ON THE THERMAL CONDUCTIVITY OF TWO-PHASE SYSTEMS

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Relationships are obtained which yield the upper and lower bounds of the coefficient of thermal conductivity for statistically homogeneous two-phase systems that have an arbitrary structure.

The problem of determining the coefficient of thermal conductivity of two-phase systems as a function of the thermal conductivity coefficients of each phase has at present been solved exactly only for a very limited class of systems having the simplest structure. The overwhelming majority of structures permits only approximate solutions based on special stipulation of the temperature field in the system. In this connection finding such estimates that would allow the range of possible values of the coefficient of thermal conductivity to be found is of definite interest.

Let us consider a statistically homogeneous two-phase system. (Statistical homogeneity here is understood to mean the following. If the system is partitioned into parts in such a way that the volume of each part is extremely large compared with the microscopic inhomogeneity of the medium, then the average values of the physical quantities characterizing the system must be identical for all the parts.) The geometry of the phase domains is arbitrary. On the phase boundary ideal conditions for thermal contact are realized (i.e., the temperature of the normal components of the thermal flux vector are continuous).

Let us define the coefficient of thermal conductivity λ_{ik} for a two-phase system by the relationship

$$\langle q_i \rangle = -\lambda_{ik} \langle \nabla_k T \rangle . \tag{1}$$

Here and below it is assumed that summation takes place over doubly repeated indices. The angular brackets indicate averaging over a physically infinitesimal volume satisfying the following two requirements:

a) a physically infinitesimal volume must be extremely large compared with the microscopic inhomogeneities of the medium;

b) a physically infinitesimal volume must be extremely small compared with the macroscopic inhomogeneities of the field (i.e., the average values of the physical quantities in this volume must differ infinitesimally from the average values of these quantities in contiguous volumes.

For a statistically anisotropic system which does not have cubic symmetry it makes sense to speak of the coefficient of thermal conductivity in a stipulated direction. Assume that this direction is characterized by the unit vector **n**. Then the coefficient of thermal conductivity in the direction of **n** is defined by the expression

$$\lambda = \lambda_{ik} n_i n_k . \tag{2}$$

As is well known, in order to find the coefficient of thermal conductivity in a stipulated direction it is necessary to specify the temperature gradient in this direction and to measure the quantity

$$\lambda = -\frac{\langle \mathbf{q} \rangle_n}{|\langle \nabla T \rangle|} . \tag{3}$$

Taking Eq. (1) into account, it can easily be shown that Eqs. (2) and (3) are equivalent.

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Let us choose the physically infinitesimal volume V in the form of a right cylinder oriented in the direction of the vector **n**. The direction of a macroscopic temperature gradient for this volume will be determined by the conditions on the boundary of the sample. It is clear that one can always stipulate boundary conditions such that the vector $\langle \nabla T \rangle$ coincides in direction with the vector **n**. This allows the equation $|\langle \nabla T \rangle| = \langle \nabla_n T \rangle$ to be written. If we now take into account the fact that $\langle q \rangle_n = \langle q_n \rangle$, then

$$\lambda = -\frac{\langle q_n \rangle}{\langle \nabla_n T \rangle} = -\frac{\int\limits_{(V)} q_n dV}{\int\limits_{(V)} \nabla_n T dV}. \tag{4}$$

Further on we shall require the inequality

$$\int\limits_a^b f(x)\,dx \int\limits_a^b g(x)\,dx \leqslant (b-a) \int\limits_a^b f(x)\,g(x)\,dx, \tag{5}$$

which was derived by Chebyshev. Here f(x) and g(x) are integrable functions which simultaneously satisfy the conditions

$$\begin{cases} f(x') \leqslant f(x''), \\ g(x') \leqslant g(x'') \end{cases} \quad \text{or} \quad \begin{cases} f(x') \geqslant f(x''), \\ g(x') \geqslant g(x'') \end{cases} \tag{6}$$

(x' and x" are any two points of the segment ab).

