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Theory of the free-carrier absorption in quantum wires with boundary roughness scattering

G.B. Ibragimov

Institute of Physics, Academy Sciences, Azerbaijan Republic, Baku-143. Pr. H.Javid 33
Fax: (99412) 39 5961, e-mail: guseyn@physics.ab.az, guseyn_gb@mail.ru

Abstract. A theory of free carrier absorption is given for quantum wires when carriers are scattered by boundary roughness and the radiation field is polarized along the length of the wire. The free-carrier absorption coefficient is found to be an oscillatory function of the photon frequency and of the wire width. The obtained results are compared with different scattering mechanisms for quasi-one-dimensional structures. It is found that boundary roughness scattering is important especially when the wire width and temperature decreases. In addition, it was found that in quantum wire the electron – boundary roughness interaction gives a greater contribution to the absorption than the electron-acoustic phonon interaction. The results are interpreted in terms of boundary roughness-assisted transitions between size quantized subbands.

Keywords: boundary roughness, quantum wire.

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1. Introduction

Recently there has been considerable interest in systems where electron movement is confined to one or two dimensions. The most interesting situation occurs when the confinement is of the order of the de Broglie wavelength for electrons. In a quantum wire, when its width becomes much less than the mean free path, the motion of electrons becomes quasi-one-dimensional (Q1D). The confinement leads to distinct quantized energy levels and to an increasing importance of boundary scattering. Physical properties of low-dimensional semiconducting structures differ from properties of bulk semiconductors because the translational symmetry is broken [1]. For carriers confined in a quantum wells (QW_s), the free-carrier absorption (FCA) is practically important for determining the optical absorption. Scattering -assisted absorption by free electrons and holes in the active QW_s then usually determines the internal loss in optically pumped laser devices with undoped claddings. Even in electrically pumped devices, assisted FCA can dominate if the lasing mode is optically confined primarily to the active region, as in the interband cascade lasers [2]. FCA in diode optical cladding layers consisting of superlattice injectors [3] can also be significant. Since FCA is one of the powerful means to understand the scattering mechanisms of carriers, it has been theoretically studied in Q2D structures for the case of absorption assisted by acoustic [4] and polar optical [5-8] phonon scattering including the effects of phonon confinement [9], piezoelectric coupling [10], ionized impurities [11], interface-roughness [12], electron-electron [13], and alloy-disorder scattering [14]. FCA has been studied theoretically in Q1D structures only (to our knowledge) for the case where the carriers are scattered by acoustic [15], acoustic and optical phonons [16] and alloy-disorder[17]. However, roughness scattering is an important scattering mechanism in QW system and some quantum-mechanical studies have been performed [18-28]. Its effect depends strongly on the height and lateral correlation length of the interface or boundary roughness.

In this paper, we present the theory of FCA for the Q1D electron gas in QW structures when carriers are scattered by boundary roughness. We consider the FCA for the cases where the radiation field is polarized along the length of the wire. Absorption coefficient will be calculated for the examples of GaAs QW wires. We shall also consider in detail the applicability of the standard semiclassical approximation to these QW wires.

2. Formalism

We assume that gas of carriers is confined to move in a long thin wire that is embedded in an insulating cladding. For simplicity, we choose the cross section of the wire to be rectangular with W and L_z the cross sectional dimensions along the y and z directions, respectively, and with L the wire length along the x direction where electrons are assumed to move freely. Assuming the usual effective-mass approximation for the conduction band , the energy eigenfunctions and eigenvalues for electrons in a rectangular thin wire can be written as

$$\mathrm{E}_{knl} = \mathrm{E}_k + \mathrm{E}_n + \mathrm{E}_l = \frac{\hbar^2 k^2}{2m^*} + n^2 \mathrm{E}_W^0 + l^2 \mathrm{E}_{L_Z}^0$$

$$\mathrm{E}_W^0 = \frac{\pi^2 \hbar^2}{2m^* W^2},\ \mathrm{E}_{L_Z}^0 = \frac{\pi^2 \hbar^2}{2m^* {L_z}^2},\ n, l = 1,2,3,\ldots \qquad (1)$$

$$\Psi_{knl} = \left|2/(WL_z L)^{1/2}\right| \sin(\pi n y/W) \sin(\pi l z/L_z) \exp(ikx)$$

