surface of inclusion are equivalent to new sources of temperature field with the intensity proportional to

$$Q(\theta,\phi) = \left(\frac{\partial T_i}{\partial r} - \frac{\partial T_m}{\partial r}\right)_{r=a} = \sum_{l,m}^{\infty}\frac{F_{lm}}{a^{l+2}}\left((2l+1) - \frac{l(2l+1)k/Bl}{1-k+lk/Bl}\right)Y_{lm}(\theta,\phi)\,, \tag{9}$$

$$D(\theta,\phi) = (T_i - T_m)_{r=a} = \sum_{l,m}^{\infty}\frac{F_{lm}(2l+1)k/Bl}{(1-k+lk/Bl)a^{l+1}}Y_{lm}(\theta,\phi)\,, \tag{10}$$

respectively. The object of this section is to derive a generalized Rayleigh identity, both inside and outside the central sphere. The sources of the temperature are the applied temperature gradient and the induced sources of the temperature field on surface of each sphere, so the temperature field at an arbitrary point $\boldsymbol{r}$ is given by

$$T(\boldsymbol{r}) = T_0 z + \frac{1}{4\pi}\sum_{i=0}^{\infty}\int\frac{Q_i(\boldsymbol{s})}{|\boldsymbol{r}-\boldsymbol{s}|}d^2\boldsymbol{s} + \frac{1}{4\pi}\sum_{i=0}^{\infty}\int D_i(\boldsymbol{s})n_\alpha(\boldsymbol{s})\partial_\alpha\frac{1}{|\boldsymbol{r}-\boldsymbol{s}|}d^2\boldsymbol{s}\,, \tag{11}$$

where $n_\alpha(\boldsymbol{s})$ is the unit normal vector on the area element $d^2\boldsymbol{s}$. In the summations i refers to the i-th sphere and the vector extends from the origin to area element $d^2\boldsymbol{s}$ on its surface. We sum over all spheres in the lattice and integrate over the entire surface of each sphere.

The evaluation of the i-th integral in Eq. (11) is facilitated by a transfer of the origin to the centre $\boldsymbol{R}_i$ of the i-th sphere. Let us write $\rho_i = \boldsymbol{r} - \boldsymbol{R}_i$, $\boldsymbol{t} = \boldsymbol{s} - \boldsymbol{R}_i$, $\boldsymbol{r} - \boldsymbol{s} = \rho_i - \boldsymbol{t}$. We first consider the case where the field point $\boldsymbol{r}$ lies inside the central sphere. We expand the denominator of integrand in Eq. (11) using the addition theorem:

$$\begin{aligned}\frac{1}{|\boldsymbol{r}-\boldsymbol{s}|} &= \sum_{l,m}^{\infty}\frac{4\pi t^l}{(2l+1)\rho_i^{l+1}}Y^*_{lm}(\theta',\phi')Y_{lm}(\theta_i,\phi_i)\,, \qquad i \neq 0\\ &= \sum_{l,m}^{\infty}\frac{4\pi r^l}{(2l+1)t^{l+1}}Y^*_{lm}(\theta',\phi')Y_{lm}(\theta_i,\phi_i)\,, \qquad i = 0\,.\end{aligned} \tag{12}$$

Here (θ',ϕ') are polar angles defining the orientation of $\boldsymbol{t}$, while (θ_i,ϕ_i) specify ρ_i. Using