Inequality (5) changes its meaning

$$\int\limits_a^b f(x)\,dx \int\limits_a^b g(x)\,dx \geqslant (b-a) \int\limits_a^b f(x)\,g(x)\,dx, \tag{7}$$

if the functions f(x) and g(x) are governed by the conditions

$$\begin{cases} f(x') \leqslant f(x''), \\ g(x') \geqslant g(x'') \end{cases} \quad \text{or} \quad \begin{cases} f(x') \geqslant f(x''), \\ g(x') \leqslant g(x''). \end{cases} \tag{8}$$

Let us arrange the coordinate system in such a way that the direction of the z axis coincides with the direction of the vector **n**, and let us transfor Eq. (4) by the following two different methods:

The first method:

$$\lambda = \frac{\int\limits_{(l)} \left(\int\limits_{(s)} \tilde{\lambda} \nabla_z T dxdy \right) dz}{\int\limits_{(l)} \left(\int\limits_{(s)} \nabla_z T dxdy \right) dz} = \frac{\int\limits_{(l)} \left(\int\limits_{(s)} \tilde{\lambda} \nabla_z T dxdy \right) dz}{\int\limits_{(l)} \left(\frac{\int\limits_{(s)} \nabla_z T dxdy \int\limits_{(s)} \tilde{\lambda} \nabla_z T dxdy}{\int\limits_{(s)} \tilde{\lambda} \nabla_z T dxdy} \right) dz}. \tag{9}$$

Here the integration is carried out over the length (l) of the cylinder and the area (s) of its perpendicular cross section. Using the fact that the resultant flux through the surface of the cylinder is zero, it can easily be shown that the inequality

$$\left| \frac{1}{l} \int\limits_{(l)} \left[\int\limits_{(s)} q_z(x, y, z)\,dxdy \right] dz - \int\limits_{(s)} q_z(x, y, z)\,dxdy \right| \ll \left| \frac{1}{l} \int\limits_{(l)} \left[\int\limits_{(s)} q_z(x, y, z)\,dxdy \right] dz \right| \tag{10}$$

is fulfilled for any values of z which vary within the limits of the cylinder length. Then

$$\lambda = l \left[\int\limits_{(l)} \left(\frac{\int\limits_{(s)} \nabla_z T dxdy}{\int\limits_{(s)} \nabla_z T \tilde{\lambda} dxdy} \right) dz \right]^{-1}. \tag{11}$$

Since the functions $\tilde{\lambda}(x, y, z)$ and $\nabla_z T(x, y, z)$ satisfy conditions of the type (8) (the variable z is considered as the parameter), then by analogy with Eq. (7) one can write

$$\int\limits_{(s)} \tilde{\lambda}\nabla_z T dxdy \leqslant \frac{1}{s}\int\limits_{(s)} \tilde{\lambda} dxdy \int\limits_{(s)} \nabla_z T dxdy. \tag{12}$$

Comparing (11) and (12), we obtain

$$\lambda \leqslant \frac{l}{s}\left[\int\limits_{(l)} \frac{dz}{\int\limits_{(s)} \tilde{\lambda}(x,\ y,\ z)\, dxdy}\right]^{-1} \tag{13}$$

or

$$\lambda \leqslant \frac{l}{s}\left[\int\limits_{(l)} \frac{dz}{\lambda^{(1)} s_1(z) + \lambda^{(2)} s_2(z)}\right]^{-1}. \tag{14}$$

The second method:

$$\lambda = -\frac{\int\limits_{(s)}\left(\int\limits_{(l)} q_z dz\right) dxdy}{\int\limits_{(s)}\left(\int\limits_{(l)} \nabla_z T dz\right) dxdy} = -\frac{\int\limits_{(s)}\left(\frac{\int\limits_{(l)} q_z dz \int\limits_{(l)} \nabla_z T dz}{\int\limits_{(l)} \nabla_z T dz}\right) dxdy}{\int\limits_{(s)}\left(\int\limits_{(l)} \nabla_z T dz\right) dxdy}. \tag{15}$$

