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Dynamic thermoelectricity in uniform bipolar semiconductor

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ABSTRACT

The theory of the dynamic thermoelectric effect has been developed. The effect lies in an electric current flowing in a closed circuit that consists of a uniform bipolar semiconductor, in which a non-uniform temperature distribution in the form of the traveling wave is created. The calculations are performed for the one-dimensional model in the quasi-neutrality approximation. It was shown that the direct thermoelectric current prevails, despite the periodicity of the thermal excitation, the circuit homogeneity and the lack of rectifier properties of the semiconductor system. Several physical reasons underlining the dynamic thermoelectric effect are found. One of them is similar to the Dember photoelectric effect, its contribution to the current flowing is determined by the difference in the electron and hole mobilities, and is completely independent of the carrier Seebeck coefficients. The dependence of the thermoelectric short circuit current magnitude on the semiconductor parameters, as well as on the temperature wave amplitude, length and velocity is studied. It is shown that the magnitude of the thermoelectric current is proportional to the square of the temperature wave amplitude. The dependence of the thermoelectric short circuit current on the temperature wave length and velocity is the nonmonotonic function. The optimum values for the temperature wave length and velocity, at which the dynamic thermoelectric effect is the greatest, have been deduced. It is found that the thermoelectric short circuit current changes its direction with decreasing the temperature wave length under certain conditions. The prospects for the possible applications of the dynamic thermoelectric effect are also discussed.

1. Introduction

Research of the thermoelectric phenomena and development of efficient thermoelectric converters represent a major challenge to the modern applied solid state physics. Currently, investigations is mainly focused on the search and creation of new efficient thermoelectric materials with a high thermoelectric figure of merit *ZT* [1–3]. However, despite a long history of thermoelectric research, because of its diversity the physics of transport phenomena under non-equilibrium energy conditions (a particular case of which is a non-uniform temperature distribution [4]) is as yet imperfectly understood. This is especially true in the case of simultaneous action of several perturbations in the semiconductor systems, as well as in the case of time-dependent temperature fields. Meanwhile, there are a number of papers demonstrating that the energy conversion in semiconductor systems under non-steady state conditions may differ significantly from the static case by its physical background. In particular, a significant increase in the thermocouple efficiency [5] (although this work does not deal with a semiconductor system), as well as an increase in the thermoelectric power at the *p–n* junction [6] are proven in the transient regime.

Note that the difference between dynamic mechanisms of the electromotive force (emf) formation and their static counterparts is not an exclusive feature of thermoelectric phenomena. It is known that, for example, a photo-emf in dynamic mode can significantly exceed the static values (for example, the Dember emf [7,8]), as well as it can appear in situations where no static emf can arise [9]. Moreover, an effective experimental technique for semiconductor parameter measurements has been developed based on the effect of the non-steady state photo-emf [10].

The main factors underlying the most significant distinctions of thermoelectric effects in the dynamics might be as follows. First, a time-dependent perturbation gives rise to an uncompensated space charge in the semiconductor. In turn, the latter affects the conventional mechanism of the thermopower generation. This way is of especial importance in multi-layer structures and polycrystalline films [6]. Second, time derivatives of the carrier densities explicitly appear in the continuity equation [11,12], and it might directly affect the magnitude of the thermo-emf. For the non-steady state photovoltaic phenomena it is the mechanism that determines the existence of the Dember emf even when the production of the static photoelectricity is basically impossible [9]. Finally, the time dependence of the temperature can influence the transport processes through changing the thermal generation rate.

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As shown in Ref. [4], in the static case the thermal generation can contribute to the emf only when there is the difference in the carrier temperatures (e.g., the electron temperature differs from the temperature of holes and phonons). If there is a single temperature of all quasiparticles in the semiconductor, the thermal generation does not affect the value of the thermopower at any static temperature distribution in the semiconductor structure.

The time dependence of the thermal generation rate can change the picture, leading to at first glance paradoxical results. Thus, it is widely assumed that two contacts at different temperatures between two media with different Seebeck coefficients are mandatory for the thermopower appearance. Or that in a uniform semiconductor sample having the same temperature of its ends, no thermoelectricity is generated at any temperature distribution inside the semiconductor. However, in the dynamic case the above is no longer true. Thus, in Ref. [13] it has been presented a physical mechanism that is responsible for the thermoelectric current generation by the temperature wave propagating in a uniform unipolar semiconductor. Below, we show that a similar phenomenon takes place in a uniform bipolar semiconductor. In the latter, as in a more complex physical system (in which there are two types of the charge carriers: electrons and holes), the nature of the dynamic thermoelectric effect is also more complicated, and the magnitude of the thermopower generated can be substantially higher than the corresponding value in the unipolar semiconductor.

The presented theory also shows that the thermoelectric short circuit current is a nonmonotonic function of the temperature wave parameters. This allows us to offer using the considered dynamic thermoelectric effect as a research technique for investigations of the bipolar semiconductor properties.

