Temperature gradient and transport of heat and charge in a semiconductor structure

(Review Article)

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A detailed analysis of the influence of thermal nonequilibrium on transport in semiconductors was carried out. It is shown that the transport of heat and electricity in bipolar semiconductors are interdependent and selfconsistent. In a general case, the distribution of the temperature in homogeneous semiconductors cannot be constant or a linear function with respect to the coordinate even in a linear approximation. The roles of nonequilibrium charge carriers and the recombination in the heat transport are established.

Keywords: thermal nonequilibrium, recombination, quasineutrality, transport phenomena.

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1. Introduction

Various quasiparticles (electrons, holes, phonons, magnons, etc.) transport heat in solids. 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. A boundary is one of the source of "mismatch" of a subsystems' temperatures. For example, the physics 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. However, in general, the temperatures of carriers and phonons in anisotropic semiconductors are unequal even in the interior of a bulk sample [3].

With a strong electron-phonon drag [4] this drag may cause the electron temperature drop to be much greater than the temperature difference between the heater and the refrigerator [5].

The heat flux may depend strongly on the distribution of electric fields in a sample [6]. Many physical phenomena, that involve thermal and charge transport of electrons and holes in semiconductor structures, create a thermal nonequilibrium of electrons, holes, and phonons. Therefore, a temperature gradient appears in the structure. First of all, these are thermoelectric [7, 8] and photothermal [9, 10] effects and devices [11, 12] operating on their basis.

Strong current flowing through a homogeneous semiconductor changes a carrier's energy, because carriers gain kinetic energy. This leads to a nonequilibrium value of energy. This affects the electrons (and/or the holes) that are known as hot electrons or hot carriers [13-16]. Electrons (holes) become much hotter that the crystal lattice. When this happens Ohm's law becomes broken so the current no longer increases linearly with voltage. It is important to consider this effect when large voltage is applied to a short structure [16].

One of the thermoelectric phenomena is the Seebeck effect: a semiconductor sample has contacts made of the same material at both sides. These contacts are kept at different temperatures (due to the presence of a heater at one contact and a cooler at the other). The contacts are connected to a resistance and there is no connection to an external voltage source. This arrangement leads to a thermodiffusion of electrons and holes from the hot junction to the cold junction, producing a thermoelectric current [7, 17]. This effect is actively used as an autonomous source of electric current [18].

Another thermoelectric phenomenon is the Peltier effect, widely used in the electronic industry for cooling. This effect states that when an electric current passes through a junction of two semiconductors, it produces a small heating or cooling effect depending on its direction [7]. The semiconductors used in this arrangement have a specific Peltier coefficient that indicates the amount of heat absorbed or generated at the junction. According to the Peltier coefficients, one of the contacts is heated and the other is cooled [19]. The temperature gradient in the Peltier effect is internal, while in the Seebeck effect it is external.

A third thermoelectric effect is present in a homogeneous conductor; it is known as the Thomson effect. It consists of reversible heating or cooling when there are a temperature gradient and a flow of electric current simultaneously [7, 18]. The absorbed or generated heat along the conductor will depend on the current direction.

Studying these three thermoelectric effects as separate phenomena can lead to misconceptions. This situation was elucidated in Ref. 19 showing that the Peltier and Thomson effects are interrelated because the flow of a current through a junction will create a temperature gradient (Peltier effect), so the Thomson effect will occur naturally.

Additionally, an electrical current across the sample will establish another thermoelectric phenomenon called Joule heating. In this process, the temperature of electrons, holes and phonons is the same and it is due to the heating of the sample.

We mentioned thermoelectric effects only as one of the reasons for the emergence of thermal nonequilibrium. It is interesting to mention that the thermoelectric devices are monopolar devices. However, thermoelectric effects manifest themselves in almost all bipolar devices (see [17, 20]).

Another source of thermal nonequilibrium is nonradiative recombination [21].

It is important to emphasize that the Peltier and Seebeck effects are linear thanks to the proportional relations, on the one hand, between the absorption of heat or cooling and the current, and, on the other, the magnitude of the voltage is proportional to the difference between the temperatures at the thermocouple junction.

The Thomson effect is proportional to the product of the current and the temperature gradient, therefore the Thomson effect is nonlinear. The Joule heating, is proportional to the square of the applied electrical current [19] resulting, also, in a nonlinear response. As stated above, in hot electron phenomena the current does not increase linearly with the applied voltage, therefore this effect is nonlinear.

For simplicity, we restrict ourselves to studying only linear phenomena. It was shown in numerous papers that the nonequilibrium effects might take place even in the linear regime (see, for example [17]).

