Calculation of the Thermoelectric Figure of Merit in Layered Structures with Quantum Wells at Different Scattering Mechanisms.

D.A. Pshenay-Severin, Yu.I. Ravich*, M.V. Vedernikov
Ioffe Physicotechnical Institute, Russian Academy of
Sciences, 194021 St. Petersburg, Russia
*St-Petersburg State Polytechnical University,
195251 St. Petersburg, Russia

Abstract

The calculations of mobility and the thermoelectric figure of merit in multiple-quantum-well (MQW) structures have been performed for the cases of different scattering mechanisms: acoustical phonon scattering, scattering by short-range impurity potential and polar scattering by optical phonons. In the first two cases, when the scattering probability is independent of the electron wave vector change Δk during the scattering act, the analytical expressions for mobility and the thermoelectric figure of merit have been obtained at the assumptions of infinite barriers height and standard dispersion law of electrons. The comparison with the case of polar scattering by optical phonons, when the scattering probability is proportional to Δk^{-2}, has shown that the enhancing of the figure of merit is possible due to the size quantum effect only if the scattering probability decreases with increasing of Δk.

Introduction

The pioneering works of Hicks and Dresselhaus [1-3] made a start on intensive study of the thermoelectric effects in quantum wells and superlattices. They performed the calculations and estimations of the thermoelectric figure of merit Z of layered structure with quantum wells and showed that the thermoelectric efficiency in such structures could be increased by a factor of 2 or 3 over the bulk value due to the rise of the density of states in quantum wells. The calculations in [1-3] were based on the constant relaxation time (CRTA) approximation, in which the relaxation time was assumed to be independent on both carrier energy and thickness of the quantum well a. In [4-6] the numerical calculations of the figure of merit were performed taking into account the variation of the relaxation time with the well thickness for different scattering mechanisms and complex charge carrier dispersion relations. These calculations showed that the rise of the density of states of electrons in quantum wells led in some cases to decrease of mobility and, hence, to diminution of the thermoelectric efficiency in comparison with the CRTA approximation.

In the present paper we have performed analytical calculations of relaxation time and the thermoelectric figure of merit for the cases of scattering by acoustical phonons, short-range impurity potential and polar scattering by optical phonons.[1] In order to compare the dependencies of relaxation time and thermoelectric efficiency on the well width at different scattering mechanisms and to achieve plain results the calculations have been performed for the case of infinite barrier height and isotropic parabolic approximation for dispersion law of electrons. In the case of polar scattering the numerical estimations of the thermoelectric efficiency have been performed, and the results of these estimations have been compared with the ones obtained in the same assumption as was made in [1], i.e. using bulk value for the relaxation time in MQW structures.

Relaxation Time for the Cases of Acoustic Scattering and Polar Scattering by Optical Phonons

The wave function of electron localized inside the quantum well (QW) with infinitely high barriers can be written as

$$\psi_{\mathbf{k}_\parallel}(\mathbf{r}) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi a}{z}\right)\frac{1}{\sqrt{S}}e^{i\mathbf{k}_\parallel \boldsymbol{\rho}}, \qquad (1)$$

where $\mathbf{k}_\parallel$ is the wave vector of an electron in the QW plane; the radius-vector $\mathbf{r}$ has two components: $\boldsymbol{\rho}$ inside the QW plane and z in the direction perpendicular to the plane; and a and S are thickness and area of the QW layer respectively.

The matrix element of scattering of electron from state with the wave vector in the plane of QW $\mathbf{k}_\parallel$ to the state $\mathbf{k}_\parallel'$ accompanied with the absorption or emission of phonon with the wave vector $\mathbf{q}$ and corresponding change of phonon occupation number from $N_\mathbf{q}$ to $N_\mathbf{q}'$ has the usual form:

$$M_{\mathbf{k}_\parallel \mathbf{k}_\parallel'} = \langle N_\mathbf{q}', \mathbf{k}_\parallel' | U(\mathbf{r}) | N_\mathbf{q}, \mathbf{k}_\parallel \rangle, \qquad (2)$$

where $U(\mathbf{r})$ is the potential energy of interaction between electron and acoustic or optical phonon.

