

Electron-acoustic phonon field induced tunnel scattering

S.V. Melkonyan, A.L. Harutyunyan, T.A. Zalinyan

Department of Physics of Semiconductors & Microelectronics, Yerevan State University, 1 Alex Manoogian St., 0025 Yerevan, Armenia

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Theory of electron-acoustic single phonon scattering has been reconsidered. It is assumed that the non-degenerate semiconductor has a spherical parabolic band structure. In the basis of the reconsideration there is a phenomenon of the tilting of semiconductor bands by the perturbing potential of an electric field. In this case, electron eigenfunctions are not plane waves or Bloch functions. In low-field regime, the expressions for electron intraband transition probability and scattering time are obtained under elastic collision approximation. Dependencies of scattering time on electron energy and uniform electric field are analyzed. The results of corresponding numerical computations for n-Si at 300 K are presented. It is established that there is no fracture on the curve of electron scattering time dependence on the electron energy.

Key words: tilted band semiconductor, electron-acoustic phonon scattering, transition probability, scattering time

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1. Introduction

Current carrier (electron) mobility μ is an important parameter characterizing many transport phenomena in semiconductors under electric field F . Electron mobility is determined as $\mu = \langle e\tau_{\mathbf{k}}/m \rangle$ [1, 2], where $\tau_{\mathbf{k}}$ is the electron quasi-momentum relaxation time, e is the electron charge magnitude, m is the electron effective mass, $\langle \dots \rangle$ is the symbol of averaging over conduction zone quantum states. Relaxation time $\tau_{\mathbf{k}}$ is determined by the electron scattering by various dynamic and static imperfections of a crystal lattice such as lattice vibrations (optic and acoustic phonons), ionized and neutral impurity atoms, vacancies, etc. For theoretical consideration of scattering probability and relaxation time $\tau_{\mathbf{k}}$, a flat-band semiconductor model is used, as a rule [1–4]. In this case, in low electric field region ($F < F_c$, where F_c is a characteristic field), the electron relaxation time $\tau_{\mathbf{k}}$ and, therefore, the mobility μ are field-independent quantities [1, 4, 5]. Particularly, the relaxation time related to electron-acoustic single phonon elastic scattering in non-degenerate n-type semiconductor with a spherical parabolic conduction band is given by [1–4]

$$1/\tau_{\mathbf{k},ac} = \frac{D_{ac}^2(2m)^{3/2}k_B T}{2\pi\hbar^4\rho_r v_0^2} \sqrt{\varepsilon_{\mathbf{k}}}. \quad (1)$$

Here, ρ_r is a reduced mass density of a crystal, D_{ac} is the acoustic deformation potential constant, k_B is the Boltzmann constant, T is temperature, v_0 is the long-wavelength longitudinal acoustic phonon velocity, $\varepsilon_{\mathbf{k}} = \hbar^2 k^2/2m$ is the electron energy, boldface \mathbf{k} is the electron wave vector (herein below, the magnitudes of vector quantities are denoted by non-boldface symbols).

At high electric fields ($F > F_c$), the time $\tau_{\mathbf{k}}$ and, therefore, the mobility μ depend on the applied electric field [4]. Thus, at electron scattering by an acoustic phonon, electron mobility decreases with an increase of electric field above F_c [5]. The magnitude of characteristic field F_c depends on semiconductor parameters such as crystallographic directions, impurity concentration, temperature, etc. It is of an order of 10^3 V/cm at 300 K, e.g., for pure Si $F_c \approx 10^3$ V/cm, for pure Ge $F_c \approx 600$ V/cm, for high purity GaAs

$F_c \approx 2.8 \cdot 10^3$ V/cm [5]. The dependence $\mu(F)$ is explained by the phenomenon of electron gas heating-up under the effect of a high electric field [1, 4]. However, in recent work [6], a new mechanism of electron lattice scattering, referred to as electron-phonon FIT (field induced tunnel) scattering, is observed. In the basis of the FIT scattering there lies a phenomenon of tilting of semiconductor bands by the perturbing potential of an electric field. The effect of the electron-phonon FIT scattering is explained in terms of penetration of an electron wave function into a semiconductor band gap in the presence of an electric field. Contrary to a flat-band semiconductor, in a tilted-band semiconductor, a conduction electron transition in the band gap region is allowed. In [6], reconsidering the electron-phonon interaction theory, the case of electron intraband FIT scattering by non-polar optical phonon is analyzed. In the present work, electron-acoustic phonon FIT intraband scattering is considered. It is assumed that the non-degenerate n-type semiconductor has a parabolic conduction band.

2. Electron-acoustic phonon FIT transition probability

To theoretically characterize the carrier scattering, it is necessary to consider the scattering probability and evaluate the relaxation time. The task of the transition probability calculation is solved based on the perturbation theory (see, e.g. [1–4]). According to this theory, the probability per unit time of quantum system transition from λ state to λ' state, to the first order in the perturbation, is determined as [1, 2]

$$W(\lambda, \lambda') = \frac{1}{\hbar^2} \frac{d}{dt} \left| \int_0^t a_{\lambda', \lambda}(t) dt \right|^2. \quad (2)$$

Here, $a_{\lambda', \lambda}(t)$ is the perturbation matrix element:

$$a_{\lambda', \lambda}(t) = \int_V d\mathbf{R} \psi_{\lambda'}^*(\mathbf{R}, t) \hat{W}(\mathbf{R}, t) \psi_{\lambda}(\mathbf{R}, t), \quad (3)$$

$\psi_{\lambda}(\mathbf{R}, t) = \psi_{\lambda}(\mathbf{R}) \exp(-iE_{\lambda} t/\hbar)$, λ is the set of quantum numbers characterizing different states of a non-perturbed system, $\psi_{\lambda}(\mathbf{R})$ and E_{λ} are the wave function and energy eigenvalues of stationary state of a non-perturbed quantum system, respectively, $\hat{W}(\mathbf{R}, t)$ is the perturbation operator, \mathbf{R} is the set of the quantum system coordinates, V is the volume, ‘*’ is the complex conjugate symbol.

