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ABSTRACT: A mixture consisting of n homogeneous phases having certain properties is considered. The geometry of the phase domains is arbitrary and the mixture as a whole is considered to be statistically homogeneous but generally anisotropic. Ideal conditions of thermal contact (a continuous temperature and thermal flux) at the phase boundary are assumed. A variational method is used to find both the upper and lower bounds of the effective thermal-conductivity coefficients of the mixture for given concentrations and the thermal-conductivity coefficients of the individual phases.

1. Let us consider some volume V of a mixture bounded by the surface S . Since the phases have different thermal conductivities, it follows that, in the case of a steady thermal flux, the temperature gradient fields τ and the thermal flux vectors f are microscopically inhomogeneous for any given temperature at S . The tensor K of the macroscopic (effective) thermal-conductivity coefficients of the mixture can be defined as follows:

$$-\langle f \rangle = K \langle \tau \rangle, \quad (1.1)$$

where the angle brackets denote averaging over the volume. We also assume that the volume over which the mean values are calculated is the "characteristic macroscopic volume" [1] of the mixture.

Let us suppose that the r -th phase with the tensor of heat-conductivity coefficients K_r occupies the volume V_r in the total volume V of the multiphase medium. Further, let the temperature $\Theta(S)$ be specified on S in such a way that

$$\Theta(S) = \tau_i \circ x_i. \quad (1.2)$$

Here x_i are the Cartesian coordinates of the surface S ; the τ_i do not depend on the coordinates. In this case $\tau^0 = \langle \tau \rangle$ in the volume V of the mixture. Let us denote, by τ^* , the gradient which results from the continuous temperature field satisfying the boundary conditions on S and, by f^* the thermal-flux vector satisfying the equation $\text{div } f^* = 0$. For the boundary-value problem, without boundary condition (1.2), we have the inequalities

$$\sum_r \int_{V_r} f^* \langle 2 \langle \tau \rangle - R_r f^* \rangle dV_r \leq 2 \langle \Phi \rangle V \leq \sum_r \int_{V_r} \tau^* K_r \tau^* dV_r. \quad (1.3)$$

These inequalities follow from the existence of the potentials

$$\Phi = 1/2 \tau K \tau, \quad \Psi = 1/2 f R f \\ (-f_i = \partial \Phi / \partial \tau_i, \quad -\tau_i = \partial \Psi / \partial f_i, \quad R = K^{-1})$$

and from the positive-definiteness of the matrices of coefficients K and R . The symbol Σ in inequalities (1.3) denotes summation over all r from 1 to n ,

$$\langle \Phi \rangle = \frac{1}{V} \int_V \Phi dV = 1/2 \langle \tau \rangle K \langle \tau \rangle, \quad R_r = K_r^{-1}. \quad (1.4)$$

2. As in the theory of elasticity [2], the above problem of determining the mean gradient of the temperature field in the mixture can be formulated as a problem for some "comparison" material L_0 with arbitrarily chosen properties. It is convenient, at this point, to introduce the "polarized" thermal-flux vector q by means of the formula

$$-f = K_0 \tau - q \quad (2.1)$$

Here K_0 is the tensor of the thermal-conductivity coefficients of the material L_0 . Since $\text{div } f = 0$, the temperature field in the material L_0 is the same as one in the mixture, if heat sources of intensity $\text{div } q$ act throughout the volume V in L_0 , where q is defined by the relation

$$-q = (K - K_0) \tau \quad (2.2)$$

Specifically, an appropriate heat-source layer must be introduced at each discontinuity surface in the mixture; the intensity of this source

per unit area is determined by the magnitude of the jump of the local "source" q .

Let q^* be an arbitrary polarized field which approximates the true field. The gradient τ^* of the continuous temperature field satisfying the conditions at S can be chosen in the form of the temperature gradient in the material L_0 with distributed heat sources of intensity $\text{div } q^*$ and with appropriate layers of sources on the discontinuity surfaces of q^* . The thermal-flux vector f^* chosen in the form $-f^* = K_0 \tau^* - q^*$ satisfies the equation $\text{div } f^* = 0$. The resulting fields can be used in inequalities (1.3). However, the final result depends on the chosen q^* . Let us take q^* in the form of a piecewise-homogeneous field which assumes the constant value

$$-q^* = (K_r - K_0) \langle \tau_r^* \rangle \quad (2.3)$$

in V_r .

Here $\langle \tau_r^* \rangle$ is the approximating field τ^* averaged over V_r . The vector f^* now becomes

$$-f^* = K_r \langle \tau_r^* \rangle + K_0 \tau_r' \quad \text{in } V_r, \quad (2.4)$$

where $\tau_r' = \tau^* - \langle \tau_r^* \rangle$ is the deviation of the gradient τ^* from the average values in V_r .