The scattering of electrons by acoustic phonons has been considered in the deformation potential approximation assuming that the phonon spectrum does not change considerably when we perform the transition from the bulk crystal to MQW structure, i.e. considering scattering of electrons by bulk acoustic phonons. In this case the potential energy of interaction between electrons and acoustic phonons can be expressed as [8]:

$$U_{ac}(\mathbf{r}) = \varepsilon_1 \operatorname{div}\mathbf{u}(\mathbf{r}) = \frac{i\varepsilon_1}{\sqrt{N M_0}}\sum_{\mathbf{q}} q\left[a_\mathbf{q}\, e^{i\mathbf{q}\mathbf{r}} + a_\mathbf{q}^{*}\, e^{-i\mathbf{q}\mathbf{r}}\right], \qquad (3)$$

where ε_1 is the deformation-potential constant; $\mathbf{u}(\mathbf{r})$ is the displacement of the point $\mathbf{r}$ in the crystal caused by acoustic lattice vibrations in the continual approximation; N is the number of unit cells in the crystal volume; M_0 is the unit-cell mass; $\mathbf{q}$ is the wave vector of a phonon; and $a_\mathbf{q}$ are the complex normal coordinates.

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[1] The results of the calculations for the cases of acoustical scattering and scattering by short-range impurity potential were published in [7] and the results concerning polar optical scattering have been revised with more accurate examination of the thin quantum well limit.

The optical phonons are more sensitive to inhomogeneities arising in layered structures with quantum wells. Calculations of optical-phonon spectra in MQW structures were performed in a number of works (see, for example, review [9] and the references therein). A comparison of charge-carrier scattering by optical phonons in MQW structures [10, 11], described with the use of optical-phonon spectra of bulk type and quantized optical-phonon spectra, showed that the differences between the obtained results are not large. Therefore, in our calculations we have considered the polar scattering of electrons by bulk optical phonons. In this case using continual approximation the potential energy of interaction between electrons and optical phonons can be written as [8]:

$$U_{opt}(\mathbf{r}) = i\sqrt{\frac{4\pi e^2 \omega_l^{\,2}}{V\varepsilon^*}} \sum_{\mathbf{q}} \frac{1}{q}\left[a_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}} - a_{\mathbf{q}}^{\;*} e^{-i\mathbf{q}\mathbf{r}}\right]. \quad (4)$$

Here, $V = S\,a$ is the volume of quantum well, ω_l is the highest frequency of longitudinal optical phonons and

$$\left(\varepsilon^*\right)^{-1} = \varepsilon_\infty^{\;-1} - \varepsilon_0^{\;-1},$$

where ε_∞ and ε_0 are the high-frequency and static dielectric constants respectively.

The calculations of matrix elements (2) for the cases of acoustic and optical phonons are rather similar. They consist of calculation of matrix element over phonon and electron coordinates. The matrix elements of $a_{\mathbf{q}}$ and $a_{\mathbf{q}}^{\;*}$ are not equal to zero only for absorption and emission of phonons respectively

$$\left\langle N_{\mathbf{q}}'|\, a_{\mathbf{q}}\, | N_{\mathbf{q}}\right\rangle = \sqrt{\hbar N_{\mathbf{q}} / 2\omega_{\mathbf{q}}} \;\; \text{for}\, N_{\mathbf{q}}' = N_{\mathbf{q}} - 1, \quad (5)$$

and

$$\left\langle N_{\mathbf{q}}'|\, a_{\mathbf{q}}^{\;*}\, | N_{\mathbf{q}}\right\rangle = \sqrt{\hbar (N_{\mathbf{q}}+1) / 2\omega_{\mathbf{q}}} \;\; \text{for}\, N_{\mathbf{q}}' = N_{\mathbf{q}} + 1, \quad (6)$$

where $\omega_{\mathbf{q}}$ is the frequency of phonon with the wave vector $\mathbf{q}$.

At the temperatures sufficiently higher than the Debye temperature Θ_D the phonon occupation numbers are much greater then unity and can be expressed as $N_{\mathbf{q}} \approx N_{\mathbf{q}} + 1 \approx k_0 T / \hbar\omega_{\mathbf{q}}$, i.e. for acoustic phonons

$$N_{\mathbf{q}} \approx \frac{k_0 T}{\hbar\omega_{\mathbf{q}}} = \frac{k_0 T}{\hbar v_0 q}, \quad (7)$$

and for optical phonons

$$N_{\mathbf{q}} \approx \frac{k_0 T}{\hbar\omega_{\mathbf{q}}} = \frac{k_0 T}{\hbar\omega_l}. \quad (8)$$

In the equation (7) v_0 is the velocity of sound.