All the effects discussed, involve charge and heat transport. There are three basic charge transport mechanisms producing carrier movement in semiconductors:

(i) drift current (the movement of charge under an applied electric field producing a force on electrons and holes);

(ii) carrier diffusion (leading to carrier migration from a region of high concentration towards a region of low concentration);

(iii) thermodiffusion (a heat transfer phenomenon in which carriers are moving in the presence of a thermal gradient [22]).

These mechanisms are important for the determination of current-voltage characteristics of a semiconductor device. It is important to note that the nonequilibrium temperature affects both the nonequilibrium concentrations of electrons and holes, and the distribution of the electric potential [8].

In order to describe carrier and heat transport in a semiconductor, recombination must be studied as well [23]. The simplest (and most used) models of recombination are band-to-band transitions [24] and Shockley-Read-Hall recombination [25]. Generation and recombination phenomena involving electrons and holes are very important processes in any nonequilibrium thermodynamics, and especially, for the study transport phenomena such as charge and heat transport. Processes like those are also essential for the designing of any solid-state device. Nevertheless, many models of recombination processes used today contradict fundamental physics such as those described by Maxwell's equations [26]. Furthermore, usually researchers ignore the influence of thermal nonequilibrium on the recombination process. Meanwhile, thermal nonequilibrium induces changes in carrier concentration in the conduction and valence bands and in the recombination rate. In case of a temperature gradient, it modifies the carrier concentrations and the space charge region [15, 26].

The purpose of this paper is to perform a consistent analysis of all the above problems. We have not considered any specific case of thermal nonequilibrium. The general case of equations was investigated. Our task is to discuss the appearance of new terms, related to the thermal nonequilibrium of any origin, in recombination and in space charge for transport phenomena. We restrict ourselves to the one-temperature approximation (all subsystems of quasiparticles — electrons, holes, and phonons — have the same temperature) and a linear approximation in perturbation.

2. General equations

The study of thermal and charge transport in nonequilibrium conditions is performed with the continuity equations for the electron and hole current densities $(\mathbf{j}_n, \mathbf{j}_p)$, the energy balance equation and the Poisson equation. This set of equations is nonlinear and it involves the recombination phenomena [22, 24, 27–29].

The continuity equations for electrons and holes in the case of the stationary transport and in the absence of radiation are:

$$div\mathbf{j}_n = eR,\tag{1}$$

$$div\mathbf{j}_p = -eR,\tag{2}$$

where *R* is the recombination rates, and e(e > 0) is the charge of a hole. In equations (1) and (2), the principle of detailed balance ($R_n = R_p = R$, R_n and R_p are the recombination rates of electrons and holes) was taken into account. For interband recombination, it performed automatically. For the Shockley–Read–Hall model, it serves as an equation to determine n_t (the concentration of electrons at the impurity level [26]).

In Eqs. (1) and (2), \mathbf{j}_n and \mathbf{j}_p are the electric currents densities of electrons and holes and their expressions are as follows [26]:

$$\mathbf{j}_n = -\boldsymbol{\sigma}_n [\nabla \boldsymbol{\psi}_n + \boldsymbol{\alpha}_n \nabla T], \qquad (3)$$

$$\mathbf{j}_p = -\boldsymbol{\sigma}_p [\nabla \boldsymbol{\psi}_p + \boldsymbol{\alpha}_p \nabla T], \qquad (4)$$

where *T* is nonequilibrium temperature, σ_n and σ_p are the electrical conductivities of electrons and holes, $\alpha_n(\alpha_p)$ are the Seebeck coefficients of electrons (holes) and:

$$\Psi_n = \varphi - \mu_n / e, \tag{5}$$

$$\psi_p = \varphi + \mu_p / e, \tag{6}$$

are the electrochemical potentials (Fermi quasi-levels) of electrons and holes (μ_n and μ_p are the nonequilibrium chemical potentials), and φ is the electrical potential [8].

For the recombination in a nondegenerate semiconductor we have [28, 29]:

$$R = \frac{1}{\tau} \left(n_0 + p_0 \right) \left[\frac{\delta n}{n_0} + \frac{\delta p}{p_0} - \left(3 + \frac{\varepsilon_g}{T_0} \right) \frac{\delta T}{T_0} \right].$$
(7)

Here n_0 and p_0 are the equilibrium concentrations of electrons and holes, δn and δp are nonequilibrium additives, T_0 is the equilibrium temperature, δT is a nonequilibrium additive to it, ε_g is the band gap.

It is necessary to emphasize that even if the parameter τ in Eq. (7) has the dimensions of time it is not the lifetime of the nonequilibrium carriers.

Expressions for τ in the cases of interband and in the Shockley–Read–Hall model with transitions due to impurity levels are given in [28, 30].

