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KINETIC PROPERTIES AND CHARGE TRANSPORT PHYSICS OF ISOTROPIC SEMICONDUCTOR CRYSTALS

WŁASNOŚCI KINETYCZNE I FIZYKA TRANSPORTU ŁADUNKU W IZOTROPOWYCH KRYSZTAŁACH PÓŁPRZEWODNIKOWYCH

Abstract

This paper presents general formulas for the kinetic properties of semiconductor crystals expressed in terms of the Fermi integrals. The formulas provide algorithms for the calculation or identification of the kinetic properties and constitute (together with the results of theoretical analysis and other presented relationships) the mathematical model of the charge carrier transport phenomena in semiconductor crystals.

Keywords: *kinetic phenomena*, *charge carriers*, *scattering mechanisms*, *semiconductor crystals*

Streszczenie

Uzyskane i przedstawione w artykule ogólne wzory opisujące własności kinetyczne kryształów półprzewodnikowych są wyrażone poprzez całki Fermiego. Te wzory są podstawą algorytmu do obliczenia i identyfikacji tych własności, stanowiąc (łącznie z wynikami analizy teoretycznej i innymi przedstawionymi zależnościami) model matematyczny zjawisk transportu nośników ładunku elektrycznego w kryształach półprzewodnikowych.

Słowa kluczowe: *zjawiska kinetyczne*, *nośniki ładunku*, *mechanizmy rozpraszania*, *kryształy półprzewodnikowe*

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1. Introduction

The theoretical problems of how to determine the kinetic properties of a semiconductor crystal are connected mainly with the following problems:

– determining the energy spectrum $\varepsilon(\overrightarrow{p})$,

– determining the scattering function $u(\varepsilon)$,

– determining the reduced chemical potential μ^*.

In this paper, a theoretical analysis of the kinetic properties of the semiconductor crystals is presented. The kinetic properties of the semiconductor crystals are considered in the framework of the statistical theory of the solid state. This discussion is based on general formulas which are expressed in terms of the Fermi integrals. These formulas provided algorithms for the calculation of the kinetic properties and, together with other relations, constitute the mathematical model of the charge carrier transport phenomena in semiconductor crystals.

The calculation or identification of the kinetic properties of a crystal and the prediction of its useful technological properties are closely related [1, 2, 4, 8, 10, 13].

2. Theoretical analysis of the kinetic properties of semiconductor crystals

According to the statistical theory of the solid state, in the presence of a weak magnetic field, or when the magnetic field is absent, the kinetic properties of isotropic doped semiconductor crystals may be described by general formulas – these are expressed in terms of the Fermi integrals.

Some of these properties are as follows:

– the resistivity $\rho\ (T, \mu^*)$

– the Hall coefficient $R\ (T, \mu^*)$,

– the thermopower (the Seebeck coefficient) $\alpha\ (T, \mu^*)$,

– the Nernst – Ettingshausen constant $N\ (T, \mu^*)$,

– the thermal conductivity $\chi\ (T, \mu^*)$,

– the conductivity $\sigma\ (T, \mu^*)$,

– the carrier density $n\ (T, \mu^*)$,

– the carrier mobility $U_D\ (T, \mu^*)$,

– the Hall mobility $U_H\ (T, \mu^*)$,

and the apprioprate formulas based on the Fermi integrals take the forms:

$$\rho(T,\mu^*) = \frac{1}{en} \frac{J00(T,\mu^*)}{J01(T,\mu^*)}, \tag{1}$$

$$R(T,\mu^*) = \frac{1}{zen} \frac{J00(T,\mu^*)J02(T,\mu^*)}{J01(T,\mu^*)^2}, \tag{2}$$

$$\alpha(T,\mu^*) = \frac{k}{ze} \left(\frac{J11(T,\mu^*)}{J01(T,\mu^*)} - \frac{\mu}{kT} \right), \tag{3}$$

$$N(T,\mu^*) = \frac{k}{e}\left|\frac{R(T,\mu^*)}{\rho(T,\mu^*)}\right|\left(\frac{J11(T,\mu^*)}{J01(T,\mu^*)} - \frac{J12(T,\mu^*)}{J02(T,\mu^*)}\right), \tag{4}$$