The integration over coordinate ρ yields the delta functions, which express the momentum conservation law in the plane of the layer:

$$\frac{1}{S}\int_S e^{i(\mathbf{k}_\parallel \pm \mathbf{q}_\parallel - \mathbf{k}_\parallel')\rho}\, d^2\rho = \delta\left(\mathbf{k}_\parallel \pm \mathbf{q}_\parallel - \mathbf{k}_\parallel'\right), \quad (9)$$

where $\mathbf{q}_\parallel$ is the projection of the phonon wave vector $\mathbf{q}$ to the plane of the layer; signs "$\pm$" correspond to the absorption and emission of phonon respectively.

The integration over coordinate z gives the form-factor

$$Y^\pm(q_z) = \frac{2}{a}\int_0^a \sin^2\left(\frac{\pi}{a} z\right) e^{\pm i q_z z}\, \mathrm{d}z = \frac{e^{\pm i\pi x}\sin(\pi x)}{\pi x\left(1 - x^2\right)}, \quad (10)$$

where q_z is the component of phonon wave vector $\mathbf{q}$ in the direction of z - axis and $x = a q_z / 2\pi$.

Gathering together equations (2), (7)-(10) the square of the modulus of the matrix element (2) can be written as

$$| M_{\mathbf{k}_\parallel \mathbf{k}_\parallel \pm \mathbf{q}_\parallel} |^2 = | M^\pm(q) |^2 \, | Y^\pm(q_z) |^2, \quad (11)$$

where the $M^\pm(q)$ are the bulk matrix elements of scattering, that are defined at the high-temperature limit for scattering by acoustic phonons as [8]

$$| M^\pm(q) |^2 = | M_{ac}(q) |^2 = \frac{\varepsilon_1^{\;2} k_0 T}{2 N M_0 v_0^{\;2}}, \quad (12)$$

and for polar scattering by optical phonons as

$$| M^\pm(q) |^2 = | M_{opt}(q) |^2 = \frac{2\pi e^2 k_0 T}{V\varepsilon^*} \frac{1}{q^2}. \quad (13)$$

The scattering by both acoustic and optical phonons at $T >> \Theta_D$ is elastic and the relaxation time in MQW-structure can be written as

$$\begin{aligned} \tau_{2D}^{\;-1} = {} & \frac{2\pi}{\hbar}\sum_{\mathbf{q}} | M_{\mathbf{k}_\parallel \mathbf{k}_\parallel + \mathbf{q}_\parallel} |^2 \frac{\mathbf{k}_\parallel \mathbf{q}_\parallel}{k_\parallel^{\;2}}\, \delta\left(\varepsilon(\mathbf{k}_\parallel + \mathbf{q}_\parallel) - \varepsilon(\mathbf{k}_\parallel)\right) \\ & - \frac{2\pi}{\hbar}\sum_{\mathbf{q}} | M_{\mathbf{k}_\parallel \mathbf{k}_\parallel - \mathbf{q}_\parallel} |^2 \frac{\mathbf{k}_\parallel \mathbf{q}_\parallel}{k_\parallel^{\;2}}\, \delta\left(\varepsilon(\mathbf{k}_\parallel - \mathbf{q}_\parallel) - \varepsilon(\mathbf{k}_\parallel)\right), \end{aligned} \quad (14)$$

where δ -functions allow for the energy conservation law; and $\varepsilon(\mathbf{k}_\parallel)$ is the energy of electron corresponding to the motion in the plane of the layer.

Replacing summation by integration in (14) leads to the following expression for τ_{2D}

$$\begin{aligned} \tau_{2D}^{\;-1} = -\frac{2\pi}{\hbar}\frac{V m^*}{8\pi^3\hbar^2} \int_{-\infty}^{\infty} dq_z \int_0^{2k_\parallel} q_\parallel\, dq_\parallel \int_0^{2\pi} d\phi \Bigg[\frac{| M(q) |^2 \cos\phi}{k_\parallel^{\;2}} \\ \times\left\{ | Y^+(q_z) |^2 \delta\left(\frac{q_\parallel}{2k_\parallel} + \cos\phi\right) - | Y^-(q_z) |^2 \delta\left(\frac{q_\parallel}{2k_\parallel} - \cos\phi\right)\right\}\Bigg], \end{aligned} \quad (15)$$

where m^* is the effective mass of electron.