Consideration of the electron scattering by phonons is based on (2) and (3) as well. In brief, the description of the probability calculation is as follows. In the present case, the quantum system consists of a conduction electron in the crystal periodic field and lattice normal vibrations. Then, λ should be replaced by an electron quasi-wave vector \mathbf{k} and by the phonon occupation numbers of all possible states. The electron-phonon interaction Hamiltonian H_{e-ph} is taken as perturbation $\hat{W}(\mathbf{R}, t)$; the \mathbf{r} radius vector and the normal coordinates of lattice vibration are taken as a quantum system coordinate \mathbf{R} . The wave function of non-perturbed state of an electron-phonon system is expressed as a product of one-electron wave function and harmonic oscillator wave functions.

In flat-band semiconductors, an electron state is described by Bloch functions. Therefore, for an electron scattered from an initial state $|\mathbf{k}\rangle$ to a final state $|\mathbf{k}'\rangle$, the transition probability per unit time $W(\mathbf{k}, \mathbf{k}')$ is evaluated based on the Bloch functions [1–4]. To simplify the calculations, a plane wave $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}} / \sqrt{L_x L_y L_z}$ (where L_x , L_y and L_z are the sizes of a semiconductor, $V = L_x L_y L_z$) is used sometimes as an electron wave function [1–4] (nearly free electron approximation). Calculations of the probability $W(\mathbf{k}, \mathbf{k}')$ based on the Bloch function or plane wave are well known and reported in detail in numerous publications (see, for example, [1–4]). However, in the present work, a semiconductor, whose bands are tilted by the perturbing potential of a uniform electric field, is of interest. In this case, electron eigenfunctions are not plane waves or Bloch functions [1, 3, 7]. Here, based on such an assumption, the probability $W(\mathbf{k}, \mathbf{k}')$ is recalculated following the above-mentioned general approach. It is assumed that the perturbation Hamiltonian H_{e-ph} , which is a harmonic function of time (harmonic perturbation), is determined using the deformation potential theory [1–4] of electron-phonon interaction. The results of our calculations show that:

- the probability of electron transition with phonon absorption can be presented as follows:

$$W_a(\mathbf{k}, \mathbf{k}') = \frac{D_{ac}^2}{2\rho_r V \hbar} \frac{d}{dt} \left| \sum_{\mathbf{q}} i q \sqrt{\frac{n_{\mathbf{q}}}{\omega_{\mathbf{q}}}} \int_0^t dt e^{i \frac{\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} - \hbar \omega_{\mathbf{q}}}{\hbar} t} \int_V d\mathbf{r} \psi_{\mathbf{k}'}^*(\mathbf{r}) e^{i\mathbf{q}\mathbf{r}} \psi_{\mathbf{k}}(\mathbf{r}) \right|^2, \quad (4)$$

- the probability of electron transition with phonon emission can be presented as follows:

$$W_e(\mathbf{k}, \mathbf{k}') = \frac{D_{ac}^2}{2\rho_r V \hbar} \frac{d}{dt} \left| \sum_{\mathbf{q}} i q \sqrt{\frac{n_{\mathbf{q}} + 1}{\omega_{\mathbf{q}}}} \int_0^t dt e^{i \frac{\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} + \hbar \omega_{\mathbf{q}}}{\hbar} t} \int_V d\mathbf{r} \psi_{\mathbf{k}'}^*(\mathbf{r}) e^{-i\mathbf{q}\mathbf{r}} \psi_{\mathbf{k}}(\mathbf{r}) \right|^2. \quad (5)$$

Here, $\psi_{\mathbf{k}}(\mathbf{r}, t) = \psi_{\mathbf{k}}(\mathbf{r}) \exp(-i\varepsilon_{\mathbf{k}} t/\hbar)$, $\psi_{\mathbf{k}}(\mathbf{r})$ is the conduction electron wave function of stationary state \mathbf{k} , $\omega_{\mathbf{q}}$ is the phonon angular frequency, $n_{\mathbf{q}}$ is the occupation number of the equilibrium phonons, which is given by the Bose-Einstein distribution:

$$n_{\mathbf{q}} = 1 / [\exp(\hbar \omega_{\mathbf{q}} / k_B T) - 1]. \quad (6)$$

The summations in (4) and (5) should be carried out in the range of the first Brillouin zone (BZ).

After integration over t , (4) and (5) are expressed as follows:

$$W_{a,e}(\mathbf{k}, \mathbf{k}') = \frac{D_{ac}^2 \hbar}{2\rho_r V} \frac{d}{dt} \left| \sum_{\mathbf{q}} \frac{q}{\sqrt{\omega_{\mathbf{q}}}} \sqrt{n_{\mathbf{q}} + \frac{1}{2}} \frac{1}{2} \frac{e^{i \frac{\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} \mp \hbar \omega_{\mathbf{q}}}{\hbar} t} - 1}{\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} \mp \hbar \omega_{\mathbf{q}}} \int_V d\mathbf{r} \psi_{\mathbf{k}'}^*(\mathbf{r}) e^{\pm i\mathbf{q}\mathbf{r}} \psi_{\mathbf{k}}(\mathbf{r}) \right|^2. \quad (7)$$

Here and below, upper and lower symbols of double signs refer to electron transitions with the \mathbf{q} phonon absorption and emission, respectively.

In the presence of a uniform electric field \mathbf{F} (which is parallel to the z -axis), the electron wave-function is determined by the stationary Schrödinger equation which in the effective mass approximation is expressed as follows:

$$\left[-\frac{\hbar^2}{2m} \left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2} \right) + eFz - \varepsilon_{\mathbf{k}} \right] \psi_{\mathbf{k}}(\mathbf{r}) = 0. \quad (8)$$

Here and below, the index \mathbf{k} of $\varepsilon_{\mathbf{k}}$ is omitted to simplify the expressions, so we can substitute $\varepsilon_{\mathbf{k}} \rightarrow \varepsilon$ and $\varepsilon_{\mathbf{k}'} \rightarrow \varepsilon'$ in further expressions.