$$\chi(T,\mu^*) = \left(\frac{k}{e}\right)^2 \frac{T}{\rho(T,\mu^*)}\left(\frac{J21(T,\mu^*)}{J01(T,\mu^*)} - \left(\frac{J11(T,\mu^*)}{J01(T,\mu^*)}\right)^2\right), \tag{5}$$

$$\sigma(T,\mu^*) = en(T,\mu^*)\frac{J01(T,\mu^*)}{J00(T,\mu^*)} = en(T,\mu^*)U_D(T,\mu^*), \tag{6}$$

$$n(T,\mu^*) = J00(T,\mu^*), \tag{7}$$

$$U_D(T,\mu^*) = \frac{J01(T,\mu^*)}{J00(T,\mu^*)}, \tag{8}$$

$$U_H(T,\mu^*) = \left|\frac{R}{\rho}\right| = \frac{J02(T,\mu^*)}{J01(T,\mu^*)}. \tag{9}$$

In the above expressions for the kinetic properties of semiconductor crystals, the symbols $Jij(T,\mu^*)$ are reserved for the Fermi integrals (the kinetic integrals) given by the following formulas:

$$Jij(T,\mu^*) = \int_0^\infty \left(\frac{\varepsilon}{kT}\right)^i u^j G(\varepsilon)\left(-\frac{df_0}{d\varepsilon}\right)d\varepsilon, \quad J00(T,\mu^*) = \int_0^\infty G(\varepsilon)\left(-\frac{df_0}{d\varepsilon}\right)d\varepsilon. \tag{10}$$

The analysis of the kinetic integrals (10) shows us that the following inequality takes place [6]:

$$\left(\frac{J01(T,\mu^*)}{J00(T,\mu^*)}\right)^2 \leq \left(\frac{J02(T,\mu^*)}{J00(T,\mu^*)}\right).$$

From this inequality, it follows that:

$$\frac{J00(T,\mu^*)J02(T,\mu^*)}{J01(T,\mu^*)^2} = f_R(T,\mu^*) \geq 1.$$

Commonly, the function $f_R(T,\mu^*)$ in lecture courses on solid state and semiconductor physics is called the Hall factor [7, 8]. It is easy to show that this function has a minimum value equal to 1 in a semiconductor crystal, where the current carriers are degenerated.

Using the function (10), formulas (8) and (9) describe the carrier and Hall mobilities:

$$U_D(T,\mu^*) = \frac{J01(T,\mu^*)}{J00(T,\mu^*)},$$

$$U_H(T,\mu^*) = \frac{J02(T,\mu^*)}{J01(T,\mu^*)}.$$

Thus, we have:

$$\frac{U_H(T,\mu^*)}{U_D(T,\mu^*)} = \frac{J00(T,\mu^*)J02(T,\mu^*)}{J01(T,\mu^*)^2} = f_R(T,\mu^*) \geq 1.$$

Consequently, we also have $U_H(T,\mu^*) = U_D(T,\mu^*)f_R(T,\mu^*)$, that is $U_H(T,\mu^*) > U_D(T,\mu^*)$.

From definition of the carrier mobility $U_D(T,\mu^*)$, there is:

$$U_D(T,\mu^*) = \frac{J01(T,\mu^*)}{J00(T,\mu^*)} = \frac{\int_0^\infty u(\varepsilon)G(\varepsilon)\left(-\frac{df_0}{d\varepsilon}\right)d\varepsilon}{\int_0^\infty G(\varepsilon)\left(-\frac{df_0}{d\varepsilon}\right)d\varepsilon}.$$

In statistical physics, this expression has mathematical sense of the average value of the function $u(\varepsilon)$, for all values ε, $\varepsilon \in [0,\infty)$ and this value is denoted by $<...>$. Clearly, in statistical physics, the carrier mobility $U_D(T,\mu^*)$ is given by:

$$U_D(T,\mu^*) = <u(\varepsilon)>_{(T,\mu^*)},$$

where the subscripts (T, μ^*) denote that the average values $<u(\varepsilon)>$ are analytically dependent of the chemical potential and temperature. Hence, the carrier mobility $U_D(T,\mu^*)$ equals the average value of the function $u(\varepsilon)$ for all values of ε.