Eq. (12) and the orthonormality properties of the spherical harmonics we find

$$\begin{aligned} T(\mathbf{r}) &= T_0 z + \sum_{l,m}^{\infty} \frac{F_{lm}}{a^{2l+1}} \frac{1-(lk/Bl)}{1-k+lk/Bl} r^l Y_{lm}(\theta,\phi) + \sum_{i\neq 0}\sum_{l,m}^{\infty} \frac{F_{lm}}{\rho_i^{l+1}} \frac{1-(lk/Bl)}{1-k+lk/Bl} Y_{lm}(\theta_i,\phi_i) \\ &\quad - \sum_{l,m}^{\infty} \frac{F_{lm}}{a^{2l+1}} \frac{(l+1)k/Bl}{1-k+lk/Bl} r^l Y_{lm}(\theta,\phi) + \sum_{i\neq 0}^{\infty}\sum_{l,m}^{\infty} \frac{F_{lm}}{\rho_i^{l+1}} \frac{lk/Bl}{1-k+lk/Bl} Y_{lm}(\theta_i,\phi_i) \qquad (13) \\ &= \sum_{l,m}^{\infty} \frac{F_{lm}}{a^{2l+1}} \left(1 - \frac{(2l+1)k/Bl}{1-k+lk/Bl}\right) r^l Y_{lm}(\theta,\phi) + \sum_{i\neq 0}^{\infty}\sum_{l,m}^{\infty} \frac{F_{lm}}{\rho_i^{l+1}} Y_{lm}(\theta_i,\phi_i) + T_0 z\,. \end{aligned}$$

We see that the terms with Bl in double summation due to $D(\mathbf{s})$ just make a compensation for that due to $Q(\mathbf{s})$, so the terms for $i \neq 0$ do not obviously depend on Bl. In Eq. (13) the first sum comes from the central sphere and the second sum is over all other spheres. Since we have assumed $|\mathbf{r}| < a$ then

$$T(\mathbf{r}) = T_i(\mathbf{r}) = \sum_{l,m}^{\infty} \left(E_{lm} + \frac{F_{lm}(1-(2l+1)k/Bl)}{(1-k+lk/Bl)a^{2l+1}}\right) r^l Y_{lm}(\theta,\phi)\,. \qquad (14)$$

The terms with Bl in Eqs. (13) and (14) are the same. Comparing Eqs. (13) and (14) we arrive at the desired identity:

$$\sum_{l,m}^{\infty} E_{lm} r^l Y_{lm}(\theta,\phi) = \sum_{i\neq 0}\sum_{l,m} \frac{F_{lm}}{\rho_i^{l+1}} Y_{lm}(\theta_i,\phi_i) + T_0 z\,. \qquad (15)$$

This identity has the same form as the original one, but the restriction on continuity of the temperature field on boundary has been removed[13,17]. A similar proof establishes the identity in the region exterior to the central sphere. We omit this proof for simplicity.

IV. The Effective Thermal Conductivities of Composite Media

In this section, we discuss only composite media with cubic symmetry. For more general systems, the procedures are more complex, but have no crucial difficulties[18]. In these systems, the thermal conductivity tensor reduces to a scalar. So calculating the effective thermal conductivity along z axis is enough for these systems. As usual, we have[19]

$$\langle q_z \rangle = -k^* \langle \partial_z T \rangle\,. \qquad (16)$$

Average value of the heat flow is

$$\begin{aligned} \langle q_z \rangle &= -\int_{\Omega_i} k_i \partial_z T_i dx - \int_{\Omega_m} k_m \partial_z T_m dx = -(k_i - k_m)\int_{\Omega_i} \partial_z T_i dx - k_m \langle \partial_z T\rangle + \frac{k_i k_m}{h_{im}} \int \frac{\partial T_i}{\partial r} e_z dS \\ &= -f D_{l,0}\left(k_i - k_m - \frac{k_i}{Bl}\right) - k_m \langle \partial_z T \rangle\,. \end{aligned} \qquad (17)$$

There is only one sphere in a unit cell of s.c. lattice. There are two spheres in a unit cell of b.c.c. lattice and four spheres in a unit cell of f.c.c. lattice. Therefore, the relationship between the volume fraction f and sphere radius a is different for different lattices (see Table 1). Combining these two formulae, we obtain

$$\frac{k^*}{k_m} = 1 + \frac{(k - 1 - k/Bl) f D_{l,0}}{\langle \partial_z T \rangle}\,. \qquad (18)$$