The solution of (8) is given by (see, e.g., [1, 7, 8])

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{L_x L_y}} e^{i(k_x x + k_y y)} \chi_n(z). \quad (9)$$

Inserting (9) into (8), the following equation is obtained [1, 7, 8]

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dz^2} + eFz - \varepsilon_n \right] \chi_n(z) = 0. \quad (10)$$

The solution of this equation is [7] as follows:

$$\chi_n(z) = C_n \text{Ai} \left[\frac{z}{l} - (k_n l)^2 \right], \quad (11)$$

where C_n is the normalization constant, $l = (\hbar^2 / 2eFm)^{1/3}$, Ai is the Airy function [8]:

$$\text{Ai}(s) = \frac{1}{\pi} \int_0^{\infty} du \cos \left(\frac{u^3}{3} + us \right). \quad (12)$$

Electron energy eigenvalues ε are determined as follows:

$$\varepsilon = \frac{\hbar^2 k_{\perp}^2}{2m} + \varepsilon_n, \quad (13)$$

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

For a semiconductor of length L_z in z -direction (i.e., $-L_z/2 \leq z \leq L_z/2$) from (9) and relation [1, 3]

$$\frac{1}{L_z} \int_{-L_z/2}^{L_z/2} dz e^{i(q_z - q_{1,z})z} = \delta_{q_z, q_{1,z}} \quad (14)$$

it follows

$$\int d\mathbf{r}^3 \psi_{\mathbf{k}'}^*(\mathbf{r}) \psi_{\mathbf{k}}(\mathbf{r}) e^{\pm i\mathbf{q}\mathbf{r}} = \delta_{k'_x, k_x \pm q_x} \delta_{k'_y, k_y \pm q_y} \int_{-L_z/2}^{L_z/2} dz \chi_{n'}^*(z) \chi_n(z) e^{\pm i q_z z}. \quad (15)$$

Inserting (15) into (7) yields

$$W_{a,e}(\mathbf{k}, \mathbf{k}') = \frac{D_{ac}^2 \hbar}{2\rho_r V} \frac{d}{dt} \left| \sum_{\mathbf{q}} \frac{q}{\sqrt{\omega_{\mathbf{q}}}} \sqrt{n_{\mathbf{q}} + \frac{1}{2} \mp \frac{1}{2}} \times \frac{e^{i \frac{\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} \mp \hbar \omega_{\mathbf{q}}}{\hbar} t} - 1}{\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} \mp \hbar \omega_{\mathbf{q}}} \delta_{k'_x, k_x \pm q_x} \delta_{k'_y, k_y \pm q_y} \int_{-L_z/2}^{L_z/2} dz \chi_{n'}^*(z) \chi_n(z) e^{\pm i q_z z} \right|^2. \quad (16)$$

The Kronecker δ in this equation expresses the laws of conservation of perpendicular to the electric field quasi-momentum x , y components of the scattered particles. Here, only the normal N-processes of scattering are considered.

After summation with respect to q_x and q_y with the help of the Kronecker δ , (16) becomes as follows:

$$W_{a,e}(\mathbf{k}, \mathbf{k}') = \frac{D_{ac}^2 \hbar}{2\rho_r V} \frac{d}{dt} \left| \sum_{q_z} \left[\frac{q}{\sqrt{\omega_{\mathbf{q}}}} \sqrt{n_{\mathbf{q}} + \frac{1}{2} \mp \frac{1}{2}} \frac{e^{i \frac{\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} \mp \hbar \omega_{\mathbf{q}}}{\hbar} t} - 1}{\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} \mp \hbar \omega_{\mathbf{q}}} \right]_{\substack{q_x = \pm(k'_x - k_x), \\ q_y = \pm(k'_y - k_y)}} \times \int_{-L_z/2}^{L_z/2} dz \chi_{n'}^*(z) \chi_n(z) e^{\pm i q_z z} \right|^2. \quad (17)$$

Taking into account that $\omega_{\mathbf{q}}$ is an even function on \mathbf{q} (and particularly on q_z), from (17) one obtains

$$W_{a,e}(\mathbf{k}, \mathbf{k}') = \frac{2D_{ac}^2 \hbar}{\rho_r V} \frac{d}{dt} \left| \sum_{q_z \geq 0} \left[\frac{q}{\sqrt{\omega_{\mathbf{q}}}} \sqrt{n_{\mathbf{q}} + \frac{1}{2} \mp \frac{1}{2}} \frac{e^{i \frac{\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} \mp \hbar \omega_{\mathbf{q}}}{\hbar} t} - 1}{\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} \mp \hbar \omega_{\mathbf{q}}} \right]_{\substack{q_x = \pm(k'_x - k_x), \\ q_y = \pm(k'_y - k_y)}} \times \text{Re} \int_{-L_z/2}^{L_z/2} dz \chi_{n'}^*(z) \chi_n(z) e^{\pm i q_z z} \right|^2. \quad (18)$$

Using the following formal transformations

$$\frac{d}{dt} \left| \sum_{\mathbf{q}} c_{\mathbf{q}}(t) \right|^2 = \frac{d}{dt} \sum_{\mathbf{q}, \mathbf{q}_1} c_{\mathbf{q}}(t) c_{\mathbf{q}_1}^*(t) = 2\text{Re} \sum_{\mathbf{q}, \mathbf{q}_1} \frac{dc_{\mathbf{q}}(t)}{dt} c_{\mathbf{q}_1}^*(t), \quad (19)$$