We will now consider the Hall mobility which by formula (9) is given as:

$$U_H(T,\mu^*) = \frac{J02(T,\mu^*)}{J01(T,\mu^*)} = \frac{J02(T,\mu^*)J00(T,\mu^*)}{J00(T,\mu^*)J01(T,\mu^*)} = \frac{<u(\varepsilon)^2>_{(T,\mu^*)}}{<u(\varepsilon)>_{(T,\mu^*)}}.$$

The Hall factor can be expressed in terms of the averages of the scattering function $u(\varepsilon)$ ($u(\varepsilon)$ is the average velocity of carriers in the presence of the unit electric field $\vec{E}$) in the following way:

$$f_R(T,\mu^*) = \frac{J00(T,\mu^*)J02(T,\mu^*)}{J01(T,\mu^*)^2} = \left(\frac{J00(T,\mu^*)}{J01(T,\mu^*)}\right)^2 \frac{J02(T,\mu^*)}{J00(T,\mu^*)} = \frac{<u(\varepsilon)^2>_{(T,\mu^*)}}{<u(\varepsilon)>^2_{(T,\mu^*)}}.$$

In statistical physics is proved that $<u(\varepsilon)^2>_{(T,\mu^*)} \geq <u(\varepsilon)>^2_{(T,\mu^*)}$, then we obtain $f_R(T,\mu^*) \geq 1$.

Analysis of formulas (1)–(10) for the kinetic properties of semiconductor crystals that is based on the above calculations shows that these kinetic properties analytically depend on the average values $<u(\varepsilon)>_{(T,\mu^*)}$ and $<u(\varepsilon)>^2_{(T,\mu^*)}$.

Carriers in semiconductor crystals are scattered by defects in the crystals hence the concept or notion of the scattering function $u(\varepsilon)$ which describes the effect of

these scattering processes on kinetic properties of these crystals is a serious problem in semiconductor and solid state physics.

Formula (10) shows that the kinetic integrals $J_{ij}(T, \mu^*)$ depend on the Fermi-Dirac equilibrium distribution function

$$f_0(\varepsilon, \mu^*) = \left(\exp\left(\frac{\varepsilon}{kT} - \mu^* \right) + 1 \right)^{-1}, \quad \mu^* = \frac{\mu}{kT}. \tag{11}$$

From this formula, and from formulas (1)–(10), it follows that all properties of the crystal, which are described by formulas (1)–(10), analytically depend on the reduced chemical potential μ^*.

There is also an analytical dependence of kinetic properties on $G(\varepsilon) = \int_0^\varepsilon g(\varepsilon) d\varepsilon$ [8] in these formulae. Here, $g(\varepsilon)$ is the density of states (DOS) lying in allowed bands which depends on the analytical form of the energy spectrum $\varepsilon_{\vec{p}} = \varepsilon(\vec{p})$.

In isotropic crystals $\varepsilon_{\vec{p}} = \varepsilon(|\vec{p}|) = \varepsilon(p)$, where $p = \sqrt{p_x^2 + p_y^2 + p_z^2}$. Thus, all kinetic properties of these crystals which are described by formulas (1)–(10) analytically depend on the energy spectrum $\varepsilon_{\vec{p}} = \varepsilon(p)$.

Formulas (1)–(10) show that with the exception of the density $n(T, \mu^*)$ of current carriers in a semiconductor (formula (7)), all kinetic properties of crystals explicitly depend on the scattering function $u(\varepsilon)$ – this describes the effect of these scattering processes on the kinetic properties of these crystals [8, 9]. Computations of values of the scattering function $u(\varepsilon)$ are connected with problems on determination the energy spectrum $\varepsilon(\vec{p})$ and scattering probability $W(\vec{p}, \vec{p}')$. The explicit form of this probability depends on the nature of the semiconductor crystal and the type of defects in this crystal by which free charge carriers are scattered [1, 10].

