Electron-polar optical phonon field-induced tunnel scatterings 
in a polar semiconductor under electric field

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Abstract - Theory of electron-phonon field-induced tunnel scattering in polar semiconductors under uniform electric field is considered. It is assumed that a non-degenerate n-type semiconductor has a spherical and parabolic simple band structure. On the basis of the study is the phenomenon of semiconductor bands tilting by the perturbing potential of an electric field. In that case electron eigenfunctions are not-plane waves or Bloch functions. They are determined by the Airy functions. An expression for the probability of electron intra-valley field-induced tunnel transitions related to polar optical phonon emission and absorption is obtained and analyzed.

Keywords: tilted band semiconductor; electron-polar optical phonon scattering; transition probability

1. Introduction

A current carrier scattering is one of important processes characterizing a number of transport phenomena in semiconductors. Many properties of a semiconductor depend on electron-phonon scattering. For theoretical consideration of scattering the flat-bands semiconductor model is used, as a rule (see, e.g., [1-4]). On the other hand, it is well-known that in the presence of an electric field semiconductor bands are tilted. In recent works [5, 6] the possible influence of the semiconductor bands tilted on the peculiarities of the electron-phonon scatterings are analyzed. As a result the new mechanism of the so-called electron-phonon FIT (field-induced tunnel) scattering is observed. The effect of the electron-phonon FIT scattering is explained in terms of the penetration of an electron wave function into a semiconductor.
forbidden-band gap in the presence of an electric field. Electron-phonon FIT scattering physical mechanism with corresponding illustrations and explanations are presented in Ref. [5] in detail.

Note that there are several mechanisms of electron-phonon interaction [1-4]. Reconsidering the electron-phonon interaction theory, in [5] the case of electron FIT scattering by non-polar optical phonons is analyzed. Other important case of electron-acoustic phonon FIT scattering is reported in [6]. The general approach developed in Refs. [5, 6] will now be applied to the case of electron interaction with polar optical phonons. The interaction of electrons with polar optical phonons is the dominating scattering mechanism at room temperatures in polar semiconductors.

Below electron-polar optical phonon FIT scattering is considered. For the qualitative study a non-degenerate n-type semiconductor with a spherical and parabolic conduction band and electron scalar effective mass \( m \) is considered.

2. Theory

The basic quantity that describes the scattering of an electron is the probability of the electron transition between two quasi-discrete states of semiconductor conduction band. According to quantum mechanics the transition probability per unit time \( W(k,k') \) for an electron scattered from an initial state \( |k\rangle \) to a final state \( |k'\rangle \) is calculated with the help of perturbation theory. The probability of the scattering of an electron with the emission or absorption of a phonon is determined by the perturbation Hamiltonian of the electron-phonon interaction and electron wave function as well. In the framework of flat-band semiconductor model as an electron wave function a plane wave or Bloch functions is used. Such calculations are well known and reported in mass of publications (see, e.g., [1-4]).

In the present work, electron-polar optical phonon scattering in a polar semiconductor, whose bands are tilted by the perturbing potential of a uniform electric field, is of interest. In that case electron eigenfunctions are not plane waves or Bloch functions [1,2]. In the presence of a uniform electric field \( F \) the electron wave-function is determined by the stationary Schrödinger equation. The solution of the Schrödinger equation in the effective mass approximation when electric field is parallel to the \( z \)-axis is given by [1-2]

\[
\psi_k (r) = \frac{1}{\sqrt{L_x L_y}} e^{i(k_xx+k_yy)} \chi_n(z). \tag{1}
\]

Here

\[
\chi_n(z) = C_n A \left( \frac{z}{l} - (k_n l)^2 \right), \tag{2}
\]
$C_n$ is the normalization constant, $l = \left( \frac{\hbar^2}{2eFm} \right)^{1/3}$, $L_x$, $L_y$ and $L_z$ are the sizes of a semiconductor, $Ai(\cdots)$ is the Airy function [7]:

$$Ai(s) = \frac{1}{\pi} \int_0^\infty du \cos \left( \frac{u^3}{3} + us \right).$$  (3)

Electron energy eigenvalues $\varepsilon_k$ is determined as [2, 6]

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m} + \varepsilon_n,$$  (4)

where $k^2 = k_x^2 + k_y^2$, $k_\perp$ is the electron wave-vector perpendicular to the electric field, $\varepsilon_n = \hbar^2 k_n^2 / 2m$, the index $n$ identifies the electron energy eigenvalues. Energy eigenvalues $\varepsilon_n$ (or $k_n$) are determined from the boundary conditions (see below) for the wave function $\chi_n(z)$.