Making use of the self-evident equation $\int_V f^* (\langle \tau \rangle - \tau) dV = 0$ and expression (2.4), we can reduce inequalities (1.3) to

$$2 \langle \Phi \rangle V \leq \Sigma \langle \tau \rangle K_r \langle \tau_r^* \rangle V_r - \Sigma \int_{V_r} \tau_r' (K_0 - K_r) \tau_r' dV_r \\ 2 \langle \Phi \rangle V \geq \Sigma \langle \tau \rangle K_r \langle \tau_r^* \rangle V_r + \\ + \Sigma \int_{V_r} \tau_r' K_0 (R_0 - R_r) K_0 \tau_r' dV_r. \quad (2.5)$$

We now define the divalent tensor H_r associated with the approximate fields $\langle \tau_r^* \rangle$, as follows:

$$\langle \tau_r^* \rangle = H_r \langle \tau \rangle, \quad (\Sigma c_r H_{ij}^r = \delta_{ij}, \quad c_r = V_r / V). \quad (2.6)$$

Next, we define the tensor K^* as the weighted mean tensor

$$K^* = \Sigma c_r K_r H_r. \quad (2.7)$$

Inequalities (2.5) now imply the following theorem: if the matrix $K_0 - K_r$ is positive-(negative-)definite for all r , the matrix $K^* - K$ is positive-(negative-)definite.

3. Let us construct the approximating field τ^* . The gradient τ^* consists of the field τ^Q generated directly by the heat sources distributed in the material L_0 and of the gradient τ^S of the temperature field satisfying the boundary conditions at S . If $G_{q_i, i}^*$ is the temperature at the point r due to the source at the point r' , τ^Q is the gradient of the temperature field

$$\theta^Q(r) = \int_{\Omega} G [q_k^*] d\Omega_k + \int_V G q_{r, k}^* dV.$$

Here $d\Omega_k$ is an element of the discontinuity surface Ω , and $[q_k^*]$ is the difference between the values of q_k^* on passage through the discontinuity surface Ω . Transforming the surface integral into a volume integral, we obtain

$$\theta^Q(r) = - \int_V \frac{\partial G}{\partial x_k} q_k^* dV.$$

Let the phases constituting the mixture be isotropic; i. e., let $K_{ij}^r = k_r \delta_{ij}$. If material L_0 is homogeneous and isotropic,

$$G = \frac{1}{4\pi k_0} \frac{1}{|\mathbf{r} - \mathbf{r}'|}$$

In this case,

$$\tau_i^* = \frac{\partial \theta^q}{\partial x_i} + \tau_i^s = \frac{1}{k_0} \sum q_k^r \varphi_{,ki}^r + \tau_i^s. \quad (3.1)$$

Here q_k^r denotes the constant value which the vector q_k^s assumes in V_r ,

$$\varphi^r(\mathbf{r}) = -\frac{1}{4\pi} \int_{V_r} \frac{dV_r}{|\mathbf{r} - \mathbf{r}'|}, \quad (\nabla^2 \varphi^r = \delta_{rm} \text{ inside } V_m). \quad (3.2)$$

The gradient τ^s is homogeneous by virtue of the special boundary conditions (1.2) and must be determined later.

4. Let the mixture be statistically isotropic; i. e., let $K_{ij} = k\delta_{ij}$. In this case, the mean value $\langle \varphi_{,ij}^r \rangle_m$ of the quantity $\varphi_{,ij}^r$ over the volume V_m must be an isotropic divalent tensor, which, with allowance for (3.2), can be written as

$$\langle \varphi_{,ij}^r \rangle_m = 1/3 \delta_{rm} \delta_{ij}. \quad (4.1)$$

Averaging expression (3.1) over the volume of each phase V_r and recalling (4.1) and (2.3), we obtain n equations for determining

$$\langle \tau_r^* \rangle = \frac{1}{3k_0} q^r + \tau^s = \frac{1}{3k_0} (k_r - k_0) \langle \tau_r^* \rangle + \tau^s. \quad (4.2)$$

Solving (4.2) for $\langle \tau_r^* \rangle$, we obtain

$$\langle \tau_r^* \rangle = a_r \tau^s, \quad a_r = \frac{3k_0}{k_r + 2k_0}. \quad (4.3)$$

Substituting (4.3) into the relation $\langle \tau \rangle = \sum c_r \langle \tau_r^* \rangle$, we obtain τ^s ,

$$\tau^s = (\sum c_r a_r)^{-1} \langle \tau \rangle. \quad (4.4)$$

Determining H_r from (4.3), (4.4), and (2.6), we finally obtain the following equation from (2.7):

$$k^* = \sum c_r k_r a_r (\sum c_r a_r)^{-1}. \quad (4.5)$$

The bounds for k can be determined as follows. Let the largest and smallest of the phase thermal-conductivity coefficients k_r be k_α and k_β . Then, in accordance with the theorem of Section 2, the best upper bound is obtainable by setting $k_0 = k_\alpha$ and the best lower bound is obtainable by setting $k_0 = k_\beta$. The bounds for k can be expressed as

$$[\sum c_r (2k_\beta + k_r)^{-1}]^{-1} - 2k_\beta \leq k \leq [\sum c_r (2k_\alpha + k_r)^{-1}]^{-1} - 2k_\alpha. \quad (4.6)$$