(18) may be written as follows:

$$\begin{aligned}
 W_{a,e}(\mathbf{k}, \mathbf{k}') &= \frac{4D_{ac}^2}{\rho_r V} \sum_{\substack{q_z \geq 0 \\ q_{1,z} \geq 0}} \operatorname{Re} \left[\frac{iqq_1}{\sqrt{\omega_{\mathbf{q}}\omega_{\mathbf{q}_1}}} \sqrt{n_{\mathbf{q}} + \frac{1}{2} \mp \frac{1}{2}} \sqrt{n_{\mathbf{q}_1} + \frac{1}{2} \mp \frac{1}{2}} \right. \\
 &\quad \times \left. \frac{e^{i(\mp\omega_{\mathbf{q}} \pm \omega_{\mathbf{q}_1})t} - e^{i\frac{\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} \mp \hbar\omega_{\mathbf{q}}}{\hbar}t}}{\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} \mp \hbar\omega_{\mathbf{q}_1}} \right]_{\substack{q_x = \pm(k'_x - k_x), \\ q_y = \pm(k'_y - k_y)}} \\
 &\quad \times \operatorname{Re} \int_{-L_z/2}^{L_z/2} dz \chi_{n'}^*(z) \chi_n(z) e^{\pm iq_z z} \operatorname{Re} \int_{-L_z/2}^{L_z/2} dz_1 \chi_{n'}^*(z_1) \chi_n(z_1) e^{\pm iq_{1,z} z_1}. \quad (20)
 \end{aligned}$$

For a sufficiently long time t , when the relation $\lim_{t \rightarrow \infty} \sin(at)/a = \pi\delta(a)$ can be used [1, 2], (20) is expressed as follows:

$$\begin{aligned}
 W_{a,e}(\mathbf{k}, \mathbf{k}') &= \frac{4D_{ac}^2}{\rho_r V} \sum_{\substack{q_z \geq 0 \\ q_{1,z} \geq 0}} \left\{ \frac{qq_1}{\sqrt{\omega_{\mathbf{q}}\omega_{\mathbf{q}_1}}} \sqrt{n_{\mathbf{q}} + \frac{1}{2} \mp \frac{1}{2}} \sqrt{n_{\mathbf{q}_1} + \frac{1}{2} \mp \frac{1}{2}} \right. \\
 &\quad \times \left. \left[-\pi \frac{(\pm\omega_{\mathbf{q}} \mp \omega_{\mathbf{q}_1})\delta(\omega_{\mathbf{q}} - \omega_{\mathbf{q}_1})}{\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} \mp \hbar\omega_{\mathbf{q}_1}} + \pi\delta(\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} \mp \hbar\omega_{\mathbf{q}}) \frac{\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} \mp \hbar\omega_{\mathbf{q}}}{\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} \mp \hbar\omega_{\mathbf{q}_1}} \right] \right\}_{\substack{q_x = \pm(k'_x - k_x), \\ q_y = \pm(k'_y - k_y)}} \\
 &\quad \times \operatorname{Re} \int_{-L_z/2}^{L_z/2} dz \chi_{n'}^*(z) \chi_n(z) e^{\pm iq_z z} \operatorname{Re} \int_{-L_z/2}^{L_z/2} dz_1 \chi_{n'}^*(z_1) \chi_n(z_1) e^{\pm iq_{1,z} z_1}. \quad (21)
 \end{aligned}$$

In this expression, the summation with respect to $q_{1,z}$ is non-zero only when $q_z = q_{1,z}$. Then, electron transition probability can be written as follows:

$$\begin{aligned}
 W_{a,e}(\mathbf{k}, \mathbf{k}') &= \frac{4\pi D_{ac}^2}{\rho_r V} \sum_{\substack{q_x, q_y, \\ q_z \geq 0}} \frac{q^2}{\omega_{\mathbf{q}}} \left(n_{\mathbf{q}} + \frac{1}{2} \mp \frac{1}{2} \right) \delta(\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} \mp \hbar\omega_{\mathbf{q}}) \\
 &\quad \times \delta_{k'_x, k_x \pm q_x} \delta_{k'_y, k_y \pm q_y} \left[\operatorname{Re} \int_{-L_z/2}^{L_z/2} dz \chi_{n'}^*(z) \chi_n(z) e^{\pm iq_z z} \right]^2. \quad (22)
 \end{aligned}$$

Here, the Dirac δ -function indicates the energy conservation law.

Note, if in (22) the plane wave ($\chi_n(z) = e^{ik_z z} / \sqrt{L_z}$) or Bloch function is taken as an electron wave function, then the well-known classical expression of probability $W_{a,e}(\mathbf{k}, \mathbf{k}')$ [1–4] (Fermi Golden rule) is derived. In the common case, the calculation of the integral and sum in (22) is complicated. On the other hand, the expression (1) for $\tau_{\mathbf{k},ac}$ is derived (within the framework of the flat-band semiconductor model) by using the approximation of elasticity of electron-acoustic phonon scattering (elastic collision approximation, $\hbar\omega_{\mathbf{q}} \ll \varepsilon_{\mathbf{k}}$) with the assumption that

$$n_{\mathbf{q}} + 1 \approx n_{\mathbf{q}} \cong \frac{k_B T}{\hbar\omega_{\mathbf{q}}} = \frac{k_B T}{\hbar v_0 q} \gg 1. \quad (23)$$

Here, $\omega_{\mathbf{q}} = v_0 q$ dispersion law of the long wavelength longitudinal acoustic phonon is used.

To reveal the difference between the results of flat and titled band approaches it is reasonable that these assumptions should be used here as well. Then, after simple summing with respect to q_x and q_y , (22) takes the following simpler form:

$$W_{a,e}(\mathbf{k}, \mathbf{k}') = \frac{4\pi D_{ac}^2 k_B T}{\rho_r V \hbar v_0^2} \delta(\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}}) \sum_{q_z \geq 0} \left[\operatorname{Re} \int_{-L_z/2}^{L_z/2} dz \chi_{n'}^*(z) \chi_n(z) e^{\pm iq_z z} \right]^2. \quad (24)$$