The FCA coefficient when boundary roughness scattering is dominant can be related to the scattering rate for free carriers to make an intraband transition from a given initial state with the simultaneous scattering of carriers by boundary roughness and can be calculated using the standard second order Born golden rule approximation. In second-order perturbation theory, the matrix element connecting the initial and final states for an optical transition in a QW wire is given by

$$< k'n'l'|M|knl >= \\ = \sum_{k''n''l''} \left[\frac{< k'n'l'|H_R|k''n''l'' >< k''n''l''|H_{BR}|knl >}{E_{knl} - E_{k''n''l''}} + \right. \\ \left. + \frac{< k'n'l'|H_{BR}|k''n''l'' >< k''n''l''|H_R|knl >}{E_{knl} - E_{k''n''l''} + \hbar\Omega} \right] \qquad (2)$$

where knl, $k'n'l'$ and $k''n''l''$ are wave vector and subband indexes for initial, final and intermediate states, respectively, $\hbar\Omega$ is the photon energy, H_R is the interaction Hamiltonian between the electrons and the radiation field, H_{BR} is the boundary roughness scattering potential.

In particular, we treat the case of photon absorption mediated by carrier scattering from boundary roughness fluctuations, although many of the qualitative conclusions will be equally applicable to other scattering mechanisms. The roughness in the wire is conventionally characterized by a fluctuation magnitude Δ and a correlation length Λ in the Gaussian autocorrellation function [1] defined by

$$\langle \Delta(x)\Delta(x') \rangle = \Delta^2 \exp\left[-\frac{(x-x')^2}{\Lambda^2} \right]$$

The square of the matrix element caused by boundary roughness along the wire direction can be approximated by the relation [19-22]

$$|\langle k'n'l'|H_{BR}|knl\rangle|^2 = \\ = \frac{\pi^{9/2} n^2 n'^2 \hbar^4 \Lambda \Delta^2}{2W^6 L} \exp\left(-\frac{q^2\Lambda^2}{4} \right) \left(1 + \frac{1}{2}\delta_{ll'} \right) \qquad (3)$$

where $q = k - k'$, Δ is the amplitude and L is the lateral correlation length of the roughness.

The matrix element of the electron-photon interaction Hamiltonians using the wave functions are

$$\langle k'n'l'|H_R|knl\rangle = -\frac{e\hbar}{m^*} \left(\frac{2\pi\hbar n_0}{V\Omega\in} \right)^{1/2} (\varepsilon\kappa) \delta_{\kappa\kappa'} \delta_{nn'} \delta_{ll'} \qquad (4)$$

when the radiation field is polarized along the wire. Here $\in$ is the dielectric constant of the material, n_0 is the number of photons in the radiation field, ε is the polarization vector of the radiation field and V is the volume of the thin wire.

From Eqs (2)–(4), the scattering rate for the electron-boundary roughness interaction and the electron-photon interaction can be obtained as

$$W_{knl,k'n'l'} = \frac{2\pi^6 e^2 n_0 \Lambda^2 \Delta^2}{m*^4\ \Omega^3 \in W^6 L^2 V} \times \\ \times \sum_{k'n'l'} n^2 n'^2 \left(1 + \frac{1}{2}\delta_{ll'} \right) \left| k' - k \right|^2 \exp\left(-\frac{q^2\Lambda^2}{4} \right) \times \\ \delta\left(E_{k'n'l'} - E_{knl} - \hbar\Omega \right) \qquad (5)$$

The absorption coefficient is calculated by summing over all occupied initial states and unoccupied final states. The coefficient FCA for a Q1D electron gas for radiation field polarized along the axis of the wire is finally given by

$$\alpha = \frac{\pi^5 e^2 \Lambda^2 \Delta^2}{8\Omega^3 m^{*2} \in^{1/2} VW^6} \times \\ \times \sum\sum n^2 n'^2 \left(1 + \frac{1}{2}\delta_{ll'} \right) \iiint \left(f_{knl} - f_{k'n'l'} \right) \times \\ \times \frac{\left(E_{k'} + E_k - 2\sqrt{E_{k'} E_k}\cos\vartheta \right)}{\sqrt{E_{k'} E_k}} \exp\left(-\frac{q^2\Lambda^2}{4} \right) \times \\ \times \delta\left(E_{k'n'l'} - E_{knl} - \hbar\Omega \right) dE_k\, dE_{k'}\, d\vartheta \qquad (6)$$

where ϑ is the scattering angle that in Q1D can have only two values, namely: π for backward scattering and 0 for the forward one. The integral over final states can be eliminated using the energy-conserving delta function.