As the bulk matrix element for the case of acoustic scattering (12) is independent of q, the integration in (15) can be performed analytically. The resulting expression for the relaxation time can be represented in the following form

$$\tau_{2D}^{(ac)^{-1}} = \frac{2\pi}{\hbar} | M_{ac}(q) |^2\, V\, g_{2D}\, X, \quad (16)$$

where $g_{2D} = m^* / (2\pi\hbar^2)$ is the two-dimensional density of states, and the quantity X can be obtained from (10) by means of integration over q_z

$$X = \int_{-\infty}^{\infty} | Y^\pm(q_z) |^2 \frac{\mathrm{d}q_z}{2\pi} = \frac{1}{a}\int_{-\infty}^{\infty}\left(\frac{\sin(\pi x)}{\pi x\left(1 - x^2\right)}\right)^2 \mathrm{d}x = \frac{3}{2}a^{-1}. \quad (17)$$

The equation (16) for relaxation time agrees with that previously reported in [12] and should be compared with the corresponding relaxation time for a bulk crystal [8]

$$\tau_{3D}^{(ac)^{-1}} = \frac{2\pi}{\hbar} |M_{ac}(q)|^2 \, V \, g_{3D}, \tag{18}$$

where $g_{3D} = m^* k / 2\pi^2 \hbar^3$ is the density of states in a bulk crystal.

The comparison of equations (16) and (18) has shown that the relaxation time in MQW structure at the acoustic scattering is less than in bulk crystal and decreases proportional to the layer thickness a

$$\frac{\tau_{2D}^{(ac)}}{\tau_{3D}^{(ac)}} = \frac{2ka}{3\pi}. \tag{19}$$

In the case of polar scattering the matrix element (13) is inversely proportional to the square of the phonon wave vector q. The expression for relaxation time in this case has the similar form as for acoustic scattering (16)

$$\tau_{2D}^{(opt)^{-1}} = \frac{2\pi}{\hbar} |M_{opt}(q)|^2 \, V \, g_{2D} \, X(u), \tag{20}$$

but in the equation (20) the quantity X becomes a function of electron wave vector

$$X(u) = \frac{3}{2a} I(u), \tag{21}$$

where $u = a k_{\|} / \pi$, and the integral $I(u)$ is defined as follows

$$I(u) = \frac{2}{3} \int_{-\infty}^{\infty} \left|Y^{\pm}(x)\right|^2 \left(1 - \frac{|x|}{\sqrt{x^2 + u^2}}\right) \mathrm{d}x. \tag{22}$$

The relaxation time in the bulk crystal at polar scattering can be obtained from (18), where $M_{ac}(q)$ should be replaced with the matrix element (13).

The comparison of the relaxation times in the MQW-structure and in the bulk crystal for the case of polar scattering by optical phonons can be represented in the following form

$$\frac{\tau_{2D}^{(opt)}}{\tau_{3D}^{(opt)}} = \frac{2ka}{3\pi} I^{-1}(u). \tag{23}$$

The integral $I(u)$ in this equation can not be expressed in analytical form. In the case of large values of u it approaches the unity, and at the small u it can be approximated by $I(u) \approx 4u/3$. As u is proportional to the thickness of layers a, the relaxation time $\tau_{2D}^{(opt)}$ decreases proportional to a in the case of relatively thick quantum wells as for the acoustic scattering. But in the case of thin QW layers $\tau_{2D}^{(opt)}$ becomes independent of layer thickness and approaches to the value $\tau_{3D}^{(opt)}/2$. Thus in the case of thin QW layers at the polar scattering the suppositions made by Hicks and Dresselhaus [1-3] becomes valid, taking into account, however, that $\tau_{2D}^{(opt)}$ is two times smaller than $\tau_{3D}^{(opt)}$.

Relaxation Time for the Case of Scattering by Short-range Impurity Potential

The scattering by short-range impurity potential is important in many thermoelectric materials with high permittivity such as PbTe [13] when the Coulomb scattering is ineffective, therefore the scattering occurs at the inner part of the impurity potential. It can be assumed that the impurity potential $U(\mathbf{r})$ has an effective radius r_0, which is of the order of the interatomic distance. In order to calculate the matrix element of scattering in this case we have used the Bloch wave function of electron in quantum well

$$\psi_{\mathbf{k}_{\|}}(\mathbf{r}) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi a}{z}\right) \frac{1}{\sqrt{S}} e^{i \mathbf{k}_{\|} \rho} u_{\mathbf{k}}(\mathbf{r}). \tag{24}$$

Then the matrix element of scattering by the impurity atom residing at the lattice site $\mathbf{r}_i$ can be written in the following form

$$\begin{aligned} M_{\mathbf{k}_{\|} \mathbf{k}_{\|}'} = \frac{1}{S} \int_S d^2 \rho \frac{2}{a} \int_0^a dz \Bigg[& e^{-i \mathbf{k}_{\|}' \rho} \sin\left(\frac{\pi z}{a}\right) \\ & \times u_{\mathbf{k}'}^*(\mathbf{r}) U(\mathbf{r} - \mathbf{r}_i) u_{\mathbf{k}}(\mathbf{r}) \, e^{i \mathbf{k}_{\|} \rho} \sin\left(\frac{\pi z}{a}\right) \Bigg]. \end{aligned} \tag{25}$$