Table 1. Coefficients and quantities in Eq. (27) for s.c., b.c.c. and f.c.c. lattices. f is the volume fraction occupied by spheres. f_c is the critical volume fraction at which the spheres touch, and a_c is the critical radius corresponding to it.

	s.c.	b.c.c.	f.c.c.
a_1	1.3045277	0.057467	0.0047058
b_1	0.0147922	0.166117	0.130683
b_2	0.4054101	1.35858	1.20500
c_1	0.1258627	0.000950738	0.00603255
c_2	0.5288918	0.733934	5.73021
c_3	0.0699313	0.134665	8.20884
c_4	6.1672713	0.0465862	0.295595
f	$(4/3)\pi a^3$	$(8/3)\pi a^3$	$(16/3)\pi a^3$
f_c	$\pi/6$	$(\sqrt{3}/8)\pi$	$(\sqrt{2}/6)\pi$
a_c	$1/2$	$\sqrt{3}/4$	$\sqrt{2}/4$

This calculation cannot be performed until an expression for $\langle\partial_z T\rangle$ built from given quantities is derived. We choose a sphere sample and apply an external temperature gradient along z axis. Imposing the boundary condition at infinity, we determine solution as

$$T_i = \alpha r \cos\theta \qquad r < R_s\,, \tag{19}$$

$$T_m = T_0\left(\frac{\beta}{r^2} + r\right)\cos\theta \qquad r > R_s\,. \tag{20}$$

The coefficients α and β are determined by matching boundary conditions on surface of the sample, which are

$$\alpha = \frac{3R_s T_0 h_{im}}{2}\left(\frac{h_{im}R_s k^*}{2k_m} + h_{im}R_s - k^*\right), \qquad \beta = \left(1 - \frac{k^*}{T_0 k_m}\right)\frac{R_s^3}{2}\,.$$

After letting R_s approach infinity, we obtain

$$\alpha = \frac{3T_0}{2 + k^*/k_m}\,, \qquad \langle\partial_z T\rangle = \frac{3T_0}{k^*/k_m + 2}\,. \tag{21}$$

It completes the formula for the effective thermal conductivity:

$$\frac{k^*}{k_m} = \frac{1 - 2fF_{l,0}/T_0a^3}{1 + fF_{l,0}/T_0a^3}\,. \tag{22}$$

V. Numerical Method and Its Convergence

In order to determine the unknown coefficients $F_{2l-1,m}$, we apply the Rayleigh identity at two points within the unit cell, namely $Q = (r_0, \theta_0, \phi_0)$ and $Q = O = (0, 0, 0)$, and equate odd order derivatives with respect to z of both sides of Eq. (15). The procedure yields a set of linear equations for the $F_{2l-1,m}$. A typical equation, obtained from the $(2n+1)$-th partial derivative is

$$\sum_{l=n+1}^{\infty}\sum_{m=0}^{2l-2n-2} A_{2n+1}^{n+2l-1} E_{2l-1,m} r_0^{2l-2n-2} P_{2l-2n-2}^{m}(\cos\theta_0)\cos(m\phi_0)$$
$$+\sum_{l=1}^{\infty}\sum_{m=0}^{L}\sum_{i=1}^{\infty} A_{2n+1}^{2l+2n-m} F_{2l-1,m}\rho_i^{-2l-2n-1} P_{2l+2n}^{m}(\cos\theta_i)\cos(m\phi_i) = T_0\delta_{n,0}\,, \tag{23}$$

where $L = 2l-1$, $A_m^n = n!/(n-m)!$. In the sums over i we run over the lattice points for all positive or negative integers (u, v, w) excluding $(0, 0, 0)$. Define

$$U_l^m(Q) = \sum_{i=1}^{\infty} \rho_i^{-l-1} P_l^m(\cos\theta_i)\cos(m\phi_i) , \tag{24}$$

where each U_l^m depends on the coordinates of Q, since

$$\rho_i = ((x_0-u)^2 - (y_0-v)^2 + (z_0-w)^2)^{1/2} , \quad \cos\theta_i = \frac{x_0-u}{\rho_i} , \quad \cos\phi_i = \frac{y_0-u}{z_0-w} .$$