In the particular case of a two-phase mixture such that $k_1 > k_2$ we have

$$\frac{3c_1 k_1 + c_2 (k_1 + 2k_2)}{k_2 \frac{3c_1 k_2 + c_2 (k_1 + 2k_2)}{k_1}} \leq k \leq k_1 \frac{3c_2 k_2 + c_1 (k_2 + 2k_1)}{3c_2 k_1 + c_1 (k_2 + 2k_1)}. \quad (4.7)$$

For $c_1 \ll 1$, the two bounds in (4.7) coincide with the expression for the macroscopic thermal-conductivity coefficient for a medium with spherical inclusions obtained in [3] (§4, Chapter XVI), under the assumption that the inclusions do not interact with each other in any way. Making use of the concept of a "spherical composite element" [4], we see that each bound in (4.7) is an exact expression for the macroscopic thermal-conductivity coefficient of a medium with spherical inclusions whose diameters vary from certain finite to vanishingly small values. This proves the fact that bounds (4.6) are the best ones for a mixture with the indicated structure.

5. Now let us consider the particular form of a mixture for which the phase domains are continuous cylinders with parallel generatrices and arbitrarily shaped cross sections. We assume that the mixture as a whole is macroscopically homogeneous and transversely isotropic. We choose the coordinate axes x_i in such a way that the x_1 -axis coincides with the cylinder generatrices. In these coordinates, the relationship between (f) and (τ) is of the form

$$- \langle f_i \rangle = k_{11} \langle \tau_i \rangle, \quad - \langle f_i \rangle = k_{22} \langle \tau_i \rangle \quad (i = 2, 3). \quad (5.1)$$

Here k_{11} and k_{22} are the effective thermal-conductivity coefficients parallel and perpendicular to the x_1 -axis respectively. All of our previous statements continue to hold in this case. The steady heat flux

along one of the x_2 - or x_3 -axes does not depend on x_1 and we have the plane analog of the problem considered above. The potential φ^r is logarithmic,

$$\varphi^r(\mathbf{r}) = -\frac{1}{2\pi} \int_{S_r} \ln |\mathbf{r} - \mathbf{r}'| dS_r, \quad (5.2)$$

and its mean value, $\langle \varphi_{,ij}^r \rangle_m$ in S_m , is given by

$$\langle \varphi_{,ij}^r \rangle_m = 1/2 \delta_{rm} \delta_{ij} \quad (i, j = 2, 3). \quad (5.3)$$

The following bounds for k_{22} are obtainable precisely as in the above case:

$$\left[\sum c_r (k_\beta + k_r)^{-1} \right]^{-1} - k_\beta \leq k_{22} \leq \left[\sum c_r (k_\alpha + k_r)^{-1} \right]^{-1} - k_\alpha. \quad (5.4)$$

Since φ^r does not depend on x_1 , we have $\langle \tau_1^r \rangle = \tau_1^s = \langle \tau_1 \rangle$. Hence, the bounds for k_{11} coincide,

$$k_{11} = \sum c_r k_r. \quad (5.5)$$

All of the statements concerning bounds at the end of Section 4 continue to hold in this case, provided the inclusions are rectilinear circular cylinders whose diameters range from certain finite to vanishingly small values.

6. In conclusion we note that the "self-consistent" model of a two-phase continuum proposed by Hill [5] can also be used in our case. In accordance with the basic postulate of Hill's model, the fields τ_r and f_r in V_r ($r = 1, 2$) are identifiable with the temperature gradient and thermal flux in a single inclusion of the r -th phase material immersed in the unbounded medium, with the required thermal-conductivity coefficient, and under the appropriate boundary conditions at infinity. If the inclusion is of simple geometric shape (e.g., a sphere or a circular cylinder), the boundary-value problems are readily solvable [3] and the fields τ_r and f_r in the inclusion turn out to be homogeneous.

Let a two-phase mixture be macroscopically isotropic. The functional equation for determining k can be obtained on the basis of our previous analysis by identifying material L_0 with the inhomogeneous medium itself. The thermal-conductivity coefficient k can then be found as the positive root of the quadratic equation

$$3c_1 k (k_1 + 2k)^{-1} + 3c_2 k (k_2 + 2k)^{-1} = 1. \quad (6.1)$$

In exactly the same way, we obtain the following equation for the coefficient k_{22} of the mixture considered in Section 5:

$$2c_1 k_{22} (k_1 + k_{22})^{-1} + 2c_2 k_{22} (k_2 + k_{22})^{-1} = 1. \quad (6.2)$$

It can be shown [5] that the values of k and k_{22} obtained from (6.1) and (6.2) always lie between bounds (4.7) and (5.4) for $n = 2$ if $k_1 > k_2$ and can therefore serve as a good approximation in those cases where empirical interpolation between the bounds is, for any reason, difficult.

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