In what follows, we use the transformation

$$\begin{aligned}
& \sum_{q_z \geq 0} \left[\operatorname{Re} \int_{-L_z/2}^{L_z/2} dz \chi_{n'}^*(z) \chi_n(z) e^{\pm i q_z z} \right]^2 \\
&= \sum_{q_z \geq 0} \left[\frac{1}{2} \int_{-L_z/2}^{L_z/2} dz \left[\chi_{n'}^*(z) \chi_n(z) e^{\pm i q_z z} + \chi_{n'}(z) \chi_n^*(z) e^{\mp i q_z z} \right] \right]^2 \\
&= \frac{1}{2} \operatorname{Re} \sum_{q_z \geq 0} \int_{-L_z/2}^{L_z/2} \int_{-L_z/2}^{L_z/2} dz dz_1 \left[\chi_{n'}^*(z) \chi_n(z) \chi_{n'}(z_1) \chi_n^*(z_1) e^{\pm i q_z z \mp i q_z z_1} \right. \\
&\quad \left. + \chi_{n'}^*(z) \chi_n(z) \chi_{n'}^*(z_1) \chi_n(z_1) e^{\pm i q_z z \pm i q_z z_1} \right] \tag{25}
\end{aligned}$$

and the relation [3]

$$\sum_{q_z} e^{i q_z (z - z_1)} = L_z \delta(z - z_1). \tag{26}$$

The result is as follows:

$$\begin{aligned}
W_{a,e}(\mathbf{k}, \mathbf{k}') &= \frac{\pi D_{ac}^2 k_B T L_z}{\rho_r V \hbar v_0^2} \delta(\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}}) \operatorname{Re} \int_{-L_z/2}^{L_z/2} \int_{-L_z/2}^{L_z/2} dz dz_1 \left[\chi_{n'}^*(z) \chi_n(z) \chi_{n'}(z_1) \chi_n^*(z_1) \delta(z - z_1) \right. \\
&\quad \left. + \chi_{n'}^*(z) \chi_n(z) \chi_{n'}^*(z_1) \chi_n(z_1) \delta(z + z_1) \right]. \tag{27}
\end{aligned}$$

Delta-integration over z_1 yields:

$$\begin{aligned}
W_{a,e}(\mathbf{k}, \mathbf{k}') &= \frac{\pi D_{ac}^2 k_B T L_z}{\rho_r V \hbar v_0^2} \delta(\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}}) \\
&\quad \times \operatorname{Re} \int_{-L_z/2}^{L_z/2} dz \left\{ |\chi_{n'}(z)|^2 |\chi_n(z)|^2 + \chi_{n'}^*(z) \chi_n(z) \chi_{n'}^*(-z) \chi_n(-z) \right\}. \tag{28}
\end{aligned}$$

Electron energy eigenvalues ε_n are determined from boundary conditions to (10). Note, there is some difference between the peculiarities of the movement of an electron under electric field in vacuum and an electron in a semiconductor. Conduction band gap ΔE_c of a semiconductor is a finite quantity. Contrary to the vacuum, the movement of a conduction electron in a semiconductor with perfect lattice has an oscillation character, as it is shown in figure 1.

Electron 'el.1' oscillates between the bottom of the conduction band and semiconductor edge; electron 'el.2' periodically reflects from the conduction band top and bottom edges. The behavior of an 'el.2' is well-known as a Bloch oscillation. Boundary conditions for Schrödinger equation (10) and, therefore, electron energy eigenvalues in case of Bloch oscillations have been reported, for example, in [9]. Here, for definiteness, neglecting the Bloch oscillations, the case of 'el.1' is considered only, i.e., it is assumed that the electric field is low and the magnitude of ΔE_c is very large. In other words, the model of a triangular quantum well with finite sizes is considered.

Here, we are interested in a large length semiconductor, particularly, in z -direction. Then, the allowed values of k_n (or ε_n) are computed from the boundary condition $\chi_n(z = -L_z/2) = 0$ as (see, [7] and figure 1)

$$\frac{L_z}{2l} + (k_n l)^2 = -a_n, \tag{29}$$

where a_n are the zeros of the Airy function which are located in the negative part of the real axis [8]. They are well approximated as $a_n \cong -(3\pi[4n-1]/8)^{2/3}$, where $n = 1, 2, \dots$. Inserting this relation into (29) we obtain

$$\frac{L_z}{2l} + (k_n l)^2 = \left[\frac{3\pi}{2} \left(n - \frac{1}{4} \right) \right]^{2/3}. \tag{30}$$

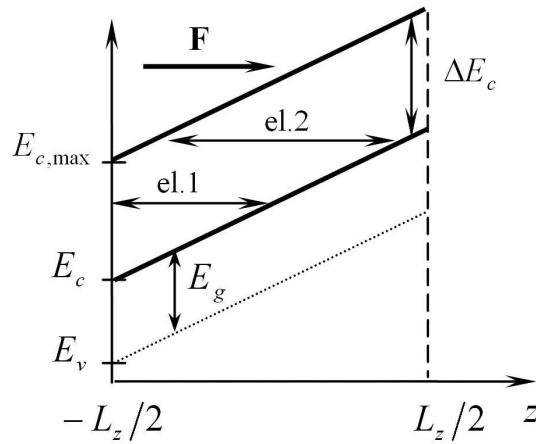


Figure 1. Semiconductor energy-band diagram in the presence of a uniform electric field F (parallel to the z -axis); el.1 – Bloch oscillations.

Solving (30) for k_n and inserting the result into (13), one obtains energy eigenvalues [7]:

$$\varepsilon = \frac{\hbar^2}{2m} \left\{ k_{\perp}^2 - \frac{L_z}{2l^3} + \frac{1}{l^2} \left[\frac{3\pi}{2}(n-1/4) \right]^{2/3} \right\}. \quad (31)$$

The values ε in (31) are obtained as a function of the electron state quantum numbers. The quantities k_x , k_y (or \mathbf{k}_{\perp}) and n (or k_n) are a set of quantum numbers which determine the conduction electron state in the presence of an electric field.

Normalization constant C_n in (11) is determined as follows:

$$C_n^{-2} = \int_{-L_z/2}^{L_z/2} dz \left| \text{Ai} \left(\frac{z}{l} - (k_n l)^2 \right) \right|^2. \quad (32)$$

It is known [7, 8] that

$$\int ds \text{Ai}^2(s) = s \text{Ai}^2(s) - \text{Ai}'^2(s), \quad (33)$$

where Ai' is the derivative of the Airy function.

