

Theory of heat conduction in solids

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The two-temperature approximation is used to study heat conduction in semiconductors. It is shown that, in general, the temperatures of carriers and phonons in anisotropic semiconductors are unequal even in the interior of a bulk sample. The effective boundary conditions are formulated for the case when these two temperatures are equal.

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1. Heat is transported in solids by various quasi-particles (electrons, holes, phonons, magnons, etc.). Frequently the interactions between these quasiparticles are such that each of these subsystems can have its own temperature and the physical conditions at the boundary of a sample can be formulated separately for each temperature. Thus, a boundary is the source of "mismatch" of a subsystem temperatures. For example, the physical conditions resulting in heat transport by electrons and phonons are given in Ref. 1 and those for the transport by phonons and magnons are given in Ref. 2, and the appropriate boundary conditions are formulated.

Since energy is exchanged between these subsystems, it may happen that a steady state of a solid can still be described by a single temperature sufficiently far from the boundaries. One of the aims of the present paper is to show that this apparent truism is not always valid. To be specific, we shall consider a semiconductor whose electron T_e and phonon T_p temperatures can be defined separately (Ref. 4).¹⁾

2. We shall begin with the cases when a rigorous analysis is not in conflict with intuition. This will help us to understand why a single temperature cannot be introduced in general.

We shall consider an isotropic semiconductor with one type of carrier. Heat is carried by electrons and phonons which interact to ensure equalization of the temperatures T_e and T_p . Steady-state heat conduction, subject to allowance for the thermoelectric effects, can be described by the following system of equations¹:

$$\operatorname{div} Q_e = -P(T_e - T_p), \quad (1)$$

$$\operatorname{curl} E = 0, \quad \operatorname{div} j = 0. \quad (2)$$

Here, P is a parameter proportional to the frequency of phonon-electron collisions and the densities of the electric current and heat flux in the electron Q_e and phonon Q_p subsystems are described by the usual relationships (the transport coefficients are labeled in accordance with the system adopted in Ref. 5):

$$Q_e = -\kappa_e \nabla T_e + \alpha T_e j, \quad Q_p = -\kappa_p \nabla T_p, \quad (3)$$

$$j = \sigma(E - \alpha \nabla T_e). \quad (4)$$

We are ignoring the drag effect, because it contributes nothing new to our problem.

If there is no electric current across a boundary s ("pure" heat conduction) and heat fluxes are governed by the differences between the temperatures T_e and T_p and the ambient temperature T_0 , the boundary conditions are as follows¹:

$$n Q_e|_s = \eta_e (T_e - T_0)|_s, \quad n Q_p|_s = \eta_p (T_p - T_0)|_s, \quad n j|_s = 0. \quad (5)$$

Here, n is a unit vector along the normal to the surface s ; η_e and η_p are the surface electron and phonon components of the thermal conductivity.²⁾

We shall assume that our semiconductor is homogeneous and that the temperature gradients are small. This allows us to regard the transport coefficients as independent of the coordinates. It follows from Eqs. (1), (2), and (3) that

$$\kappa_e \Delta T_e = P(T_e - T_p), \quad \kappa_p \Delta T_p = -P(T_e - T_p), \quad (6)$$

and the equations of electrostatics (2), together with Eq. (4), allow us to find the distributions of the current $j(r)$ and field $E(r)$.

Instead of T_e and T_p , we shall introduce the "average" temperature

$$T = \frac{\kappa_e T_e + \kappa_p T_p}{\kappa_e + \kappa_p} \quad (7)$$

and the temperature difference

$$\Theta = T_e - T_p, \quad (8)$$

which satisfy the following equations:

$$\Delta T = 0, \quad \Delta \Theta = k^2 \Theta, \quad k^2 = P(\kappa_e^{-1} + \kappa_p^{-1}). \quad (9)$$

The boundary conditions (5) rewritten in terms of Θ and T are

$$\left. \begin{aligned} n \nabla T &+ \frac{k_e^2}{k^2} n \nabla \Theta &= -\xi_e (T_e - T_0) - \xi_e \frac{k_e^2}{k^2} \Theta_s, \\ n \nabla T &- \frac{k_p^2}{k^2} n \nabla \Theta &= -\xi_p (T_p - T_0) + \xi_p \frac{k_p^2}{k^2} \Theta_s, \end{aligned} \right\} \quad (10)$$

where

$$\kappa_{e,p}^2 = \frac{P}{\kappa_{e,p}}, \quad \xi_{e,p} = \frac{\eta_{e,p}}{\kappa_{e,p}}.$$