It is convenient to make a substitution $\mathbf{r} = \mathbf{r}' + \mathbf{r}_i$. Then using periodicity of the Bloch amplitude $u_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r}')$, equation (25) can be expressed as

$$\begin{aligned} M_{\mathbf{k}_{\|} \mathbf{k}_{\|}'} = \frac{2 e^{-i \rho_i (\mathbf{k}_{\|}' - \mathbf{k}_{\|})}}{S a} \int_S d^2 \rho' \int_{-z_i}^{a - z_i} dz' \Bigg[& \sin^2\left(\frac{\pi (z' + z_i)}{a}\right) \\ & \times e^{-i \mathbf{k}_{\|}' \rho'} u_{\mathbf{k}'}^*(\mathbf{r}') U(\mathbf{r}') u_{\mathbf{k}}(\mathbf{r}') \, e^{i \mathbf{k}_{\|} \rho'} \Bigg]. \end{aligned} \tag{26}$$

Taking into account that the short-range potential differs from zero in a small region $\Omega_0 \sim r_0^3$ the domain of integration in (25) can be replaced with Ω_0. If we consider scattering of electrons with the small wave vectors, we have $k r' << 1$ for the radius vectors $\mathbf{r}'$ in the region Ω_0. Then all the exponential functions under the integral in (26) are close to unity and sine can be replaced with $\sin(\pi z_i / a)$. In addition, for small values of the wave vector, the dispersion law of electrons is almost parabolic; therefore, in the same approximation, the Bloch amplitudes $u_{\mathbf{k}}(\mathbf{r}')$ can be assumed to depend on $\mathbf{k}$ weakly and can be replaced with $u_0(\mathbf{r}')$. Taking into considerations all this assumptions the matrix element (26) can be rewritten in the following form

$$M_{\mathbf{k}_{\|} \mathbf{k}_{\|}'} = \frac{2 e^{-i \rho_i (\mathbf{k}_{\|}' - \mathbf{k}_{\|})} C}{S a} \sin^2\left(\frac{\pi z_i}{a}\right), \tag{27}$$

where the quantity C is independent of the electron wave vectors $\mathbf{k}_{\|}$ and $\mathbf{k}_{\|}'$

$$C = \int_{\Omega_0} u_0^*(\mathbf{r}') U(\mathbf{r}') u_0(\mathbf{r}') \, d^3 r'. \tag{28}$$

Note, that the square of the module of matrix element in this case is independent of the electron wave vector change as in the case of acoustic scattering.

The relaxation time of electrons in QW independently scattering by the short-range potential of impurities uniformly distributed in the QW volume with the concentration n_I is given by

$$\tau_{2D}^{-1} = -\frac{2\pi}{\hbar}\int_V d^3 r_i \left\{ n_I \sum_{\mathbf{k}_\parallel'} \left[|M_{\mathbf{k}_\parallel \mathbf{k}_\parallel'}|^2 \frac{k_\parallel' - k_\parallel}{k_\parallel} \delta\left(\varepsilon(\mathbf{k}_\parallel') - \varepsilon(\mathbf{k}_\parallel)\right) \right] \right\}. \quad (29)$$

The averaging over impurity coordinates in (29) results in the following factor in the expression for relaxation time

$$\int_V d^3 r_i \left(n_I \sin^4\left(\frac{\pi}{a} z_i\right)\right) = \frac{3}{8} n_I V. \quad (30)$$

Using (30), after summation over $k_\parallel'$ we obtain

$$\tau_{2D}^{(i)\,-1} = \frac{2\pi}{\hbar} |C|^2 n_I \, g_{2D} \, X. \quad (31)$$

The corresponding expression for relaxation time in bulk crystal can be obtained in a similar way

$$\tau_{3D}^{(i)\,-1} = \frac{2\pi}{\hbar} |C|^2 n_I \, g_{3D}. \quad (32)$$

As can be seen from equations (31) and (32), the ratio of relaxation times in MQW-structure and in bulk crystal is the same as in the case of scattering by acoustic phonons (19). The common feature of these two scattering mechanisms is that the squared modules of matrix elements are independent of the change of electron wave vector during the scattering act. The relaxation time in these cases appears to be proportional to the small thickness of QW layer and decreases with the reducing of a due to the rise of density of final states during electron scattering.