Consequently, normalization constant C_n can be presented as follows:

$$C_n^{-2} = l \left[s \text{Ai}^2(s) - \text{Ai}'^2(s) \right] \Big|_{a_n}^{L_z/l + a_n}. \quad (34)$$

For a semiconductor with large length L_z one has

$$C_n^{-2} = l \text{Ai}'^2(a_n). \quad (35)$$

Here, we used the fact that $\text{Ai}(a_n) = 0$; functions $\text{Ai}(s)$ and $\text{Ai}'(s)$ exponentially vanish for positive large argument s [8]. On the other hand, the value $\text{Ai}'(a_n)$ is well approximated as [8]

$$\text{Ai}'(a_n) \cong (-1)^{n-1} \frac{1}{\sqrt{\pi}} (-a_n)^{1/4}. \quad (36)$$

Insertion of (36) into (35) yields:

$$C_n^2 = \pi/l \sqrt{-a_n}. \quad (37)$$

Thus, using (11), (29) and taking into account that $\chi_n(z)$ is the real function [see, (11), (12)] the expression (28) can be presented as follows:

$$W_{a,e}(\mathbf{k}, \mathbf{k}') = \frac{\pi D_{ac}^2 k_B T L_z l}{\rho_r V \hbar v_0^2} \delta(\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}}) C_{n'}^2 C_n^2 \left\{ \int_{-L_z/2l}^{L_z/2l} du |\text{Ai}(u - (k_{n'} l)^2)|^2 |\text{Ai}(u - (k_n l)^2)|^2 + \int_{-L_z/2l}^{L_z/2l} du [\text{Ai}(u - (k_{n'} l)^2) \text{Ai}(-u - (k_{n'} l)^2) \text{Ai}(u - (k_n l)^2) \text{Ai}(-u - (k_n l)^2)] \right\}, \quad (38)$$

where $u = z/l$ is the dimensionless variable of integration. (38) describes electron transition probability in the presence of an electric field. Transition probability depends on the electric field and it is a symmetric function: $W_{a,e}(\mathbf{k}, \mathbf{k}') = W_{a,e}(\mathbf{k}', \mathbf{k})$.

3. Electron-acoustic phonon FIT scattering time

The scattering time is defined by [3]:

$$\tau_{\mathbf{k}, \text{sc}}^{-1} = \sum_{\mathbf{k}'} W(\mathbf{k}, \mathbf{k}') \quad (39)$$

(38) shows that in the present case, the probabilities of phonon absorption and emission by electron are the same: $W_a(\mathbf{k}', \mathbf{k}) = W_e(\mathbf{k}, \mathbf{k}')$. Then, (39) can be written as follows:

$$\tau_{\mathbf{k}, \text{sc}}^{-1} = 2 \sum_{\mathbf{k}'} W_e(\mathbf{k}, \mathbf{k}'). \quad (40)$$

In the common case, the scattering time (the inverse of the scattering rate) differs from the relaxation time although sometimes both of them are equivalent (for example, the above-mentioned case of (1)) [3]. To calculate $\tau_{\mathbf{k}, \text{sc}}^{-1}$ in (40), we replace the sums over k'_x and k'_y by integrals over k'_x and k'_y , respectively. The transition from the sum to integral with the help of the relation $dk'_x dk'_y = \pi dk'^2_{\perp}$ can be presented as follows:

$$\sum_{\mathbf{k}'} \rightarrow \frac{2L_x L_y}{(2\pi)^2} \int_{\text{BZ}} dk'_x dk'_y \sum_{n'} = \frac{L_x L_y}{2\pi} \int_{\text{BZ}} dk'^2_{\perp} \sum_{n'}. \quad (41)$$

Here, coefficient 2 in the numerator is related to the electron spin.

From (30) it follows that $k_{n+1}^2 - k_n^2 \sim 1/l^2$. The distance between k_n and k_{n+1} depends on n and it is small for large l . Therefore, at low-field regime, one can change the summation over n' by an integral over $k_{n'}$:

$$\sum_{n'} \rightarrow \int dk_{n'} \frac{dn'}{dk_{n'}}. \quad (42)$$

The derivative $dn'/dk_{n'}$ can be evaluated based on (30). The solution of (30) for n is given the following expression for n' :

$$n' = \frac{2}{3\pi} \left(\frac{L_z}{2l} + (k_{n'} l)^2 \right)^{3/2} + \frac{1}{4}. \quad (43)$$

Therefore,

$$\frac{dn'}{dk_{n'}} = \frac{2l^2 k_{n'}}{\pi} \sqrt{\frac{L_z}{2l} + (k_{n'} l)^2}. \quad (44)$$

Based on (29), the derivative $dn'/dk_{n'}$ can be presented as follows:

$$\frac{dn'}{dk_{n'}} = \frac{2l^2 k_{n'}}{\pi} \sqrt{-a_{n'}}. \quad (45)$$

Thus, transition (41) can be presented as follows:

$$\sum_{n'} \longrightarrow \frac{L_x L_y l^2}{2\pi^2} \int_{k_{\perp,\min}^{\prime 2}}^{k_{\perp,\max}^{\prime 2}} \int_{k_{n',\min}^2}^{k_{n',\max}^2} dk_{\perp}^{\prime 2} dk_{n'}^2 \sqrt{-a_{n'}}. \quad (46)$$