For the case of a nondegenrate, Q1D electron gas, the electron distribution function is

$$f_{knl} = \frac{(2\pi)^{1/2}\hbar n_e ab}{\gamma\delta\left(m^* k_B T\right)^{1/2}} \times \exp\left[-\frac{n^2 E_W^0 + l^2 E_{L_Z}^0}{k_B T}\right] \exp\left(-\frac{\hbar^2 k^2}{2m^* k_B T}\right) \quad (7)$$

$$\gamma = \sum_n \exp\left(-\frac{n^2 E_W^0}{k_B T}\right), \ \delta = \sum_l \exp\left(-\frac{l^2 E_{L_Z}^0}{k_B T}\right)$$

where n_e is the concentration of the electrons. Using Eq. (7) in Eq. (6) we obtain the FCA

$$\alpha = \frac{\pi^{11/2} e^2 \hbar n_e \Lambda^2 \Delta^2}{\sqrt{2}\Omega^3 m^{*5/2} c \in^{1/2} VW^6 (k_B T)^{1/2}} \times \left[1 - \exp\left(-\frac{\hbar\Omega}{k_B T}\right)\right] \sum\sum n^2 n'^2 \left(1 + \frac{1}{2}\delta_{ll'}\right) \times \exp\left(-\frac{n^2 E_W^0 + l^2 E_{L_Z}^0}{k_B T}\right) Z \exp\left(\frac{Z}{2k_B T}\right) \times \left\{\frac{1}{2}\left[\left(\frac{p+b}{p-b}\right)^{1/2} + \left(\frac{p+b}{p-b}\right)^{-1/2}\right] K_1\left(\frac{Z}{2}\sqrt{p^2 - b^2}\right)_1 + \frac{b}{\sqrt{p^2 - b^2}} K_1\left(\frac{Z}{2}\sqrt{p^2 - b^2}\right)\right\} \quad (8)$$

where

$$Z = \hbar\Omega - \left(n'^2 - n^2\right)E_W^0 + \left(l'^2 - l^2\right)E_{L_Z}^0,$$

$$p = \frac{1}{k_B T} - \frac{m^* \Lambda^2}{\hbar^2}, \ b = \frac{m^* \Lambda^2}{2\hbar^2}$$

and K_l(y) is the modified Bessel function of the second kind.

It is interesting to note that in the quantum size limit, in temperature range where the intersubband transitions are not allowed due to the energy differences between the subbands being very large(i.e. $E_W/k_B T > 1$, $E_{L_Z}/kBT > 1$, and $E_W > \hbar\Omega$, $E_{L_Z} > \hbar\Omega$), we can assume $n = n' = l = l' = 1$ and $p = \frac{1}{k_B T}$ ($p >> b$). In this limit, the absorption coefficient of equation (8) can be rewritten

$$\alpha = \frac{3\pi^{11/2} e^2 \hbar^2 n_e \Lambda^2 \Delta^2}{2\sqrt{2}c\Omega^2 \in^{1/2} m^{*5/2} W^6 L (k_B T)^{1/2}} \times \left[1 - \exp\left(-\frac{\hbar\Omega}{k_B T}\right)\right] \exp\left(\frac{\hbar\Omega}{2k_B T}\right) K_1\left(\frac{\hbar\Omega}{2k_B T}\right) \quad (9)$$

In the limit of very long wavelengths, the absorption coefficient is known to reduce to the semiclassical form , which scales as λ^2. The semiclassical expression becomes a reasonable approximation in the limit of $K_B T >> \hbar\Omega$ for nondegenerate statistics. In this limit, the absorption coefficient of equation (9) can be rewritten

$$\alpha^{sc} = \frac{3\pi^{11/2} e^2 \hbar^2 n_e \Lambda \ \Delta^2}{\sqrt{2}c\Omega^2 \in^{1/2} m^{*5/2} W^6 (k_B T)^{1/2}} \quad (10)$$

3. Discussion

We have obtained general expressions for the quantum wires when the carriers are scattered by boundary roughness. The FCA coefficient is expressed as a function of $\hbar\Omega$ and also depends on W and T. We have evaluated, numerically, the above expressions for FCA coefficient at 300K and parameters characteristic of GaAs and electron concentration $n_e = 10^{17}$cm^{-3}, $\Delta = 4.2$ Å and $\Lambda = 50$ Å. On the basis of expressions obtained, we have constructed Fig.1–2.

In Fig. 1, we plot the FCA coefficient α_{BR}^{1D} as a function of the photon energy $\hbar\Omega$. The curves 1 and 4 refers to polar-optic and acoustic phonon modes [16] and curves 2 and 3 to alloy-disorder and boundary roughness. It is shown that α_{BR}^{1D} decreases monotonically with increasing photon energy. The kinks in the curves indicate boundary roughness-assisted transition between the subbands. The enhancement of the absorption coefficient associated with scattering to higher subbands also holds for other scattering mechanisms [15-17]. It is shown that in quantum wire the electron boundary roughness interaction gives a greater contribution to the absorption than the electron-acoustic phonon interaction. It can also be seen that FCA coefficients due to boundary roughness and to alloy disorder and polar-optic phonons are of the same order.