It follows directly from the second equation in the system (9) that Θ differs from zero only near the boundaries; at distances $L \sim k^{-1}$ from the boundaries the electron and phonon temperatures are identical ($\Theta = 0$,

$T_e = T_p = T$) even when they differ in the surface layer because of the boundary conditions (10). This surface layer is the region that determines the dependence of the average temperature T on the coordinates in the bulk of the sample (see, for example, Ref. 5).

In those cases when the temperatures of the quasiparticle subsystems participating in heat conduction are identical in the bulk of the sample, we can formulate the boundary-value problem in the one-temperature approximation, i.e., we can consider conduction of heat in a sample ignoring the existence of several quasiparticle subsystems. The solution for T applies everywhere outside the boundary layer which sets the effective boundary conditions for T .

It follows from the definition of T given by Eq. (7) that in the region where Θ vanishes the value of T is identical with the carrier and phonon temperatures. Therefore, the first equation in the system (9) describes heat conduction in the one-temperature approximation (when the divergence of the total heat flux vanishes). Our problem is to formulate the boundary conditions for T .

It follows from $\Delta\Theta = k^2\Theta$ that $n\nabla\Theta \approx k\Theta$ at the surface of the sample. This estimate is valid if the characteristic size of a sample l is such that $kl \gg 1$. Moreover, it is assumed that the surface bounding our semiconductor is smooth. Otherwise, the above estimate is valid at distances $\sim k^{-1}$ from surface singularities.³⁾

It follows from the system (10) that

$$\left. \begin{aligned} n\nabla T &+ \xi_e(T_s - T_0) = -\frac{k_e^2}{k^2}(\xi_e + k)\Theta_e, \\ n\nabla T &+ \xi_p(T_s - T_0) = \frac{k_p^2}{k^2}(\xi_p + k)\Theta_p. \end{aligned} \right\} \quad (11)$$

Eliminating the function Θ_s from the boundary conditions (11), we finally obtain the following equations for T :

$$\Delta T = 0, \quad n\nabla T|_{s=0} = -\xi(T_s - T_0), \quad (12)$$

where

$$\xi = k \frac{\xi_e \xi_p k + \xi_e k_p^2 + \xi_p k_e^2}{k^3 + \xi_e k_e^2 + \xi_p k_p^2} \quad (13)$$

is the effective surface thermal conductivity.

3. We shall now consider an anisotropic gyrotropic semiconductor in the case when the problem can be regarded as one-dimensional (all the quantities depend on just one coordinate, for example, on x). To be specific, we shall consider an infinite plate ($0 \leq x \leq l$) of thickness l much greater than all the transport lengths, in particular, much greater than k^{-1} .

The material equations (3) and (4) can be replaced by the tensor relationship between the fluxes and fields⁶⁾:

$$Q_e - T_s \hat{\alpha} j = -\hat{\chi}_e \nabla T_e, \quad Q_p = -\hat{\chi}_p \nabla T_p, \quad j = \sigma(E - \hat{\alpha} \nabla T_s). \quad (14)$$

It follows from the condition $\text{curl } E = 0$ that E_x and E_z are independent of the coordinates and that their values are governed by the boundary conditions. Since we are interested in "pure" heat conduction, we can naturally assume that $E_y = E_z = 0$ [the component of the current j_x vanishes throughout a sample treated in the one-dimen-

sional approximation if the boundary condition (5) is applied]. However, we must bear in mind that it is not possible to suppress completely charge transport in a truly anisotropic case when the x axis does not coincide with one of the principal directions in a crystal: it does not follow from $\text{div } j = 0$ ($j_x = 0$) that

$$\frac{d}{dx}(\alpha_{xz}j_z) = 0; \quad i = y, z.$$

This results in "renormalization" of the thermal conductivity.⁴⁾ It follows from Eq. (14) that

$$\text{div } Q_e = -\bar{\chi}_{exx} \frac{d^2 T_s}{dx^2}, \quad (15)$$

where

$$\bar{\chi}_{exx} = \chi_{exx} - \frac{T_s}{\sigma_{xx}} \alpha_{xz}\sigma_{zx}\alpha_{xz}\sigma_{zx} + T_s \alpha_{xz}\alpha_{xz}\sigma_{zx}; \quad i, k = y, z. \quad (16)$$