Inserting (38) into (40), simultaneously taking into account (37) and transition (46), for the scattering time one obtains:

$$\begin{aligned} \tau_{\mathbf{k},\text{sc}}^{-1} = & \frac{D_{\text{ac}}^2 k_{\text{B}} T C_n^2}{\rho_r \hbar^3 v_0^2} \int_{k_{\perp,\min}^{\prime 2}}^{k_{\perp,\max}^{\prime 2}} \int_{s'_{\min}}^{s'_{\max}} dk_{\perp}^{\prime 2} ds' \delta(\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}}) \left\{ \int_{-L_z/2l}^{L_z/2l} du |\text{Ai}(u - s')|^2 |\text{Ai}(u - (k_n l)^2)|^2 \right. \\ & \left. + \int_{-L_z/2l}^{L_z/2l} du \text{Ai}(u - s') \text{Ai}(-u - s') \text{Ai}(-u - (k_n l)^2) \text{Ai}(u - (k_n l)^2) \right\}. \quad (47) \end{aligned}$$

Here, $s' = (lk_{n'})^2$ is the dimensionless variable of integration, Brillouin zone is replaced by the infinite range: $0 \leq k_{\perp}^{\prime 2} < \infty$. The limits of integration over s' are determined by the δ -function

$$\delta(\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}}) = \frac{2m}{\hbar^2} \delta(k_{\perp}^{\prime 2} + k_{n'}^2 - k_{\perp}^2 - k_n^2), \quad (48)$$

as: $s'_{\min} = -a_1 - L_z/2l$, $s'_{\max} = (k_{\perp}^2 - k_n^2) l^2$, where $a_1 = -(9\pi/8)^{2/3}$ is the first zero of the Airy function [8]. δ -integration over s' in (47) yields

$$\begin{aligned} \tau_{\mathbf{k},\text{sc}}^{-1} = & \frac{2D_{\text{ac}}^2 m k_{\text{B}} T C_n^2}{\rho_r \hbar^3 v_0^2} \int_0^{\infty} ds'_{\perp} \left\{ \int_{-L_z/2l}^{L_z/2l} du |\text{Ai}(u + s'_{\perp} - \Delta)|^2 |\text{Ai}(u - (k_n l)^2)|^2 \right. \\ & \left. + \int_{-L_z/2l}^{L_z/2l} du \text{Ai}(u + s'_{\perp} - \Delta) \text{Ai}(-u + s'_{\perp} - \Delta) \text{Ai}(-u - (k_n l)^2) \text{Ai}(u - (k_n l)^2) \right\}. \quad (49) \end{aligned}$$

Here, $s'_{\perp} = k_{\perp}^{\prime 2} l^2$ is the dimensionless variable of integration, $\Delta \equiv k_{\perp}^2 l^2 + k_n^2 l^2 = 2m\varepsilon l^2 / \hbar^2$ is the dimensionless energy of an electron.

In (49), evaluations of the first and second the integrals over s'_{\perp} can be carried out based on (33) and following the integral of the product of two Airy functions [8], respectively,

$$\int_0^{\infty} ds \text{Ai}(b + s) \text{Ai}(c + s) = \frac{1}{b - c} [\text{Ai}(b) \text{Ai}'(c) - \text{Ai}'(b) \text{Ai}(c)]. \quad (50)$$

The result is as follows:

$$\tau_{\mathbf{k},\text{sc}}^{-1} = \frac{D_{\text{ac}}^2 m k_{\text{B}} T C_n^2}{\rho_r \hbar^3 v_0^2} [I_1 + I_2], \quad (51)$$

where

$$I_1 = \int_{-L_z/2l}^{L_z/2l} du \{(\Delta - u) \text{Ai}^2(u - \Delta) + \text{Ai}'^2(u - \Delta)\} |\text{Ai}(u - (k_n l)^2)|^2, \quad (52)$$

$$I_2 = \int_{-L_z/2l}^{L_z/2l} du \frac{1}{2u} [\text{Ai}(u - \Delta) \text{Ai}'(-u - \Delta) - \text{Ai}'(u - \Delta) \text{Ai}(-u - \Delta)] \text{Ai}(-u - (k_n l)^2) \text{Ai}(u - (k_n l)^2). \quad (53)$$

The functional analyses of the sub-integral expression show that the main contribution in integrals (52) and (53) is given by the range near $u \sim 0$. An approximate estimation of the integral (53) is carried out with the help of L'Hopital's rule. The result is as follows:

$$I_1 + I_2 \approx \frac{1}{lC_n^2} [\Delta \text{Ai}^2(-\Delta) + \text{Ai}'^2(-\Delta)]. \quad (54)$$

Therefore, the electron scattering time can be presented as follows:

$$\tau_{\mathbf{k},\text{sc}}^{-1} = \frac{D_{\text{ac}}^2 m k_B T}{\rho_r \hbar^3 v_0^2 l} [\Delta \text{Ai}^2(-\Delta) + \text{Ai}'^2(-\Delta)]. \quad (55)$$

4. Summary

The electron-acoustic phonon scattering theory has been reconsidered. In semiconductors, whose bands are tilted under uniform electric field, the time of electron scattering by acoustic phonon is determined by (55). Scattering time depends on the electron energy ε . It depends on the electric field as well, because $\Delta \sim \varepsilon l^2$; $l \sim F^{-1/3}$. Those dependencies are determined by the Airy function properties [8]. Thus, for negative arguments, the Airy function oscillates. From the asymptotic series of the Airy function $\text{Ai}(\Delta)$ and of their derivative $\text{Ai}'(\Delta)$ it follows that for large negative argument [8]

$$|\Delta| \text{Ai}^2(-|\Delta|) + \text{Ai}'^2(-|\Delta|) = |\Delta|^{1/2} / \pi. \quad (56)$$

The Airy function decays exponentially for positive arguments. The first terms of asymptotic series of the Airy function and of their derivative for positive arguments are as follows:

$$\text{Ai}(|\Delta|) = \frac{1}{2\sqrt{\pi}|\Delta|^{1/4}} \exp(-2|\Delta|^{3/2}/3), \quad \text{Ai}'(|\Delta|) = -\frac{|\Delta|^{1/4}}{2\sqrt{\pi}} \exp(-2|\Delta|^{3/2}/3). \quad (57)$$

Then, from (55), (56) and (57) it follows:

- for positive large Δ

$$\tau_{\mathbf{k},\text{sc}}^{-1} = \frac{D_{\text{ac}}^2 m k_B T |\Delta|^{1/2}}{\pi \rho_r \hbar^3 v_0^2 l}, \quad (58)$$