The third term in the right-hand side Eq. (7) is related to local "equilibrium" temperature at every point of the semiconductor in the presence of the inhomogeneous space nonequilibrium energy. Equilibrium carrier concentrations depend on the equilibrium temperature; therefore, in the presence of a temperature gradient, the "equilibrium" concentrations are different at different points in the sample (for more details see [28]). It is interesting to note that in the literature it is usually believed that in the case of strong recombination ($\tau \rightarrow 0$), nonequilibrium carriers disappear ($\delta n, \delta p \rightarrow 0$). However, as it follows from Eq. (7), in the presence of nonequilibrium energy it is not so.

The Poisson equation is used to describe the charge transport in semiconductor structures [31]:

$$div \mathbf{E} = 4\pi \rho/\mathbf{b},\tag{8}$$

where E is electric field,

$$\rho = e \left(N_t - n - n_t + p \right) \tag{9}$$

is the bulk charge density, \ni is the permittivity, N_t is the concentration of impurities, (for simplicity, we assume that there is one impurity level).

The solution of Eq. (8) is substantially simplified if we use the quasineutrality approximation [32-34]. It establishes that if the Debye length is very small, then the space charge spreads over a length comparable to the Debye length in the semiconductor. With this condition, the space charge density ρ is equal to zero and an algebraic equation is obtained, instead of the differential Poisson equation (see [32] and book by Lampert and Mark [35]). The quasineutrality is a fundamental physical mechanism with its own manifestation: the quasineutrality is the cause that forms a quasineutral region in the study of injection of minority carriers in drift-diffusion equilibrium [27, 33]. Nonequilibrium current carriers can move in a semiconductor structure only if they form a quasineutral packet [27]. In this case, ambipolar diffusion and drift will manifest themselves [20, 27, 36].

The system of equations (1), (2), and (8) is closed by the heat balance equation. We will look at it in the next Section.

3. Heat balance equation

Let us consider a uniform bipolar semiconductor for which the conditions of a quasineutral approximation take place. In this case, the equilibrium concentrations of electrons, n_0 , and holes, p_0 , do not depend on the coordinate [21].

The energy balance equation has practically never been investigated for bipolar transport, when, even in the linear approximation with respect to the gradient of the temperature (small mismatch of the temperatures), the nonequilibrium charge carriers arise, and consequently, it is natural that the generation–recombination processes must be taken into account [8]. The latter is important in an optimization of various bipolar devices, since all of them (with few exceptions) operate in the regime of bipolar transport where the problem of heat dissipation and removing it is one of the concerns for the parameters that characterize the work of the device.

The energy balance equation in a stationary state in a one-dimensional case in a bipolar semiconductor that does not both radiate and absorb light in a linear approximation with respect to a perturbation is as follows [21, 28, 30]:

$$div\mathbf{q} = -\varepsilon_g R, \qquad (10)$$

where \mathbf{q} is the heat flux density. It is equal to:

$$\mathbf{q} = \mathbf{q}_{dr} + \mathbf{q}_{diff}.$$

Here the \mathbf{q}_{dr} is the drift heat flux, $\mathbf{q}_{dr} = \prod_n \mathbf{j}_n + \prod_p \mathbf{j}_p (\prod_{n,p} \mathbf{a}_r)$ are the Peltier coefficients for electrons and holes). The \mathbf{q}_{diff} is the density of the diffusion heat flux, $\mathbf{q}_{diff} = -\kappa \nabla T$ ($\kappa = \kappa_{ph} + \kappa_n + \kappa_p$ is the thermal conductivity of the bipolar semiconductor, where κ_{ph} is the phonon thermal conductivity, κ_n is the thermal conductivity of electrons from a conduction band, and κ_p is the thermal conductivity of holes). The term $\varepsilon_g R$ describes the emission of heat due to nonradiative recombination.

This equation can be rewritten as [30]:

$$\left(\prod_{n0} + \psi_{n0}\right) \frac{dj_n}{dx} + \left(\prod_{p0} + \psi_{p0}\right) \frac{dj_p}{dx} - \kappa_0 \frac{d^2 \delta T}{dx^2} = 0, \quad (11)$$

where the subscript n indicates electron; the subscript p indicates holes; the subscript 0 indicates that the magnitude corresponds to the equilibrium.