It is worth noting that renormalization of $\hat{\chi}$ does not imply the existence of any restrictions on the values of the components of the tensors $\hat{\chi}$, $\hat{\sigma}$, and $\hat{\alpha}$, because the expression for the formation of the entropy S has its "initial" form [see Eq. (25.5 in Ref. 5)]. Renormalization is important only in the calculation of ∇T (see below for the boundary conditions).

Then, the equations for T_e and T_p again assume the form given by Eq. (6) (if we use $\Delta = d^2/dx^2$), so that all the conclusions reached in Sec. 2 are still valid. For example, the temperature T (naturally at distances from the boundaries large compared with k^{-1}) satisfies

$$d^2 T / dx^2 = 0, \quad (17)$$

subject to the boundary condition

$$\left. \frac{dT}{dx} \right|_{x=0,l} = \mp \xi_{s,i}(T - T_{s,i})|_{x=0,l}, \quad (18)$$

where ξ is described by Eq. (13) and χ is replaced with $\bar{\chi}_{ixx}$.

Since the linear function $T = Ax + B$, i.e., the function corresponding to $\nabla T = \text{const}$, is the solution of the problem (17)–(19), the bulk current (in the interior of the plate) can be compensated by selecting suitable electric fields E_y and E_z . However, we must bear in mind that this changes the expression for the x component of the flux Q_e :

$$\left. \begin{aligned} Q_e^z &= -\bar{\chi}_{exx} \frac{dT_s}{dx} + \gamma_{xi} E_i, \\ \gamma_{xi} &= -\frac{T_s}{\sigma_{xx}} \alpha_{xz}\sigma_{zx} + T_s \alpha_{xz}\sigma_{zx}, \quad i, k = y, z, \end{aligned} \right\} \quad (19)$$

which alters the boundary conditions at $x = 0$ and l :

$$\left. \frac{dT}{dx} \right|_{x=0,l} - \frac{k + \xi_p}{k(\bar{\chi}_{exx} + \chi_{pxx}) + \xi_p \bar{\chi}_{ixx} + \xi_e \chi_{pxx}} = -\xi(T - T_{s,i})|_{x=0,l}. \quad (20)$$

4. We shall consider one other situation in which the electron and phonon subsystems have the same temperatures in the interior of a bulk sample. We have in mind gyrotropic media in which the densities of the electric current and heat fluxes are given by⁶⁾:

$$\left. \begin{aligned} Q_e &= -\chi_e \nabla T_e + \alpha T_j j + L[H \times \nabla T_e] + NT_e[H \times j], \\ Q_p &= -\chi_p \nabla T_p, \\ j &= \sigma(E - \alpha \nabla T_e) - R\sigma[H \times E] - (N - R\alpha\sigma)[H \times \nabla T_e], \end{aligned} \right\} \quad (21)$$

where the transport coefficients are independent of H .

For example, this applies to isotropic semiconductors in weak magnetic fields.

The quantity N in the system (21) represents the transverse Nernst-Ettingshausen effect,⁹ R -the Hall effect,⁵ and L -the Righi-Leduc effect.⁹ Substituting Eq. (21) into Eq. (1), we find that the balance equations have the form (6), i.e., in the interior of a sample the electron and phonon temperatures are indeed identical: $T_e = T_p = T$. In contrast to the above cases, the heat conduction and electrodynamic problems are not separated. If \mathbf{E} is sought in the form

$$\mathbf{E} = \alpha \nabla T - \nabla \varphi, \quad (22)$$

the system (1)-(2) reduces to

$$\Delta \varphi = 0, \quad \Delta T = 0, \quad \Delta \Theta = k^2 \Theta. \quad (23)$$

It follows from the third equation of the system (23) that in the case of bulk sample ($kl \gg 1$), we have

$$n \nabla \Theta |_s \approx k \Theta, \quad [n \times \nabla \Theta]_s \approx \frac{\Theta_s}{l}.$$

Subject to the above expression, we find that the second boundary condition of Eq. (5) expressed in terms of Θ and T allows us to find easily Θ_s in terms of T_o , T , and $n \cdot \nabla T$. The above estimate and the knowledge of Θ_s can be used to find $[n \times \nabla \Theta]_s$. Substituting the above expressions in the first and third boundary conditions (5), we can eliminate Θ_s and obtain the boundary conditions for the potential φ and common temperature T in the first two equations of the system (23). These conditions are of the second order relative to the operator ∇ .