- for negative large Δ

$$\tau_{\mathbf{k},\text{sc}}^{-1} = \frac{D_{\text{ac}}^2 m k_B T |\Delta|^{1/2}}{\pi \rho_r \hbar^3 v_0^2 l} \frac{1}{2} \exp(-4|\Delta|^{3/2}/3). \quad (59)$$

Insertion Δ and l into (59) yields:

$$\tau_{\mathbf{k},\text{sc}}^{-1} = \tau_{\mathbf{k},\text{ac}}^{-1} \frac{1}{2} \exp\left(-4\sqrt{2m|\varepsilon|^3/\hbar^2}/3eF\right). \quad (60)$$

General expression (55) for the electron-acoustic phonon scattering time can be modified by inserting Δ into (55). Then, one has

$$\tau_{\mathbf{k},\text{sc}}^{-1} = \frac{D_{\text{ac}}^2 m k_B T}{\rho_r \hbar^3 v_0^2 l} \left[\frac{2m\varepsilon l^2}{\hbar^2} \text{Ai}\left(-\frac{2m\varepsilon l^2}{\hbar^2}\right) + \text{Ai}'^2\left(-\frac{2m\varepsilon l^2}{\hbar^2}\right) \right]. \quad (61)$$

It is easy to establish that (58) and (1) are the same. As equation (60) shows, the scattering time of low energy electron depends on the electric field. The dependence has exponential character. This effect has been explained in terms of the penetration of the electron wave function into a band gap of a semiconductor [6]. As a result, for low energy electrons, which are located near the bottom edge of the conduction band, the transition with phonon emission becomes allowable in the region below the conduction band edge. Note, at flat-bands approach, there is a threshold of a phonon emission by a low energy electron, for details see [10]. All these peculiarities are well displayed in figure 2, where the dependencies of $\tau_{\mathbf{k},\text{ac}}^{-1}$

and $\tau_{\mathbf{k},sc}^{-1}$ on electron dimensionless energy $\varepsilon/k_B T$ are plotted for n-Si at $T = 300$ K with the following parameters [5]: $m = 0.32m_0$, $\rho_r = 2329$ kg/m³, $v_0 = 8.43 \cdot 10^3$ m/s, $D_{ac} = 9$ eV. The dependence $\tau_{\mathbf{k},sc}^{-1}(\varepsilon/k_B T)$ (curve 'a') is calculated at $F = 800$ V/cm based on (61). The dependence $\tau_{\mathbf{k},ac}^{-1}(\varepsilon/k_B T)$ (curve 'b') is calculated based on (1). As shown in figure 2, the curve 'a' has a character of light oscillations around the curve 'b'. At a low field regime $F < \sim 400$ V/cm, the curves 'a' and 'b' practically coincide in the range of positive energy. Other important peculiarities are as follows: on the curve 'b' there is a fracture, i.e., $d\tau_{\mathbf{k},ac}^{-1}/d\varepsilon|_{\varepsilon=0} = \infty$ [see, equation (1)]; on the curve 'a' there is no fracture [see, (61)].

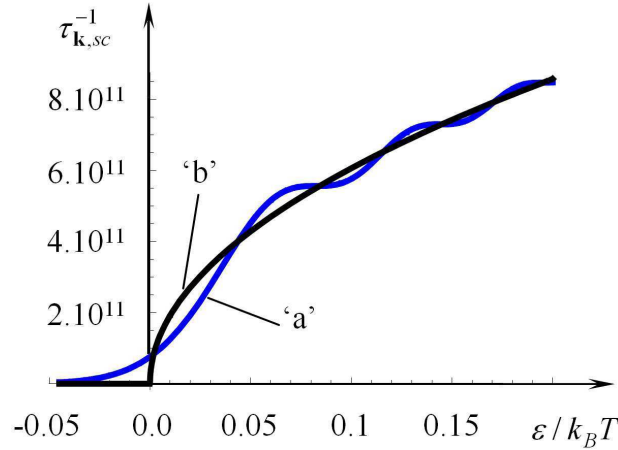


Figure 2. (Color online) The dependencies of $\tau_{\mathbf{k},sc}^{-1}$ (curve 'a' – $F = 800$ V/cm) and $\tau_{\mathbf{k},ac}^{-1}$ (curve 'b' – $F = 0$) on electron dimensionless energy $\varepsilon/k_B T$ for n-Si at $T = 300$ K.

Taking into account the problem solution reported in [6] it can be stated that the results of the present study can have a principal effect on the mobility fluctuation theory, especially. It should be noted that in the above-presented electron-acoustic phonon FIT scattering study, the electron quasi-momentum relaxation time and its relation to the scattering time is not included. It requires a separate consideration.

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Індуковане електронноакустичним фононним полем тунельне розсіяння

С.В. Мелконян, А.Л. Харатюнян, Т.А. Залінян

Факультет фізики напівпровідників і мікроелектроніки, Єреванський державний університет, 0025
Єреван, Вірменія

У статті подано новий погляд на теорію електронноакустичного розсіювання одного фонона. При цьому припускається, що невироджений напівпровідник має сферичну параболічну зонну структуру. В основу перегляду теорії покладено ефект нахилу напівпровідникових зон при накладанні збурюючого потенціалу електричного поля. У цьому випадку власні функції електрона вже не є плоскими хвилями чи функціями Блоха. В режимі слабких полів отримано вирази для ймовірності електронних внутрішньозонних переходів і для часу розсіяння в наближенні пружних зіткнень. Також проаналізовано залежність часу розсіяння від енергії електрона та напруженості однорідного електричного поля. Представлено результати відповідних числових обчислень для n-Si при температурі 300 К. Встановлено відсутність зламу на кривій залежності часу розсіяння електрона від енергії електрона.

Ключові слова: напівпровідник з нахиленою зоною, електронноакустичне фононне розсіяння, ймовірність переходу, час розсіяння