2. Mathematical model of dynamic thermoelectric effect

Consider a slab of uniform bipolar semiconductor of the length L, in which a stationary (but not static) temperature distribution in the form of a traveling wave is maintained by an external heating:

$$T = T_0 + \delta T_0 \cos \Phi, \tag{1}$$

where $\Phi = kx + \omega t$, $k = 2\pi/\Lambda$, Λ is the temperature wave length, $\omega = k\nu$, ν is the temperature wave velocity. To simplify the calculations, we assume that the slab length is divisible by the temperature wave length, i.e. let $kL/(2\pi)$ be an integer.

We will not dwell on methods for creating the temperature distribution of the form in Eq. (1) in the specimen. For discussion of this matter see the Appendix Appendix A.

We will restrict our consideration to the one-dimensional model, supposing all physical values in directions normal to the temperature wave propagation to be uniform. Then, under the drift-diffusion model one can write the following continuity equations for the electron (j_n) and hole (j_p) current densities [11,12,14]:

$$\frac{\partial n}{\partial t} = \frac{1}{e}\frac{\partial j_n}{\partial x} - R_n, \tag{2}$$

$$\frac{\partial p}{\partial t} = -\frac{1}{e}\frac{\partial j_n}{\partial x} - R_p, \tag{3}$$

with

$$j_n = e\mu_n nE + T\mu_n \frac{\partial n}{\partial x} - e\mu_n \alpha_n n \frac{\partial T}{\partial x}, \tag{4}$$

$$j_p = e\mu_p pE - T\mu_p \frac{\partial p}{\partial x} - e\mu_p \alpha_p p \frac{\partial T}{\partial x}, \tag{5}$$

where n and p are the electron and hole densities, respectively; e is the elementary charge, $R_{n,p}$ are the recombination rates of electrons and holes, $\mu_{n,p}$ are the electron and hole mobilities, E is the electric field in the semiconductor, $\alpha_{n,p}$ are the Seebeck coefficients for the electron and hole subsystems.

Brief mention should be made of the following. In modern literature, Eqs. (4) and (5) are written frequently in the following form [15–17]:

$$j_{n,p} = -\sigma_{n,p}\left(\frac{\partial \psi_{n,p}}{\partial x} - \alpha^*_{n,p}\frac{\partial T}{\partial x}\right), \tag{6}$$

where $\psi_{n,p} = \varphi \mp \zeta_{n,p}/e$ are the electrochemical potentials of the carriers (here, sign "−" refers to the electrons, and "+" to holes), φ is the electric potential, $\zeta_{n,p}$ are the chemical potentials of the carriers, $\sigma_n = e\mu_n n$ and $\sigma_p = e\mu_p p$ are the conductivity of the electron and hole subsystems, respectively. Introduced in that way the Seebeck coefficients $\alpha^*_{n,p}$ differ from the phenomenologically introduced Seebeck constants in Eqs. (4) and (5) and are related to them as follows:

$$\alpha^*_{n,p} = \alpha_{n,p} \mp \frac{1}{e}\frac{\partial \zeta_{n,p}}{\partial T}. \tag{7}$$

Below we will use the Seebeck coefficients $\alpha_{n,p}$, and the resulting expression can be rewritten in terms of $\alpha^*_{n,p}$ in an obvious way, using Eq. (7).

Here we restrict ourselves to the quasi-neutrality approximation by assuming the Debye screening length to be the smallest spatial parameter and the Maxwell relaxation time to be the smallest temporal parameter of the problem [18,19]. Under these conditions there is no space charge in the semiconductor: $\rho = e(p - n_t - n) = 0$, where n_t is the charged impurities density (to be specific, the density of negatively charged impurity levels).

Suppose that the dominant mechanism of recombination is the interband recombination (if so, the calculations are less bulky). Then [20,21]:

$$R_n = R_p = R = \gamma(np - n_0 p_0), \tag{8}$$

where γ is the capture coefficient, n_0 and p_0 are the electron and hole densities in the thermodynamic equilibrium (i.e. at T_0), respectively.

To simplify the calculations we assume that the charged impurity density remains constant. This assumption is valid at sufficiently high temperatures, when in the thermodynamic equilibrium the majority of dopant atoms are already ionized. Thus, the local change in temperature has no effect on them. The appearance of nonequilibrium electrons and holes does not affect the equilibrium of the impurity subsystem due to the interband transitions dominate. In these conditions, the lack of space charge imposes the following relation between the nonequilibrium electron density $\delta n = n - n_0$ and the nonequilibrium hole density $\delta p = p - p_0$: $\delta n = \delta p$ [19].

In the quasi-neutrality from Eqs. (2) and (3) follows $\partial j/\partial x = 0$, where $j = j_n + j_p$ is the total electric current density. Adding up Eqs. (4) and (5), one gets:

$$j(t) = \sigma E + T\left(\mu_n - \mu_p\right)\frac{\partial \delta n}{\partial x} - \left(\alpha_n \sigma_n + \alpha_p \sigma_p\right)\frac{\partial T}{\partial x}, \tag{9}$$

where $\sigma = \sigma_n + \sigma_p$ is the total conductivity of the semiconductor.

The system of differential Eqs. (2) and (3) must be supplemented by boundary conditions (BCs). To avoid issues related to influence of contacting media and physical processes at the interfaces we choose the cyclic BCs. From a physical point of view,