It follows from the equation for T in the system (23) that the characteristic length of variation of T is l . Therefore (since $H n \cdot \nabla T \sim H \cdot [n \times \nabla T]$) in one of the boundary conditions the term with the second derivative is of the order of

$$\frac{k_e^2}{k^2 + \xi_e k_e^2 + \xi_p k_p^2} \frac{LR - N^2 T^*}{R \chi_e} \frac{T}{l^2} H$$

(T^* is the average temperature of the sample).

The term with the first derivative is not smaller than T/l and

$$\frac{k_p^2 + k \xi_p}{k^2 + \xi_e k_e^2 + \xi_p k_p^2} \frac{LR - N^2 T^*}{R \chi_e} \frac{T}{l}.$$

If the dimensions of the sample are such that

$$kl \gg \max \left[\frac{k_e^2}{k_p^2}, \frac{k_e^2}{k_p^2} \frac{LR - N^2 T^*}{R \chi_e} H \right], \quad (24)$$

we can ignore the term with the second derivative of T with respect to the coordinate in the boundary conditions in question.

In the second boundary condition the term with the second derivative can be ignored if $kl \gg k_e^2/k_p^2$.

Therefore, if the dimensions of a sample are sufficiently large to satisfy the conditions (24), the boundary conditions for T and φ become

$$\left. \begin{aligned} & n \nabla T |_s + k \frac{k_e^2 + k \xi_p}{k^2 + \xi_e k_e^2 + \xi_p k_p^2} \frac{LR - N^2 T^*}{R \chi_e} H [n \times \nabla T]_s, \\ & + \frac{k_p^2 (k + \xi_p)}{k^2 + \xi_e k_e^2 + \xi_p k_p^2} \frac{NT^*}{R \chi_e} n \nabla \varphi |_s = -k \frac{\xi_e \xi_p + \xi_e k_e^2 + \xi_p k_p^2}{k^2 + \xi_e k_e^2 + \xi_p k_p^2} (T_s - T_o), \\ & n \nabla \varphi |_s + R \Theta H [n \times \nabla \varphi]_s - k \frac{k_e^2 + k \xi_p}{k_p^2 (k + \xi_p)} N \times H [n \nabla T]_s = 0. \end{aligned} \right\} \quad (25)$$

It must be stressed that the first two equations in the system (23) and the boundary conditions (25) represent a complete formulation of the macroscopic problem of determination of the temperature T and potential φ of a body whose dimensions are greater than all the transport characteristics λ_i with the dimensions of length. We must bear in mind that all the coefficients λ_i are essentially various mean free paths. Therefore, the conditions (24) imply that the dimensions of the investigated body are large compared with the mean free paths of quasiparticles.

5. We shall now consider the general situation of an anisotropic (and gyrotropic) semiconductor of arbitrary shape when the heat conduction problem is three-dimensional. Substituting the expressions for the electric current and heat fluxes (14) in Eqs. (1) and (2), we obtain

$$E = -\nabla \varphi, \quad (26)$$

$$\left. \begin{aligned} & (\chi_e^{ik} + T^* \sigma_{in} \alpha_{in} \alpha_{ik}) \frac{\partial^2 T_e}{\partial x_i \partial x_k} + T^* \sigma_{ik} \alpha_{ii} \frac{\partial^2 \varphi}{\partial x_i \partial x_k} = P(T_e - T_p), \\ & \sigma_{ik} \frac{\partial^2 \varphi}{\partial x_i \partial x_k} + \alpha_{ik} \sigma_{ii} \frac{\partial^2 T_e}{\partial x_i \partial x_k} = 0, \quad \chi_p^{ik} \frac{\partial^2 T_p}{\partial x_i \partial x_k} = -P(T_e - T_p). \end{aligned} \right\} \quad (27)$$

It follows from the form of the system (27) that it admits the solution $T_e = T_p = T$ only if T is a linear function of the coordinates. Such a situation arises only under special conditions.