3. The energy spectrum and the discrete density of states (DOS) of the charge carrier energy in a semiconductor crystal

In the quantum theory of crystal structure, the energy spectrum is called the function – this describes the dependence of the total charge carrier energy ε on this carrier quasimomentum $\vec{p}$ in this crystal, that is $\varepsilon_{\vec{p}} = \varepsilon(\vec{p})$ [8].

According to quantum mechanics, the charge carrier quasimomentum $\vec{p}$ in crystals varies discretely and there are as many values of $\vec{p}$ as there are structure particles in the crystal. In this connection, it should be noted the charge carrier energy is quantised. Moreover, it was proved [7] that the energy spectrum has symmetry properties being a periodic and

even function of the vector $\vec{p}$: $\varepsilon(\vec{p}) = \varepsilon(-\vec{p})$, $\varepsilon(\vec{p}) = \varepsilon(-\vec{p} + \vec{P})$, where $\vec{P} = \hbar \vec{K}_n$. In this relationship, $\hbar$ is the Planck's constant, $\vec{K}_n$ is the reciprocal lattice vector.

A free charge carrier with energy $\varepsilon_{\vec{p}} = \varepsilon(\vec{p})$ in crystals has the velocity of chaotic motion $\vec{v}_{\vec{p}} = \nabla_{\vec{p}}\, \varepsilon(\vec{p})$ and this carrier subjected to the action of a force $\vec{F}$ will acquire an acceleration $\vec{a}_{\vec{p}}$, which is defined by formula [8]:

$$\vec{a}_{\vec{p}} = \left(\frac{\partial^2 \varepsilon(\vec{p})}{\partial p_i \partial p_k} \right) \vec{F} = \left(\frac{1}{m_{ik}(\vec{p})} \right) \vec{F},$$

where the tensor $\left(\dfrac{\partial^2 \varepsilon(\vec{p})}{\partial p_i \partial p_k} \right) = \left(\dfrac{1}{m_{ik}(\vec{p})} \right)$ is called the reciprocal effective mass tensor. Once the symmetry properties of the energy spectrum are known, it is easy to approximate this energy spectrum of the free energy carriers in a semiconductor crystal.

It can be seen from these calculations that in the case of anisotropic crystals, the energy spectrum is described by the constant energy ellipsoid S, having the following anisotropic parabolic form:

$$\varepsilon_{\vec{p}} \cong \frac{p_1^2}{2m_{11}} + \frac{p_2^2}{2m_{22}} + \frac{p_3^2}{2m_{33}},$$

and in isotropic crystals, it is the constant energy sphere S, having the isotropic parabolic form:

$$\varepsilon_{\vec{p}} \cong \frac{p_1^2 + p_2^2 + p_3^2}{2m} = \frac{p^2}{2m},$$

where m_{11}, m_{22}, m_{33} are the diagonal components of the charge carrier effective mass tensor [8].

In quantum mechanics, the quantity $G(\varepsilon)$, which determines the number of states of particles in a crystal, with the energy range between $\varepsilon = 0$ and $\varepsilon(\vec{p})$, is given by the well--known general expression:

$$G(\varepsilon) = \int_0^\varepsilon d\varepsilon\, \frac{2}{h^3} \oint_S \frac{dS}{\left| \nabla_{\vec{p}}\, \varepsilon_{\vec{p}} \right|}, \quad S = \{(\vec{p}, \varepsilon) : \varepsilon_{\vec{p}} = \varepsilon(\vec{p}),\ \varepsilon = \text{const}\}. \quad (12)$$

From the definition of the density of the energy states (DOS), we obtain:

$$g(\varepsilon) = \frac{dG(\varepsilon)}{d\varepsilon}. \quad (13)$$

Substituting the value $G(\varepsilon)$ into equation (13), we have:

$$g(\varepsilon) = \frac{2}{h^3} \oint_S \frac{dS}{\left|\nabla_{\vec{p}}\, \varepsilon_{\vec{p}}\right|}, \tag{14}$$

where the integral has to be evaluated for the constant energy surface S, which is defined by the energy spectrum $\varepsilon_{\vec{p}} = \varepsilon(\vec{p})$.

