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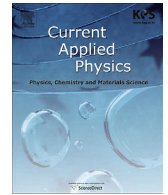

Mechanisms of charge carriers nonequilibrium in transport processes in bipolar semiconductors

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The interplay between physical origins of the nonequilibrium and their influence on the linear steady state transport processes in bipolar semiconductors are under investigation. Particular attention is paid to the influence of the energy nonequilibrium on the generation-recombination processes under various conditions. It is shown that in the case of the same (even if coordinate-dependant) temperature of the charge carriers and the phonons the volume recombination rate of the charge carriers in the steady state is completely determined by the splitting of the quasi-Fermi levels.

Particular emphasis has been placed on the manifestation of the energy nonequilibrium in the presence of hot charge carriers in a semiconductor. It is shown that in this case the generation-recombination balance shifts, being completely equivalent to the appearance of an additional external generation of electron-hole pairs. The two-temperature model (with electron temperature being different from the single temperature of holes and phonons) of the Dember photovoltaic effect is used to illustrate that the electromotive force (emf) may differ significantly from its corresponding values with no hot electrons. This additional contribution to the emf does not depend neither on the Seebeck coefficient nor on the temperature gradient and the electron-hole pair generation rate. This contribution to the emf is exclusively determined by the magnitude of the electron heating.

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1. Introduction

Semiconductor materials are widely used in the electronics industry because of their nonlinear properties, which in turn, are due to the fact that the nonequilibrium charge carriers and phonons readily appear even with relatively weak external excitation [1,2]. The electric field, light, ionizing radiation, heat and other external influences easily disturb the thermodynamic equilibrium in the semiconductor system, leading to the emergence of the nonequilibrium charge carriers.

Since a bipolar semiconductor is a system of three interacting subsystems (electrons, holes and phonons), the emergence of nonequilibrium in one of them disturbs the equilibrium state of the rest. In general, to study transport processes in semiconductors one needs to find a nonequilibrium distribution function of the charge carriers and phonons, e.g., by solving the Boltzmann equation [3,4]. However, in most cases of practical importance it is possible to introduce the nonequilibrium thermodynamic characteristics: the nonequilibrium chemical potentials, the electrochemical potentials (so called the quasi-Fermi levels or imrefs) and the temperature for each subsystem of the charge carriers and phonons. Accordingly, special cases of the nonequilibrium can be distinguished, depending on which parameter differs from its value in the thermodynamic equilibrium. For example, in the cases of the injection of charge carriers into the semiconductor from the contacting medium (as well as in the case of the generation of charge carriers by lighting or by heating the sample) the concentration of the charge carriers changes [5]. As a result, the carrier concentration usually becomes nonuniform in space. This type of the nonequilibrium is appropriately called the concentration nonequilibrium.

In general, due to the physical nature of the semiconductor, the concentration nonequilibrium disturbs the dynamic balance of the other processes; in particular, the ratio of the diffusion and drift components of the electron and hole currents changes [6]. Also, the balance between the capture of electrons and holes by impurity levels (i.e., recombination of electrons) and the thermal generation

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of charge carriers shifts. This means that e.g. the nonequilibrium electrons, appearing in the conduction band, give rise to the generation-recombination nonequilibrium, which in turn generates nonequilibrium holes in the valence band [5]. At the same time, such processes as the Peltier effect, Joule heating and nonradiative recombination disturb the energy equilibrium as well, making the temperatures of electrons, holes and phonons spatially nonuniform.

From the point of view of the thermodynamic characteristics of the semiconductor both the concentration nonequilibrium and the generation-recombination nonequilibrium are caused by the deviation of the electrochemical potential from its equilibrium value: the concentration nonequilibrium corresponds to the spatial inhomogeneity of the electrochemical potential, and the generation-recombination nonequilibrium corresponds to the difference in the electrochemical potential of electrons and holes (to the splitting of the quasi-Fermi levels) [6]. Similarly, the spatial inhomogeneity of the temperature and the differences in temperature between the three subsystems (charge carriers and phonons) are the physical mechanisms of the energy nonequilibrium in transport processes in semiconductors [4].

In turn, the energy nonequilibrium rarely can be analyzed independently of the other mechanisms of the nonequilibrium. For instance, the energy nonequilibrium caused by spatial nonuniformity of the charge carrier temperature disturbs the drift-diffusion balance due to the appearance of the thermoelectric field [7]. Additionally the temperature dependence of the cross sections of the rate of electron capture by impurities leads to a modification of the generation-recombination balance that is directly reflected on the charge carrier concentration, i.e. it leads to the concentration nonequilibrium [8].

