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Free-carrier absorption in quantum wires for boundary roughness scattering

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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 width of the wire. 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 width of the wire and the temperature decrease. In addition, it was found that in quantum wires 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.

1. Introduction

Recently there has been considerable interest in systems in which the electron motion 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. The physical properties of low-dimensional semiconducting structures differ from the properties of bulk semiconductors because the translational symmetry is broken [1]. For carriers confined in a quantum wells (QWs), the free-carrier absorption (FCA) is practically important for determining the optical absorption. Scattering-assisted absorption by free electrons and holes in the active QWs then usually determines the internal loss in optically pumped laser devices with undoped cladding. Even in electrically pumped devices, assisted FCA can dominate if the lasing mode is optically confined primarily to the active region, as in interband cascade lasers [2]. FCA in diode optical

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cladding layers consisting of superlattice injectors [3] can also be significant. Since FCA offers a powerful means for understanding the scattering mechanisms of carriers, it has been studied theoretically 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 systems 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 cases where the radiation field is polarized along the length of the wire. The 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 a 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 length of the wire 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

$$E_{knl} = E_k + E_n + E_l = \frac{\hbar^2 k^2}{2m^*} + n^2 E_W^0 + l^2 E_{L_Z}^0$$

$$E_W^0 = \frac{\pi^2\hbar^2}{2m^* W^2}, \quad E_{L_Z}^0 = \frac{\pi^2\hbar^2}{2m^* {L_z}^2} \quad n, l = 1, 2, 3, \ldots \tag{1}$$

$$\Psi_{knl} = [2/(WL_zL)^{1/2}] \sin(\pi ny/W) \sin(\pi lz/L_z) \exp(\mathrm{i}kx).$$

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

$$\langle k'n'l'|M|knl\rangle = \sum_{k''n''l''} \left[\frac{\langle k'n'l'|H_R|k''n''l''\rangle\langle k''n''l''|H_{BR}|knl\rangle}{E_{knl} - E_{k''n''l''}} + \frac{\langle k'n'l'|H_{BR}|k''n''l''\rangle\langle k''n''l''|H_R|knl\rangle}{E_{knl} - E_{k''n''l''} + \hbar\Omega} \right] \tag{2}$$

where $knl, k'n'l'$ and $k''n''l''$ are the wavevector and subband indices for initial, final and intermediate state respectively, $\hbar\Omega$ is the photon energy, H_R is the interaction Hamiltonian between the electrons and the radiation field and 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 autocorrelation 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]

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

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

The matrix elements of the electron–photon interaction Hamiltonians using the wavefunctions are

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

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 equations (2)–(4) the scattering rate for the electron–boundary roughness interaction and the electron–photon interaction can be obtained as

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

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 a radiation field polarized along the axis of the wire is finally given by

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

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

For the case of a non-degenerate, Q1D electron gas, the electron distribution function is

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

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

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

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

where

$$Z = \hbar\Omega - (n'^2 - n^2) E_W^0 + (l'^2 - l^2) E_{L_Z}^0,\ p = \frac{1}{k_B T} - \frac{m^* \Lambda^2}{\hbar^2},\ b = \frac{m^* \Lambda^2}{2\hbar^2}$$

and $K_1(y)$ is the modified Bessel function of the second kind.

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

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

This expression can be compared with the following expression for the FCA in a non-degenerate Q1D electron gas when acoustic phonon scattering via the deformation potential dominates [15]

$$\alpha_{ac}^{1D} = \frac{2^{5/2}\sqrt{\pi} n_e e^2 E_d^2 (k_B T)^{1/2}}{\in^{1/2} c\rho \upsilon_s^2 m^{*1/2} W^2 \gamma \delta} \frac{\left[1 - \exp\left(-\frac{\hbar\Omega}{k_B T}\right)\right]}{(\hbar\Omega)^3} \sum_{nl} \sum_{n'l'} \left(1 + \frac{1}{2}\delta_{nn'}\right)\left(1 + \frac{1}{2}\delta l_{ll'}\right)$$
$$\times \exp\left(-\frac{n^2 E_n^0 + l^2 E_l^0}{k_B T}\right) Z \exp\left(\frac{Z}{2k_B T}\right) K_1\left(\frac{Z}{2k_B T}\right) \tag{10}$$