In Fig. 2, we plot the FCA coefficient α_{alloy}^{1D} in GaAs quantum wire as a function of the wire width. The absorption coefficient shows the oscillatory behavior as a function of $1/W^6$ whenever the photon energy is such that boundary roughness-assisted transition takes place to one of the higher subbands of the QW wire. It is shown that FCA becomes considerably enhanced as wire width decreases. It was predicted in [19-22] that the relaxation rate due to boundary roughness scattering in Q1D structures increases as the transverse dimensions of the wire diminish. This increase in the scattering rate explains the increase in the FCA coefficient predicted in our

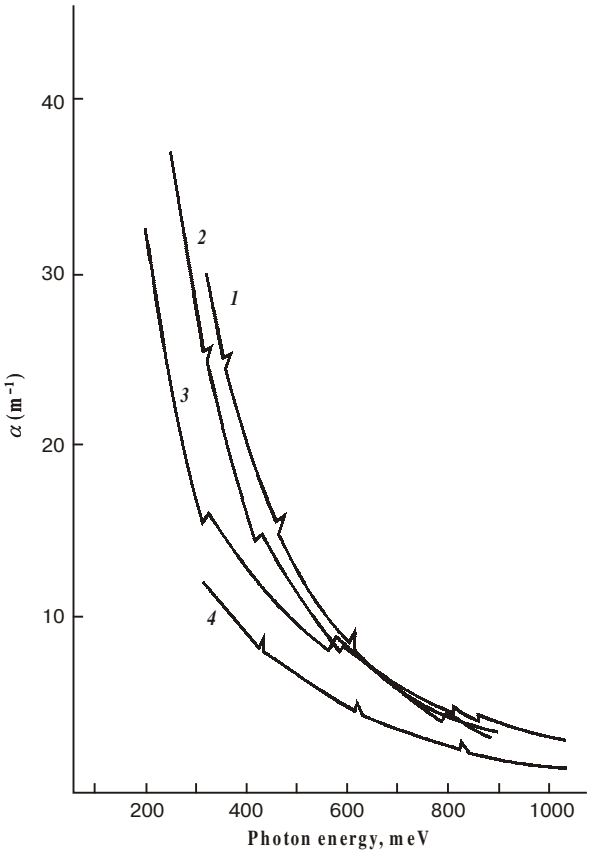

Fig. 1. FCA coefficient in a GaAs quantum wire due to boundary roughness scattering as a function of the photon frequency for T = 300 K. Curves 1 and 4 correspond to the FCA for GaAs quantum wire when the carrier are scattered by polar optical and acoustic phonons [16]. Curves 3 correspond to the FCA for $Ga_{0.47}In_{0.53}As$ quantum wire when the carrier are scattered by alloy-disorder [17]. In the all cases transverse dimensions is same, $W = L_z = 10^{-6}$ cm.

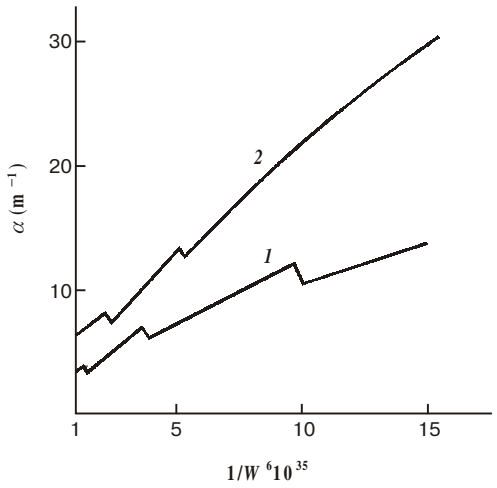

Fig. 2. The FCA coefficient is shown as a function $1/W^6$. Curve 1 is for the wavelength λ = 3 μm and curve 2 is for λ = 5 μm.

present numerical results for a quantum wire. As the wavelength decreases more and more oscillations are observed and the absorption coefficient increases linearly with $\alpha_{BR} \propto 1/W^6$.

In conclusion, we predict that when boundary roughness scattering is dominant, the FCA coefficient should increase with decreasing transverse dimensions of the wire for radiation polarized along the length of the wire. We also predict an oscillatory dependence of the FCA on the wire width and photon frequency. The oscillatory behaviour is explained in terms of boundary roughness transitions between quantised subbands arising from the confinement of electrons in the Q1D semiconducting structure. The electron-boundary roughness scattering is important especially when the wire width W decreases. The electron-boundary roughness interaction gives a greater contribution to the absorption than the electron-acoustic phonon interaction in Q1D structures made from the same materials.

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