Since $g(\varepsilon) = \dfrac{dG(\varepsilon)}{d\varepsilon}$, then $G(\varepsilon) = \displaystyle\int_0^\varepsilon g(\varepsilon)d\varepsilon.$

It is clear from formulas (12) and (14), that to determine the density of state (DOS), the constant-energy surface S must be known.

4. The calculation of the kinetic properties of isotropic doped semiconductor crystals

The presented formulas provide algorithms for the calculation of the kinetic properties (1)–(9) of isotropic doped semiconductor crystals.

In isotropic crystals, the energy spectrum is isotropic and it takes the form: $\varepsilon_p = \varepsilon(p)$, where $p = |\vec{p}| = \sqrt{p_1^2 + p_2^2 + p_3^2}$. It can then also be rewritten in the form: $p = p(\varepsilon)$.

We shall use formulae (12) and (14) to determine the quantities $G(\varepsilon)$ and $g(\varepsilon)$, taking into consideration the crystal with the isotropic energy spectrum. Now, the quantities $G(\varepsilon)$ and $g(\varepsilon)$ have the following forms:

$$G(\varepsilon) = \frac{8\pi}{3h^3} p^3(\varepsilon), \tag{15}$$

$$g(\varepsilon) = \frac{dG(\varepsilon)}{d\varepsilon} = \frac{8\pi}{3h^3} p^2(\varepsilon)\frac{dp(\varepsilon)}{d\varepsilon}. \tag{16}$$

In the above formulae, the function $p = p(\varepsilon)$ is defined by the isotropic energy spectrum $\varepsilon_p = \varepsilon(p)$.

There are the different modes of the charge carriers scattering in semiconductors [1, 8, 9, 13]. Here, the main mechanisms of interest are scattering by the acoustic phonons, the optical phonons, the point defects in semiconductors, and the charged impurities (the ions).

The scattering function of the main scattering modes is given by [1, 2, 3, 10]:

$$u(\varepsilon) = U^{(r)}(T)p^{(2r-3)}\left(\frac{d\varepsilon}{dp}\right)^2, \tag{17}$$

where $U^{(r)}(T)$ is the temperature dependent function known for the actual scattering mode, r is the parameter and it has the following values [1]:
– $r = 0$ for the scattering by the acoustic phonons and the point defects in semiconductors.
– $r = 1$ for the scattering by the optical phonons when the crystal's temperature is larger than the Debay temperature Θ.
– $r = 2$ for the scattering by the charged impurities (the ions) in the crystal lattice.

In the case of the combined scattering mode, the general scattering function u is given by the formula:

$$\frac{1}{u} = \frac{1}{u(r_1)} + \frac{1}{u(r_2)} + \ldots + \frac{1}{u(r_n)}, \tag{18}$$

where $\dfrac{1}{u(r_i)}$ is the scattering function of the simple scattering mode with the parameter r_i,

$i = 0, \ldots, 2$.

Now, we can use the formulae (1)–(9) to the calculation of the kinetic properties of isotropic doped semiconductor crystals with a narrow energy gap E_g.

In these crystals, the electrons and holes energy spectra are described by the nonparabolic Kane's band [1, 5]:

$$\frac{p^2}{2m^*} = \varepsilon + \frac{\varepsilon^2}{E_g}, \quad \text{that is} \quad p = \sqrt{2m^*\varepsilon(1+\frac{\varepsilon}{E_g})}, \tag{19}$$

where m^* is the parameter of the spectrum which plays a role of the electron or hole effective mass, E_g is the energy gap width.