In the case of polar scattering by optical phonons the probability of scattering is inversely proportional to the square of phonon wave vector. This fact results in independence of the relaxation time $\tau_{2D}^{(opt)}$ of the layer thickness in the limiting case of thin QW layers and, as will be shown in subsequent sections, gives the possibility to increase the thermoelectric figure of merit in QW in comparison with the bulk value due to the rise of density of states.

The Kinetic Coefficients and the Thermoelectric Efficiency

Using the equations for relaxation time (16), (20) and (32), the expressions for kinetic coefficients and the thermoelectric figure of merit can be easily obtained.

For example for the electric conductivity in the plane of QW one can write

$$\sigma_{2D} = \frac{2e^2}{m^*}\int_0^\infty \left(-\frac{\partial f_0(\varepsilon)}{\partial \varepsilon}\right) \tau_{2D} \frac{g_{2D}}{a} \varepsilon \, d\varepsilon, \quad (33)$$

where $f_0(\varepsilon)$ is the Fermi-Dirac distribution.

For simplification of the further treatment it is convenient to write the expression for relaxation time as a function of dimensionless electron energy

$$\tau_{2D} = \frac{2}{3}\tau_0 \frac{w \, x^{r+1/2}}{I^s\left(w\sqrt{x}\right)}, \quad (34)$$

where $w = a\sqrt{2m^* k_0 T} / \pi\hbar$; integral $I(u)$ is given by equation (22); and τ_0 is the coefficient of proportionality in energy dependence of the relaxation time in the bulk case

$$\tau_{3D} = \tau_0 \, x^r. \quad (35)$$

In the equations (34), (35) the exponents r and s are defined for acoustic scattering and scattering by short-range impurity potential as

$$r = -\frac{1}{2}, \; s = 0, \quad (36)$$

and for the case of polar scattering by optical phonons as

$$r = \frac{1}{2}, \; s = 1. \quad (37)$$

After substitution of (34) in (33), the expression for electric conductivity in QW can be written in the following form

$$\sigma_{2D} = \frac{2^{3/2} e^2 m^{*1/2} (k_0 T)^{3/2}}{3\pi^2 \hbar^3} \tau_0 \left(r + \frac{3}{2}\right) J_{r+1/2}^s\left(\mu^*, w\right), \quad (38)$$

where μ^* is the chemical potential in $k_0 T$ units measured from the bottom of the lowest subband of dimensional quantization, and

$$J_m^n\left(\mu^*, w\right) = \int_0^\infty \left(-\frac{\partial f_0(x, \mu^*)}{\partial x}\right) \frac{x^m}{I^n\left(w\sqrt{x}\right)} dx. \quad (39)$$

The expressions for the Seebeck coefficient α_{2D} and electronic component of the thermal conductivity κ_{2D} can be obtained in a similar way

$$\alpha_{2D} = -\frac{k_0}{e}\left(\frac{r + 5/2}{r + 3/2} \frac{J_{r+3/2}^s\left(\mu^*\right)}{J_{r+1/2}^s\left(\mu^*\right)} - \mu^*\right), \quad (40)$$

$$\kappa_{2D} = \frac{2^{3/2} m^{*1/2} (k_0 T)^{5/2} k_0}{3\pi^2 \hbar^3} \tau_0 \left(\left(r + \frac{7}{2}\right) J_{r+5/2}^s\left(\mu^*\right) - \frac{\left(r + 5/2\right)^2}{r + 3/2} \frac{J_{r+3/2}^{s\;2}\left(\mu^*\right)}{J_{r+1/2}^s\left(\mu^*\right)} \right). \quad (41)$$

The expressions for the thermoelectric figure of merit in QW layers can be easily obtained using equations (38), (40) and (41)

$$Z_{2D} T = \left(\left(r + \frac{5}{2}\right) J^s_{r+\frac{3}{2}}(\mu^*, w) - \mu^* \left(r + \frac{3}{2}\right) J^s_{r+\frac{1}{2}}(\mu^*, w) \right)^2 \Bigg/ \left[\left(r + \frac{3}{2}\right) J^s_{r+\frac{1}{2}}(\mu^*, w) \left(\frac{1}{B} + \left(r + \frac{7}{2}\right) J^s_{r+\frac{5}{2}}(\mu^*, w) \right) - \left(r + \frac{5}{2}\right)^2 J^{s\;2}_{r+\frac{3}{2}}(\mu^*, w) \right], \quad (42)$$

where the material parameter B is determined by the following expression

$$B = \frac{2^{3/2} m^{*1/2} (k_0 T)^{5/2} k_0}{3\pi^2 \hbar^3 \kappa_{ph}} \tau_0. \quad (43)$$