From Eqs. (1), (2), and (11), taking into account Eq. (7), and expressions $\prod_{n,p}$ for nondegenerate electrons and holes, $\prod_{n,p} = \mp \frac{1}{e} \left[T \left(r_{n,p} + \frac{5}{2} \right) - \mu_{n,p} \right]$ [7, 24, 37, 38], where $r_n(r_p)$

is the exponent in the momentum relaxation time for electrons (holes) [39]; $\tau_{n,p} = \tau_{n,p;0} (\varepsilon/T)^{r_{n,p}}$, where ε is the energy of the carriers (the constant quantities $\tau_{n,p;0}$ and $r_{n,p}$ for different relaxation mechanisms can be found in Ref. 39), and also an expression $\mu_{n,0} + \mu_{p,0} = -\varepsilon_g$ [8], the following equation for the temperature δT can be obtained:

 $L_0^2 \frac{d^4 \delta T}{dx^4} - \frac{d^2 \delta T}{dx^2} = 0,$

(12)

where

×

$$L^{2} = \frac{\tau_{0}T_{0}}{e^{2}} \left(\frac{1}{n_{0}} + \frac{1}{p_{0}} \right) \times \left(\frac{\sigma_{n,0} + \sigma_{p,0}}{\sigma_{n,0}\sigma_{p,0}} + \frac{(r_{n} + r_{p} + 5)\left[(r_{n} + r_{p} + 5)T_{0} + \varepsilon_{g}\right]}{e^{2}\kappa_{0}} \right)^{-1}$$
(13)

is the generalized diffusion length [30].

It follows from Eqs. (12) to (13) that the heat and electrical transport processes cannot be separated in a general case.

The fields of the temperature and the concentrations of electrons and holes are interdependent and establish selfconsistently, because they have the same characteristic length L_0 , which depends on the properties of electrical transport (electrical conductivities of electrons and holes), on the properties of heat transport (thermal conductivity), and also on the properties of recombination (lifetime of charge carriers).

It is important to note that Eq. (10) does not contain thermoelectric heating or cooling (Peltier effect). They arise at the interface between two media due to a change in the drift component of the heat flux \mathbf{q}_{dr} [40, 41]. According to the Le Chatelier-Braun principle in the irreversible thermodynamics, "some internal fluxes appear in the system in the stationary state when an external influence affects this system, and these internal fluxes weaken the results of this influence" [42]. Applying this principle to our problem, one can say that the discontinuity in the drift fluxes at the junction that appears because of the different Peltier coefficients must lead to other thermal fluxes tending to reduce this discontinuity [40]. These thermal fluxes can only be thermal diffusion fluxes because the other drift heat fluxes are absent. The occurrence of these thermal diffusion fluxes leads to temperature heterogeneity in the structure and, as a result, to a cooling or heating of the junction. Thus, we have to understand the Peltier effect as a lowering or raising of the junction temperature (depending on the current direction) due to the appearance of induced thermal diffusion fluxes in the structure, and not as an evolution or absorption of the additional heat on the junction.

Let us note that the Peltier effect strongly depends on the junction surface thermal conductivity [40]. The contribution of this effect to the total effect of thermoelectric cooling increases with an increase in surface thermal conductivity, and slackens with a decrease in surface thermal conductivity.

The Peltier effect is frequently considered the opposite of the Seebeck effect [43] and vice versa. The reason for this is that in the case of the Peltier effect an electric current generates a nonuniform spatial temperature distribution, while in the case of the Seebeck effect a given nonuniform temperature distribution creates an electric current in a closed thermoelectric circuit.

From our point of view, the theoretical basis of this discussion lies in the Le Chatelier–Braun principle. Indeed, the appearance of temperature heterogeneity in the Peltier effect is caused by the appearance of an induced compensating thermal diffusion flux. A thermal diffusion flux a priori is given in the Seebeck effect. According to the Le Chatelier– Braun principle, in this case some compensatory thermal flux must also appear in a thermoelectric circuit. Only the drift thermal flux accompanied by the electric current appears, tending to compensate for the thermal diffusion flux.

It is clear that the system of equations (1), (2), (8), and (10) must be supplemented with boundary conditions for currents and heat flux. They were discussed in detail in [44–46].

4. Conclusions

A detailed analysis of the influence of thermal nonequilibrium on transport in semiconductors was carried out. The resulting equations are extremely simple and transparent. It has been proved that for thermal nonequilibrium conditions, nonequilibrium carriers do not disappear for strong recombination. Recently, a number of publications have appeared in which individual issues from those considered in this review were discussed in terms of experimental research and computational approaches [47–58]. These publications confirm the relevance of this review, since the number of theoretical articles in this area is small. At the same time, the review may stimulate the emergence of new theoretical and experimental studies and new interpretations of the known results.

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Градієнт температури і транспорт тепла та заряду в напівпровідниковій структурі (Огляд)

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Проведено детальний аналіз впливу теплової нерівноваги на транспорт у напівпровідниках. Показано, що транспорт тепла та заряду в біполярних напівпровідниках взаємозалежні та самоузгоджені. У загальному випадку розподіл температури в однорідних напівпровідниках не може бути постійним, або лінійною функцією щодо координати навіть у лінійному наближенні. Встановлено ролі нерівноважних носіїв заряду та рекомбінації в транспорті тепла.

Ключові слова: термічна нерівновага, рекомбінація, квазінейтральність, транспортні явища.