For a semiconductor with large length $L_z$ in z-direction ($-L_z/2 \leq z \leq L_z/2$) normalization constant $C_n$ is presented as [6]

$$C_n^2 = \pi/2 \sqrt{-a_n}.$$  (5)

Here $a_n$ are the zeros of the Airy function which are located in the negative part of the real axis. They are well approximated as [7]

$$a_n \approx -(3\pi[4n-1]/8)^{2/3},$$  (6)

where $n = 1, 2, \cdots$.

Based on the electron wave function Eq.(1) and taking into account well known expression of electron-polar optical phonon interaction Hamiltonian [1-4] the probability of electron FIT scattering by polar optical phonons $W_{el-opt}(k,k')$ can be calculated following to general approach developed in Ref. [6]. However, as the analysis shows, there is no necessity for caring out such long and complicated mathematical calculations in details. Here one can use the results of the reconsidered theory of electron scattering by acoustic phonons presented in Ref. [6]. So, in Ref. [6] based on the Eq.(1) and used the deformation potential interaction Hamiltonian the following expression for electron-acoustic phonon FIT scattering probability per unit time is obtained:

$$W(k,k') = \frac{4\pi D_{el}}{h} \sum_{q,\omega_{q}} \frac{q^2}{\omega_{q}} \delta(n_q + \frac{1}{2} \pm \frac{1}{2}) \delta(\varepsilon_k' - \varepsilon_k \mp \hbar\omega_{q})$$

$$\times \delta(k_x',k_x) \delta(k_y',k_y) \left[ \text{Re} \left( \int_{-L_z/2}^{L_z/2} \chi_{n_k'}^*(z) \chi_n(z) e^{i\omega_{q} z} \right)^2 \right].$$  (7)
Here $\rho_r$ is the reduced mass density of the crystal, $D_{ac}$ is the acoustic deformation potential constant, $\varepsilon_k = \hbar^2 k^2 / 2m$ is the conduction electron energy, bolded $k$ and $q$ are the electron and phonon wave vector (below the magnitudes of vector quantities are denoted by non-bolded symbols), respectively, $V = L_x L_y L_z$ is the semiconductor volume $n_q$ is the occupation numbers of the equilibrium acoustic phonons which are determined by the Bose-Einstein distribution function:

$$n_q = \frac{1}{\exp(\hbar \omega_q / k_B T) - 1},$$

$\omega_q$ is the longitudinal acoustic phonon angular frequency, $k_B$ is the Boltzmann constant, $T$ is the temperature.

In Eq.(7) upper and lower symbols of double signs refer to electron transitions with the $q$ phonon absorption and emission, respectively. The summations should be carried out in the range of the first Brillouin zone. The Dirac $\delta$-function indicates the energy conservation law. The Kronecker parameter $\delta$ expresses the laws of conservation of perpendicular to electric field quasi-momentum $x$ and $y$ components of the scattered particles. Here the normal N-processes of scattering are considered.

As is known [1, 2] with the help of the formal substitution

$$D_{ac} \to \frac{\varepsilon \omega_{q,LO}}{q^2 + q_i^2} \sqrt{\frac{\rho_r}{\varepsilon_{r,LO}}},$$

from the Hamiltonian for the electron – acoustic phonon deformation-potential interaction the Hamiltonian for the electron – polar optical phonon interaction is derived.

In Eq.(9) $\omega_{q,LO}$ is the longitudinal polar optical phonon frequency, $1/\varepsilon_r = [1/\varepsilon_r(\infty)]^{-1/\varepsilon_r(0)}$, $\varepsilon_r(0)$ and $\varepsilon_r(\infty)$ are the low and high frequency relative dielectric constants, respectively. In Eq.(8) the screening effect (static screening) is taken into account by $q_s$, where $q_s$ is the inverse screening length. In the Debye formulation, for non-degenerate statistics:

$$q_s = \left( \frac{e^2 n}{\varepsilon_0 \varepsilon_r k_B T} \right)^{1/2},$$

where $n$ is the electron density [2].