If the phonon thermal conductivity of QW layer does not change in comparison with the bulk case, the value of material parameter B for the bulk case is determined by equation (43), and the corresponding expressions for kinetic coefficients and thermoelectric efficiency in this case has the similar form as (38), (40), (41) and (42). But for the bulk crystal the values of energy and chemical potential are measured from the bottom of the conduction band, and the integral (39) should be replaced with the corresponding Fermi integral $F_m\left(\mu^*\right)$, which can be obtained from (39) by setting $n = 0$.

In the case of acoustic scattering and scattering by short-range impurity potential $s = 0$. Therefore, the integral (39) equals to the Fermi integral $F_m\left(\mu^*\right)$, and the expressions for kinetic coefficients and the figure of merit Z in bulk case and in QW layers has exactly the same form. This means that the optimal values of chemical potential are the same for the both cases, and, hence, the maximum values of thermoelectric efficiencies $Z\left(\mu^*_{opt}\right)T$ are equal. But in the QW layers the maximum value of the figure of merit is reached at higher concentrations and lower mobilities than in bulk crystal.

In the case of polar scattering $s = 1$ and the expressions for Z_{2D} and Z_{3D} differs from each other. In the relatively thick QW layers the integral $I(u)$ in (39) approaches the unity and the kinetic coefficients and the thermoelectric efficiency in QW layers are close to the bulk values. In the limiting case of thin QW layers the integral $I(u)$ in (39) is proportional to the layer thickness a, the relaxation time (see equations (20), (21)) becomes independent of the layer thickness, and the electric conductivity σ_{2D} and the figure of merit increase with the reducing a due to the rise of the density of states in quantum wells.

If we assume that the relaxation time in QW structure does not differ from the one in the bulk crystal, as was made by Hicks and Dresselhaus [1], the expression for electric conductivity σ^*_{2D} for polar scattering can be easily obtained by substituting $\tau^{(opt)}_{2D} = \tau^{(opt)}_{3D}$ in equation (33):

$$\sigma^*_{2D} = \frac{e^2 k_0 T \tau_0}{\pi \hbar^2 a} F_{3/2}\left(\mu^*\right). \qquad (44)$$

The expression for thermoelectric efficiency in this case can be written in the following form

$$Z^*_{2D}T = \frac{\left(F_{5/2}(\mu^*) - \mu^* F_{3/2}(\mu^*)\right)^2}{F_{3/2}(\mu^*)\left(1/B^* + F_{7/2}(\mu^*)\right) - F_{5/2}{}^2(\mu^*)}, \qquad (45)$$

where the parameter B^* is related to the material parameter B by the following equation

$$B^* = B\frac{3}{2w}. \qquad (46)$$

Using equations (42) and (45), it is possible to compare the dependencies of the thermoelectric efficiencies on QW thickness in the two approximations: the first, which takes into account the change of the relaxation time with the layer thickness, and the second, which assumes, that the relaxation time in QW is equal to that in the bulk crystal. The estimations have been performed for the case of polar scattering, when the rise of the figure of merit in MQW structure is expected. For this case the material parameter B has been chosen to be equal to 0.073, which gives the maximum thermoelectric efficiency in the bulk crystal of the order of unity, $Z^{\max}_{3D}T \approx 1$. The dependencies of optimized thermoelectric efficiencies $Z^{\max}_{2D} / Z^{\max}_{3D}$ and $Z^{*\max}_{2D} / Z^{\max}_{3D}$ on the parameter w are presented on the figure 1.

In order to obtain the dependencies of the figures of merit on the thickness of QW layer a the following parameters were chosen: the average value of electron effective mass $m^* = 0.07\,m_0$ and the Debye temperature $\Theta_D \approx 150\,\mathrm{K}$, that correspond to the parameters of PbTe. At the room temperature $T = 300\,\mathrm{K}$ in this material the polar scattering by the optical phonons can be considered elastic.