As a consequence of the fact that the macroscopic temperature gradient is directed along the cylinder axis, the following inequality is valid for the quantity $\int\limits_{(l)} \nabla_z T(x,\ y,\ z) dz$:

$$\left|\frac{1}{s}\int\limits_{(s)}\left[\int\limits_{(l)} \nabla_z T(x,\ y,\ z)\, dz\right] dxdy - \int\limits_{(l)} \nabla_z T(x,\ y,\ z)\, dz\right| \ll \frac{1}{s}\int\limits_{(s)}\left|\int\limits_{(l)} \nabla_z T(x,\ y,\ z)\, dz\right| dxdy, \tag{16}$$

which is satisfied for any pairs of values x and y which vary within the limits of the domain (s). Therefore,

$$\lambda = \frac{1}{s}\int\limits_{(s)}\left(\frac{\int\limits_{(l)} q_z dz}{\int\limits_{(l)} q_z \tilde{\lambda}^{-1} dz}\right) dxdy. \tag{17}$$

The functions $q_z(x,\ y,\ z)$ and $(x,\ y,\ z)/\tilde{\lambda}$ are governed by conditions of the type (6) (the variables x and y are treated as parameters); therefore, by analogy with (5) one can write

$$\int\limits_{(l)} q_z \tilde{\lambda}^{-1} dxdy \geqslant \frac{1}{l}\int\limits_{(l)} q_z dz \int\limits_{(l)} \tilde{\lambda}^{-1} dz. \tag{18}$$

Substituting this expression into (17), we obtain

$$\lambda \geqslant \int\limits_{(s)}\left[\int\limits_{(l)} \frac{dz}{\tilde{\lambda}(x,\ y,\ z)}\right]^{-1} dxdy \tag{19}$$

or

$$\lambda \geqslant \frac{l}{s}\int\limits_{(s)}\left[\frac{l_1(x,\ y)}{\lambda^{(1)}} + \frac{l_2(x,\ y)}{\lambda^{(2)}}\right]^{-1} dxdy. \tag{20}$$

Using Eqs. (14) and (20), one can determine the upper and lower boundaries of the coefficient of thermal conductivity of any statistically homogeneous two-phase system.

If Eq. (4) and the inequalities

$$\int\limits_{(V)} \tilde{\lambda}\nabla_n T dV \leqslant \frac{1}{V}\int\limits_{(V)} \tilde{\lambda} dV \int\limits_{(V)} \nabla_n T dV,$$

$$\int\limits_{(V)} \tilde{\lambda}^{-1} q_n dV \geqslant \frac{1}{V} \int\limits_{(V)} \tilde{\lambda}^{-1} dV \int\limits_{(V)} q_n dV \tag{21}$$

(instead of (12) and (18)) were to be used directly in the derivation, then we would obtain the well-known relationship

$$\left[\frac{1-P}{\lambda^{(1)}} + \frac{P}{\lambda^{(2)}}\right]^{-1} \leqslant \lambda \leqslant \lambda^{(1)}(1-P) + \lambda^{(2)}P. \tag{22}$$

Let us now show that the domain of values of λ given by the relationships (14) and (20) lies inside the old domain (22). For this purpose we make use of the well-known inequality

$$\int\limits_a^b \frac{dz}{f(z)} \geqslant \frac{(b-a)^2}{\int\limits_a^b f(z)\,dz}\,, \tag{23}$$

which is valid if $\int\limits_a^b f(z)dz > 0$.

In Eq. (13) the quantity $\int\limits_{(s)} \tilde{\lambda}(x, y, z)dxdy$ is a positive function of z. Comparing (13) and (23), we obtain

$$\lambda \leqslant \frac{l}{s}\left[\int\limits_{(l)} \frac{dz}{\int\limits_{(s)} \tilde{\lambda}(x, y, z)\,dxdy}\right]^{-1} \leqslant \frac{l}{s} \frac{\int\limits_{(l)}\left[\int\limits_{(s)} \tilde{\lambda}(x, y, z)\,dxdy\right] dz}{l^2}\,, \tag{24}$$

where the expression at the right is

$$\lambda^{(1)} \frac{V_1}{V} + \lambda^{(2)} \frac{V_2}{V} = \lambda^{(1)}(1-P) + \lambda^{(2)}P. \tag{25}$$

Analogously, it may be shown that

$$\lambda \geqslant \frac{l}{s} \int\limits_{(s)} \left[\frac{l_1(x, y)}{\lambda^{(1)}} + \frac{l_2(x, y)}{\lambda^{(2)}}\right]^{-1} dxdy \geqslant \left[\frac{1-P}{\lambda^{(1)}} + \frac{P}{\lambda^{(2)}}\right]^{-1}. \tag{26}$$

Thus, relationships (14) and (20) yield a more accurate estimate of the values of λ than do the old relationships (23). However, in order to use the relationships (14) and (20) more information than previously is required on the system.