This paper deals with the peculiarities and the interrelation between various mechanisms of the nonequilibrium in bipolar semiconductors in the steady state. Note that in the steady state, when the nonequilibrium space charge in the semiconductor does not depend on time, the mathematical description of transport processes is simplified. However, the physics of nonequilibrium transport processes is more complex and richer. This is due to the fact that in the steady state we have an additional relation $\operatorname{div}\boldsymbol{j}=0$ (here, $\boldsymbol{j}$ is the total electric current density in the circuit), therefore an additional mechanism for the interaction among the nonequilibrium of different types appears. For non-stationary (e.g., high-frequency) processes this interaction does not have enough time to manifest itself, and it is possible to analyze some mechanisms of the nonequilibrium independently [9].

2. Energy nonequilibrium and generation-recombination balance in uniform bipolar semiconductor

Evidently a nonuniform heating of an uniform sample of a bipolar semiconductor gives rise to nonequilibrium electron-hole pairs whose concentration profile will be non-uniform and, therefore, modifying the original homogeneity of the sample. There are two physical reasons for this: the appearance of thermoelectrical currents (causing the spatial redistribution of the charge carrier concentration) and thermal generation. The same result is obtained by the action of light and ionizing radiation, as well as by the injection of charge carriers from contacting media. Are these sources of nonequilibrium charge carriers equivalent in terms of the formation of the current–voltage characteristics (CVC) and the possibility of generating electromotive forces (emf)? To answer this question, we shall take a closer look at the energy nonequilibrium and its impact on the generation-recombination balance in bipolar semiconductors. Mathematically, to do this one needs to calculate the displacement of the dynamic equilibrium between the thermal generation and the recombination of electrons and holes; and then to determine the concentration of nonequilibrium charge carriers caused by this displacement.

For this purpose we use the drift-diffusion approximation, that is widely used and adequately describes the operation of the most modern solid-state microelectronics devices [10].

The continuity equation for the electron and hole current densities $\boldsymbol{j}_{n,p}$, describing the stationary transport processes are as follows [11]:

$$\operatorname{div}\boldsymbol{j}_n = e(R_n - G_n), \quad \operatorname{div}\boldsymbol{j}_p = e(G_p - R_p), \tag{1}$$

where e is the electron charge, $R_{n,p}$ are the electron (n) and hole (p) recombination rates, and $G_{n,p}$ are the external generation rates of charge carriers (the photo-generation rates). Note that the recombination rates $R_{n,p}$ are defined as the difference between the capture rate of a conduction electron or hole by impurity levels (or by holes and electrons, respectively, in interband recombination) and the rate of the reverse process — the thermal generation of free charge carriers.

In interband recombination [13] and recombination via an impurity level in the Shockley-Read-Hall (SRH) model in the steady state [14] the recombination rate can be written as $R_n = R_p = \chi(np - n_i^2)$, where χ is the capture factor, n and p are the concentrations of electrons and holes, respectively; n_i is the intrinsic charge carrier concentration [15]. Note that in the stationary SRH recombination the capture factor χ is a function of impurity level parameters and the charge carrier concentration [15]. However, this dependence is not relevant in the linear approximation, since, as will be shown below, drops out of the expression for the recombination rate (see Eq. (2), as well as the discussion at the end of the Section 3).

Following Ref. [15], we write the expression for the recombination rate in the linear approximation (with respect to the perturbation of any type) for stationary processes, as follows (recall, that according to the Ref. [15] this expression has been developed for the interband recombination and can be extended to the trap-assisted recombination only if $G_n = G_p$):

$$R_n = R_p = \frac{1}{T}\left(\frac{p_0}{n_0+p_0}\delta_n + \frac{n_0}{n_0+p_0}\delta_p - \beta\delta T + \eta(\delta T_n - \delta T)\right), \tag{2}$$

where $\delta n = n - n_0$, $\delta p = p - p_0$; n_0, p_0 are respectively the electron and hole concentrations in the state of the thermodynamic equilibrium at the temperature T_0; $\delta T_n = T_n - T_0$, $\delta T = T - T_0$, T_n is the electron temperature, T is the temperature of phonons and holes, $\tau = [\chi(T_0)(n_0+p_0)]^{-1}$ is the lifetime of the nonequilibrium charge carriers [15],

$$\beta = \frac{n_0 p_0}{n_0+p_0}\frac{1}{T_0}\left(3 + \frac{\varepsilon_g}{T_0}\right), \tag{3}$$

$$\eta = \frac{1}{\chi(T_0)}\frac{\partial\chi(T_0)}{\partial T_n}\frac{n_0 p_0}{n_0+p_0}, \tag{4}$$

ε_g is the semiconductor band gap. Let us note that for simplification when deriving Eq. (2) heating was assumed to affect only the conduction electrons while holes quickly transfer excess energy to phonons (inelastic scattering of holes by phonons [3], $m_n \ll m_p$, where m_n and m_p are the effective masses of electrons and holes, respectively), so that the temperatures of the hole subsystem and the lattice match.

The densities of electron and hole currents in the nonequilibrium case are conveniently expressed by the quasi-Fermi level

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