By using Eq. (24), equation (23) becomes

$$\sum_{l=n+1}^{\infty} \sum_{m=0}^{2l-2n-2} \frac{A_{2n+1}^{m+2l-1} F_{2l-1,m} r_0^{2l-2n-2} P_{2l-2n-2}^m(\cos\theta_0)\cos(m\phi_0)}{G_{2l-1}a^{4l-1}} + \sum_{l=1}^{\infty}\sum_{m=0}^{L} A_{2n+1}^{2l+2n-m} F_{2l-1,m} U_{2l+2n}^m(Q) = T_0\delta_{n,0} . \tag{25}$$

In the case of electrical conduction, when the conductivity of the inclusions is infinite and nearly touching, the conductivity of the composite medium will develop a singularity. This singularity will not occur in the case of the thermal conduction of composite media, because of the presence of contact resistance. We expect, therefore, that the convergence of numerical method will be much better. We shall show this fact by a set of evaluations.

We wish to consider the general solution, and will suppose that we have to determine M_θ coefficients of the form $F_{2l-1,0}$ and M_ϕ coefficients of the form $F_{2l-1,m}$. We take $Q = O$, the corresponding equations are

$$\frac{F_{2n+1,0}}{G_{2n+1}a^{4n+3}} + \sum_{l=1}^{\infty}\sum_{m=0}^{L} A_{2n+1}^{2l+2n-m} U_{2l+2n}^m(O) F_{2l-1,m} = T_0\delta_{n,0} . \tag{26}$$

Thus, if we write down the first M_θ equation from Eq. (26), there will occur therein M_θ unknowns of the form $F_{2l-1,0}$, as well as the M_ϕ unknowns $F_{2l-1,m}$. In order to get the extra M_ϕ equations required to solve the field identity, we use Eq. (25) for a point Q lying away from O. We take this point in $Q(x_0, x_0, x_0)$ with $x_0 = 1/4\sqrt{3}$. We calculate the thermal conductivity for a composite medium with simple cubic symmetry, the results are tabulated in Table 2. In order to show amply the convergence of the numerical method, we had chosen a much small contact resistance (with Biot number 100) and a rather large volume fraction of inclusion. From Table 2, we draw two useful conclusions. The convergence of numerical method is rather rapidly and azimuthal terms have little influence on the thermal conductivity of composite media.

VI. Formulae for Effective Thermal Conductivities of Composite Media

Owing to the rapid convergence of the numerical method, we can derive neat formulae for the effective thermal conductivity of composite media with cubic symmetry, which may find applications in engineering.

The solution of Eq. (25) to order 4, without azimuthal terms, yields the following formulae

Table 2. Convergence of the numerical method.

		$Bl = 100$					
M_θ	$M_\phi f$	0.32	0.38	0.42	0.46	0.48	0.50
0	2	2.4083	2.9036	3.3433	3.7317	4.3124	4.7795
	3	2.4092	2.9095	3.3627	3.9955	4.4308	5.0055
	4	2.4096	2.9117	3.3699	4.0224	4.4867	5.1313
	6	2.4096	2.9119	3.3710	4.0296	4.5074	5.1987
	8	2.4096	2.9119	3.3710	4.0301	4.5094	5.2099
1	3	2.4096	2.9108	3.3653	4.0010	4.4390	5.0182
	4	2.4098	2.9123	3.3710	4.0244	4.4894	5.1349
	6	2.4098	2.9125	3.3720	4.0313	4.5095	5.2015
	8	2.4098	2.9125	3.3720	4.0318	4.5116	5.2127
6	4	2.4097	2.9118	3.3694	4.0196	4.4812	5.1208
	6	2.4099	2.9127	3.3725	4.0325	4.5113	5.2046
	8	2.4099	2.9127	3.3724	4.0325	4.5125	5.2139