Actually, whereas only the factor P appears in the expression (22), the parameters $s_1(z)$ and $l_1(x, y)$ reflecting the structural characteristics of the system participate in the new relationship. (For example, in the case of matrix structures these parameters will depend on the shape of the inclusions and their mutual disposition.)

For any specific structure the functions $s_1(z)$ and $l_1(x, y)$ may be written in analytic form, which leads to estimates of the coefficient of thermal conductivity of this structure after they have been substituted into expressions (14) and (20). As an example, let us investigate the structure of a cube in a cubic stack. Let $\lambda^{(2)}$ be the coefficient of thermal conductivity of the cubic inclusion. As a consequence of symmetry, all quantities in expressions (14) and (20) shall be referred to the unit cell. If the origin is placed at the center of the cubic inclusion and the z axis is directed along an edge of the cube, then $s_1(z) = L^2$ for $|z| > a/2$ and $s_1(z) = L^2 - a^2$ for $|z| < a/2$; $l_1(x, y) = L$ for $|x| > a/2$ or $|y| > a/2$, and $l_1(x, y) = L - a$ for $|x| < a/2$, $|y| < a/2$. Substituting these expressions into (14) and (20) and integrating, we obtain

$$\frac{\lambda}{\lambda^{(1)}} \leqslant \frac{(1-P^{2/3}) + \lambda^{(2)}/\lambda^{(1)} \cdot P^{2/3}}{(1-P^{2/3}+P) + \lambda^{(2)}/\lambda^{(1)} \cdot (P^{2/3}-P)} \tag{27}$$

and

$$\frac{\lambda}{\lambda^{(1)}} \geqslant \frac{(P^{1/3}-P) + \lambda^{(2)}/\lambda^{(1)} \cdot (1-P^{1/3}+P)}{P^{1/3} + \lambda^{(2)}/\lambda^{(1)} \cdot (1-P^{1/3})}\,. \tag{28}$$

Thus, in the particular case of the structure of a cube in a cubic stack we have arrived at the well-known estimates given by Frey [1] which he found on the basis of other notions. The relationship (27) (having in mind the equality sign) was found somewhat later in [2] and is better known in the literature as the Russel formula.

NOTATION

q_i $(i = 1, 2, 3)$	is the thermal-flux vector (microscopic);
$\nabla_i T$ $(i = 1, 2, 3)$	is the microscopic temperature gradient;
$\lvert \langle \nabla T \rangle \rvert$	is the modulus of the macroscopic temperature gradient;
$\langle \nabla T \rangle_n$, $\langle q \rangle_n$	are the projections of the macroscopic temperature gradient and thermal-flux vector onto the direction of **n**;
$\nabla_n T$, q_n	are the projections of the microscopic temperature gradient and thermal-flux vector onto the direction of **n**;
$\tilde{\lambda} = \lambda^{(1)}$	in the domain occupied by the first phase;
$\tilde{\lambda} = \lambda^{(2)}$	in the domain occupied by the second phase;
$\lambda^{(1)}$, $\lambda^{(2)}$	are the coefficients of thermal conductivity in the first and second phases;
l, s	are the length and perpendicular cross-section area of the physically infinitesimal volume;
$l_1(x, y)$, $s_1(z)$	are the length and perpendicular cross-section area of the physically infinitesimal volume assigned to the first phase;
$l_2(x, y) = l - l_1(x, y)$;	
$s_2(z) = s - s_1(z)$;	
V_1	is the volume occupied by the first phase;
$V_2 = V - V_1$;	
P	is the volume concentration of the second phase;
L	is the parameter of the unit cell;
a	is the length of a cube edge.

LITERATURE CITED

1. G. S. son Frey, Z. Elektrochem., 38, 260 (1932).
2. H. W. Russel, J. Am. Ceram. Soc., 18, No. 1 (1935).