In general, the electron and phonon temperatures are nonlinear functions of the coordinates and, consequently, these temperatures are not identical in any finite region of a sample, no matter how large is the sample. In other words, the total heat flux in anisotropic and gyrotropic samples of arbitrary shape cannot be described by a gradient of a single scalar function even in the interior of a bulk sample.

We can easily demonstrate the physical meaning of this conclusion. Let us assume that in a certain region the temperatures T_e and T_p are identical. Then, the heat fluxes along the x axis give rise to heat fluxes along the y and z axes, which are related by

$$Q_e^{iz}/Q_p^{iz} \neq Q_e^{iy}/Q_p^{iy} \neq Q_e^{ix}/Q_p^{ix}. \quad (28)$$

The inequalities (28) mean that in a finite region the values of $\text{div} Q_e$ and $\text{div} Q_p$ differ from zero, i.e., there should be a redistribution of heat between the electron and phonon subsystems. This is why T_e begins to differ from T_p .

If the anisotropy is such that rotation of the coordinate axes and their compression or stretching makes it possible to reduce simultaneously all the quadratic forms in the system (27) to $\gamma_e \Delta T_e$, $\gamma_p \Delta T_p$, and $\varepsilon \Delta \varphi$ ($\gamma_{e,p}$ and ε are certain combinations of the transport coefficients), the temperatures T_e and T_p in the interior of a bulk sample are identical and all the conclusions drawn in the earlier sections still apply.

It should be stressed that simultaneous reduction of the tensors \hat{n}_e , \hat{n}_p , $\hat{\sigma}$, etc. in Eq. (27) to the principal axes is insufficient for a macroscopic description of heat conduction.

If frequency happens (this applies to isotropic gyroscopic semiconductors in a magnetic field $H = H_z$) that, instead of the inequalities (28), we have

$$Q_e^x/Q_p^x = Q_e^y/Q_p^y \neq Q_e^z/Q_p^z. \quad (29)$$

In this case the electron and phonon temperatures are not equal anywhere in a three-dimensional body. However, if the problem is two-dimensional (if all the quantities depend on x and y only), the temperatures T_e and T_p are identical in the interior of a bulk sample.^{1,7,8}

We shall conclude by drawing attention to the following point. Our analysis has revealed two circumstances which complicate the standard macroscopic description of heat conduction: first of all, the thermoelectric effects may make it necessary to solve a coupled system of heat conduction and electrostatics equations, i.e., the heat flux may depend strongly on the distribution of electric fields in a sample¹⁰, secondly, in general the difference between the quasiparticle temperatures does not tend to zero as we go away from the boundaries of a body which are the sources of the mismatch between these temperatures. Naturally, in determining the transport coefficients we can always artificially create conditions permitting a simplified description (see Sec. 3). Therefore, the results given here apply to the problems whose formulation is dictated by some special need. In particular, this applies to the nonlinear galvanomagnetic effects in bounded semiconductors^{11,12} and to the thermomagnetic effects,¹ since it is shown in Ref. 13 that η_e (if no special measures are taken) differs from zero on all the walls (we usually find that $\eta_e \rightarrow \infty$).

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Note added in proof (November 15, 1978). It should be stressed that the possibility introducing of a single temperature implies, as shown in Secs. 2–4, that $T_e = T_p$, with exponential precision, i.e., $T_e - T_p \approx T \exp(-\lambda_e/l)$. In general, (Sec. 5) we have $T_e - T_p \approx T(\lambda_e/l)^2$, where λ_e is the energy relaxation length ($\lambda_e < l$).

¹In some cases one of the quasiparticle subsystems participating in heat conduction consists of electrons and long-wavelength phonons which have the same temperature T_e and the other subsystem comprises short-wavelength phonons of temperature T_p (Ref. 3).

²It should be noted that the temperature T_0 depends on the coordinates of the surface s . Moreover, the values of $\eta_{e,p}$ may depend on the coordinates.

³The replacement of $\mathbf{n} \cdot \nabla \Theta$ with $k\Theta$ corresponds to averaging of Eq. (9) in an interval large compared with k^{-1} but small compared with l .

⁴This situation is considered in Refs. 7 and 8 for isotropic gyroscopic semiconductors.

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