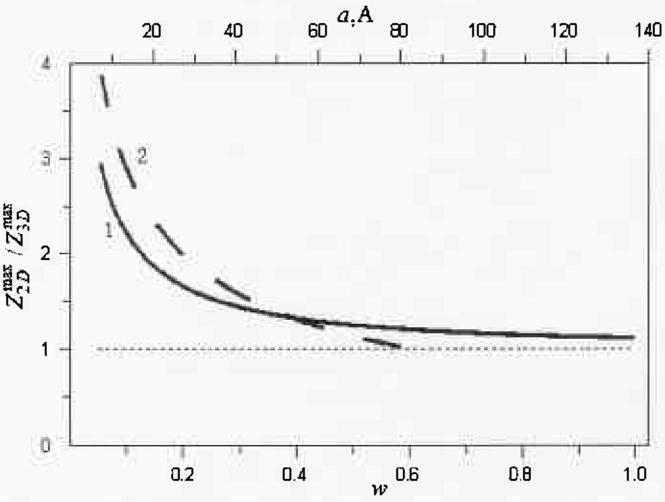

Figure 1. The optimized thermoelectric figures of merit in MQW structure for the polar scattering. The curve 1 is calculated taking into account the change of relaxation time in QW, the curve 2 is calculated using bulk value for relaxation time.

The calculations in the present paper have been performed in the assumption that the lowest conduction subband in QW makes the main contribution to the kinetic effects. This assumption requires that the energy difference between the two lowest subbands $\Delta\varepsilon = 3\pi^2\hbar^2 / 2m^* a^2$ is less than $k_0 T$ or the value of chemical potential in the case of degenerate statistics. The first of these conditions determines the upper bound for the parameter w, which appears to be equal to $\sqrt{3}$. The verification of the second condition has shown that in the region of parameter w, where the value μ_{opt} is positive, its value is less than the thermal energy. Thus the contribution to the kinetic coefficient from the upper subbands can be neglected.

The curve 1 on the figure 1 corresponds to the thermoelectric efficiency in the MQW structure calculated taking into account the change of the relaxation time with the layer thickness. The curve 2 on the figure 1 corresponds to the figure of merit calculated using bulk value of the relaxation time. The comparison has shown that in the case of polar scattering in the both approximations the value of $Z_{2D}T$ increases over the bulk value with the reducing QW layer thickness. However, in the approximation considering the relaxation time change the figure of merit is increasing slightly less, because the limiting value of $\tau^{(opt)}_{2D}$ in this case is two times less than in the bulk crystal.

Conclusions

In the present paper the thermoelectric figure of merit in MQW structures at different scattering mechanisms was theoretically investigated. It has been shown that in the cases of scattering by acoustic phonons and short-range impurity potential the relaxation time in QW layer decreases in comparison with the bulk value proportional to the small value of the layer thickness a. This effect is the consequence of the fact, that the scattering probability is independent of the electron wave vector change during the scattering act. The decrease of the relaxation time in QW layers completely compensate the rise of the figure of merit due to the increase of the density of states in the two-dimensional systems, and the expression for the kinetic coefficients and the figure of merit have exactly the same form. Therefore, the optimal values of the chemical potential are equal and corresponding magnitudes of $Z_{2D}^{\max} T$ and $Z_{3D}^{\max} T$ are the same.

In the case of polar scattering by the optical phonons the probability of scattering is inversely proportional to the square of the phonon wave vector, and the relaxation time $\tau_{2D}^{(opt)}$ in the limiting case of small a becomes independent of the layer thickness and approaches to one-half of the bulk value. In this case the electric conductivity and the thermoelectric efficiency increase with the QW layer thickness as was predicted by Hicks and Dresselhaus [1-3]. These analytical calculations have been illustrated with the numerical estimations, which have shown that the figure of merit in QW can be by a factor of 1.5 or 2 higher then in the bulk case. The comparison has been made of the figure of merit calculated using equation (20) for $\tau_{2D}^{(opt)}$, which takes into account the variation of the relaxation time with the layer thickness, and the figure of merit, calculated in the approximation similar to that used in [1], which utilizes the bulk value of the relaxation time for $\tau_{2D}^{(opt)}$. It has been shown that in the both cases the values of $Z_{2D}^{\max} T$ increase with the diminishing of the QW layer thickness, but the first approximation leads to the smaller values of the figure of merit as the relaxation time for this case is limited to one-half of the bulk value.

Thus, the calculations performed in the present paper have shown that the thermoelectric figure of merit in the MQW structures can be enhanced over the bulk value only if the probability of scattering decreases with the rise of the electron wave vector change during the scattering act.

The numerical results, obtained in the present paper, are reasonable only for the aid of comparison of two approximations, mentioned above. The more realistic results [4-6, 14-17] can be obtained taking into account the dimensional quantization of the phonon spectrum, tunneling of electrons through the barriers between the QW layers and the phonon thermal conductivity through the barriers.

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