For the energy spectrum (19) and the actual scattering modes (which are defined by the parameter r in formula (17)) taking into consideration formulae (15) and (17), the kinetic integral (10) takes form:

$$Jij(T,\mu^*) = [U^{(r)}(T)]^j N_c(T) I_{ij}(T,\mu^*). \tag{20}$$

In formula (20), the following notations were used:

$N_c(T)$ is the conduction band effective density of states and is defined by [8]:

$$N_c(T) = \frac{8}{3\sqrt{\pi}}(\frac{2m^*kT}{h^2})^{3/2}. \tag{21}$$

$U^{(r)}(T)$ is the temperature dependent function, which has dimension of the mobility and is defined by [1, 3, 10]:

$$U^{(r)}(T) = \left[\frac{1}{T}(U_A\delta(0,r) + U_O\delta(1,r) + U_I\delta(2,r))\right](m^*)^{(r-5/2)}T^{(r-1/2)}, \tag{22}$$

where U_A, U_O, U_I are the constants, which depend on the nature of the semiconductor crystal and the scattering mode of charge carriers in the crystal – the subscripts A, O, I are for the scattering by the acoustic phonons, the optical phonons, and the ions in the crystal lattice, respectively. $\delta(\ldots)$ is the Kronecker symbol.

$Iij(T,\mu^*)$ is the dimensionless functional and is given by:

$$Iij(T,\mu^*) = \int_0^\infty x^i \frac{(x+\beta(T)x^2)^{(rj-j/2+3/2)}}{(1+2\beta(T)x)^{2j}}\left(-\frac{df_0}{dx}\right)dx. \tag{23}$$

In formula (23), $\beta(T) = \dfrac{kT}{E_g}$ is the parameter of nonparabolicity of the energy spectrum – this parameter is near zero in the semiconductor crystals with a wide energy gap E_g, and the nonparabolic Kane's band turns into a parabolic band, i. e. the semiconductor crystal has a parabolic energy spectrum, $x = \varepsilon / kT$.

We substitute the value $Jij(T, \mu^*)$ from (20) in formulae (1)–(9) of the kinetic properties. For example, the selected kinetic properties of the crystal take the forms:

$$n(T, \mu^*) = N_c(T)I00(T, \mu^*), \tag{24}$$

$$R(T, \mu^*) = \frac{1}{zen(T, \mu^*)} \frac{I00(T, \mu^*)I02(T, \mu^*)}{I01(T, \mu^*)^2}, \tag{25}$$

$$\alpha(T, \mu^*) = \left(\frac{k}{ze}\right)\left(\frac{I11(T, \mu^*)}{I01(T, \mu^*)} - \mu^*\right), \tag{26}$$

$$N(T, \mu^*) = \left(\frac{k}{e}\right)U_H(T, \mu^*)\left[\frac{I11(T, \mu^*)}{I01(T, \mu^*)} - \frac{I12(T, \mu^*)}{I02(T, \mu^*)}\right], \tag{27}$$

$$\sigma(T, \mu^*) = en(T, \mu^*)U^{(r)}(T)\frac{I01(T, \mu^*)}{I00(T, \mu^*)}, \tag{28}$$

$$U_D(T, \mu^*) = U^{(r)}(T)\frac{I01(T, \mu^*)}{I00(T, \mu^*)}, \tag{29}$$

$$U_H(T, \mu^*) = |\sigma R| = U^{(r)}(T)\frac{I02(T, \mu^*)}{I01(T, \mu^*)} = U_D(T, \mu^*)\frac{I00(T, \mu^*)I02(T, \mu^*)}{I01(T, \mu^*)}. \tag{30}$$

From formulae (24)–(30) for the kinetic properties of the semiconductor crystals, it will be obvious that in order for the theoretical determination of these properties, the following experimental data should be known: the parameter of scattering r (i. e. the actual scattering mode or modes in the crystal), the reduced chemical potential μ^*, and the carriers' effective mass m^*. There are well-known experimental techniques capable of determining these experimental data [11–13] including the actual scattering modes from the temperature dependence of the Hall mobility U_H.

5. Conclusions

We have proposed general formulae for the kinetic properties of semiconductor crystals expressed in terms of the Fermi integrals.

The formulae constitute the mathematical model of the charge carriers transport phenomena in the semiconductor crystals.

Possibly, it is useful to have a method of evaluating these properties without resorting to the Boltzmann equation, we do then not use this equation as the basis for our model and our analysis of the kinetic properties of semiconductor crystals.

The theoretical analysis of the model shows that for the calculation of the kinetic properties of isotropic doped semiconductor crystals, the following experimental data should be known: the actual scattering mode or modes in the crystal, the reduced chemical potential, and the carriers' effective mass.

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