Therefore, Eq.(7) can be modified for electron-polar optical phonon scattering by a simple replacing according to Eq.(9). As a result of such replacement one obtain the following expression for the probability of electron FIT scattering by polar optical phonon,
\[ W_{\text{el-oph}}(k, k') = \frac{4\pi e^2}{V\varepsilon_\ell \varepsilon_r} \sum_{q, q' \geq 0} \frac{q^2 \omega_{q,q'}^{LO}}{q^2 + q'^2} \left( n_q + \frac{1}{2} \mp \frac{1}{2} \right) \delta(\varepsilon_{k'} - \varepsilon_k \mp \hbar \omega_{q,q'}) \times \delta_{k',k',q,q'} \delta_{k',k',q,q'} \left[ \text{Re} \int_{-L_z/2}^{L_z/2} dz \chi_{s'}^*(z) \chi_s(z) e^{\pm i q z} \right]^2. \] (10)

Eq.(10) describes electron transition probability in the presence of an electric field. It has a general character and is applicable for low as well as for high electric fields.

3. Discussion and conclusion

Thus, in semiconductors, whose bands are tilted under uniform electric field, the probability of the electron scattering by polar optical phonons is determined by Eq.(10). Scattering probability depends on electric field. It depends on electron energy as well. Those dependencies are determined by the Airy function properties [7]. Electron energy eigenvalues \( \varepsilon_k \) are determined from boundary conditions for the Schrödinger equation. So, the allowed values of \( \varepsilon_k \) are computed from the boundary condition \( \chi_s(z = -L_z/2) = 0 \) as [1, 6]

\[ \varepsilon_k = \frac{\hbar^2}{2m} \left\{ k_\perp^2 - \frac{L_z}{2} - \frac{1}{2} \left[ \frac{3\pi}{2} \left( \frac{n - 1/4}{2} \right) \right]^{2/3} \right\}. \] (11)

Note that Eq.(10) can be a little simplified. The dispersion curve of optical phonons is quite flat. For long-wavelength range it can be assumed that \( \omega_{q,q'}^{LO} \) is the independent of phonon wave vector \( q \) constant. Then, to first order approximation, can be assumed that \( \omega_{q,q'}^{LO} \equiv \omega_0 = \text{const} \). For the same reason, \( n_q \) becomes \( q \)-independent:

\[ n_q \equiv N_0 = \frac{1}{\exp(\hbar \omega_0 / k_B T) - 1}. \] (12)

For more simplicity, let the screening wavenumber be taken \( q_s = 0 \). The probability Eq.(10) is then given by

\[ W_{\text{el-oph}}(k, k') = \frac{4\pi e^2 \omega_0}{V\varepsilon_\ell \varepsilon_r} \left( N_0 + \frac{1}{2} \pm \frac{1}{2} \right) \delta(\varepsilon_{k'} - \varepsilon_k \mp \hbar \omega_0) \]
\[ \times \sum_{q, q' \geq 0} \frac{1}{q^2} \delta_{k',k',q,q'} \delta_{k',k',q,q'} \left[ \text{Re} \int_{-L_z/2}^{L_z/2} dz \chi_{s'}^*(z) \chi_s(z) e^{\pm i q z} \right]^2. \] (13)

As it is known [3] there are definite restrictions associated with the quasi-momentum and energy conservation laws for the electron-phonon scattering process in flat-band semiconductor.
For an electron with the initial energies $\varepsilon_k < \hbar \omega_0$, optical phonon emission is impossible. However in tilted band semiconductor for electron FIT transitions there are no restrictions. In the presence of an electric field the electron can penetrate into the band gap. Then for an electron with $\varepsilon_k < \hbar \omega_0$ the probability of optical phonon emission is not zero. This is one of notable particularity of FIT transitions.

It should be noted that Eqs.(10) and (13) are a good background for the future evaluation of such important transport parameters of a polar semiconductor as electron quasi-momentum relaxation time or scattering rate related to electron-polar optical phonon scattering under electric field.

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**References**