r the effective thermal conductivity of composite media:

$$\frac{k^*}{k_m} = \frac{D - 2f}{D + f}\,,$$
$$D = G_1^{-1} - b_1 G_5 f^{14/3} - c_1 G_7 f^6 - a_1 f^{10/3} \frac{1 - c_2 G_5 f^{11/3} + c_3 G_5^2 f^{22/3}}{G_3^{-1} + b_2 f^{7/3} - c_4 G_5 f^6}\,. \tag{27}$$

he coefficients a_1, b_1, b_2, c_1, c_2, c_3 and c_4 for different lattices are listed in Table 1. Using ese formulae, we study the dependences of the effective thermal conductivities of composite edia on Biot number, which are depicted in Fig. 1. If $h_{im} = \infty$ these formulae coincide with e formulae for the effective electrical conductivity of composite media.

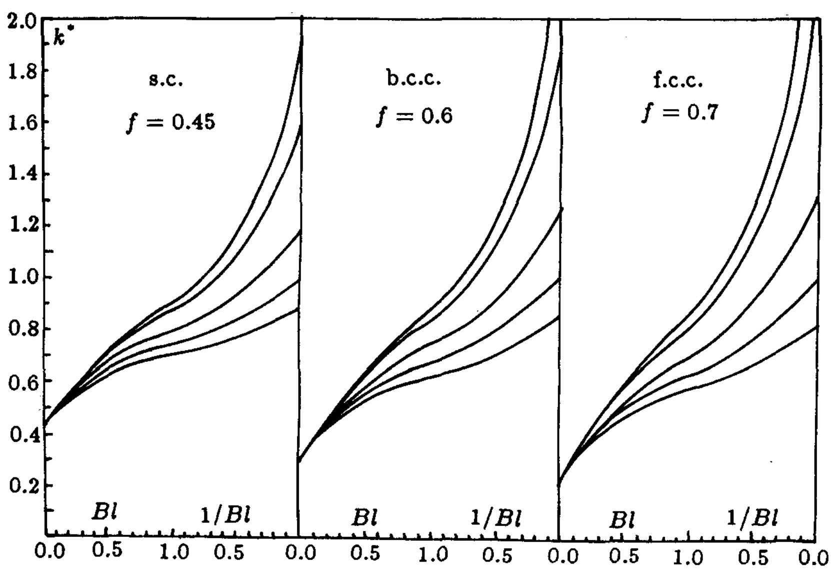

Fig. 1. Dependence of the effective thermal conductivity of composite media on Biot number. The curves along the positive orientation of ordinate correspond successively to $k = 0.75$, 1.0, 1.5, 3.0 and 4.5.

VII. Conclusion

Much effort had been invent in wide and comprehensive exploration on the electrical conductivity of composite media and some efficient methods have been developed. The thermal conductivity constitutes also an important aspect of the theoretical approach of the properties of composite media. In article [5], we had expounded that the existence of the contact resistance on surfaces between different phases of composite media changes the thermal properties dramatically. Unfortunately, the boundary conditions for the thermal conduction complicate the problem and are an obstacle for theoretical treatment of thermal properties. As the awareness of authors, among the present methods for treating the electrical properties of composite media, only the Rayleigh method and the method of long waves[20], invented by M. Born, can be generalized to deal with the thermal conduction of composite medium. The former is the most efficient first-principle approach; but it has a strict restriction on geometry of the microstructure of composite media, only the composite medium with spherical or cylindric inclusions can be treated by this method. The solution of the thermal conduction for these two cases provides, therefore, reasonable data for developing new method in treating the thermal properties of composite media.

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