where ρ is the density of the semiconductor, υ_s is the velocity of sound and E_d is the deformation potential. The coefficients have an identical variation with photon frequency Ω, which may be seen from (9) and (10). The identical nature of the variation for the two scattering processes may be explained by examining the matrix elements for scattering. For the case $n = n' = l = l' = 1$ the ratio $\alpha_{BR}^{1D}/\alpha_{ac}^{1D}$ is

$$\frac{\alpha_{BR}^{1D}}{\alpha_{ac}^{1D}} = \frac{\pi^5 \hbar^4 \Lambda \Delta^2 \rho \upsilon_s^2}{12 E_d^2 k_B T W^4 m^{*2}}. \tag{11}$$

In this form, the ratio depends only upon material parameters and absolute temperature and does not depend upon photon frequency.

In the quantum limit, using the expression for the FCA coefficient α_{alloy}^{1D} taking into consideration the alloy-disorder scattering given by (12) in [17] and (9), we obtain

$$\frac{\alpha_{BR}^{1D}}{\alpha_{alloy}^{1D}} = \frac{\pi^4 \hbar^4 \Lambda \Delta^2}{6(\delta V)^2 \Omega_0 x(1-x) m^{*2} W^4} \tag{12}$$

where Ω_0 is the volume of the unit cell and $\delta V = 0.6$ eV is the alloy-disorder scattering potenial. In this form, the ratio $\alpha_{BR}^{1D}/\alpha_{alloy}^{1D}$ depends only material parameters and increases with increasing transverse dimension of the quantum wire.

In the limit of very long wavelengths, the absorption coefficient is known to reduce to the semiclassical form [29], which scales as λ^2. The semiclassical expression becomes a

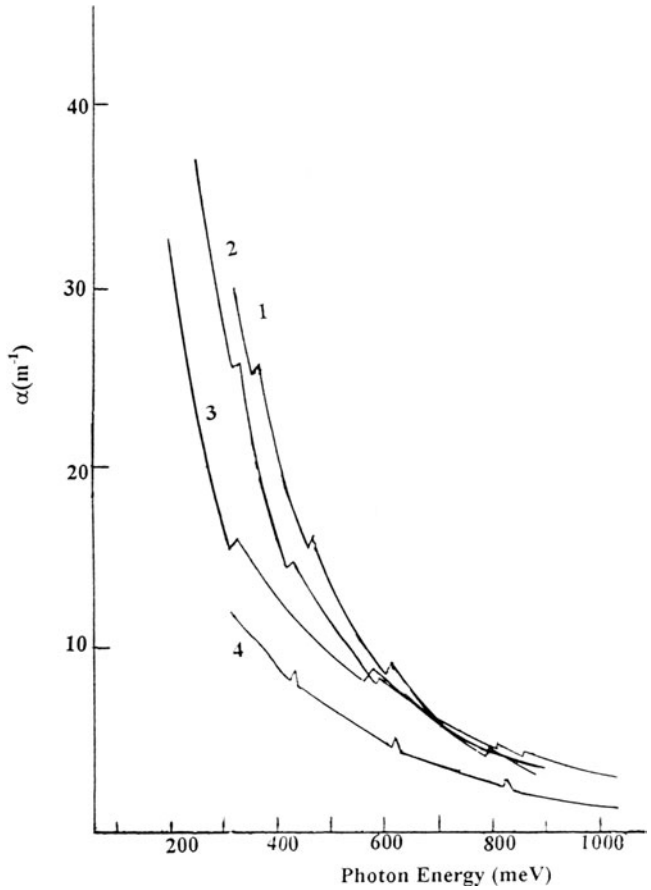

Figure 1. FCA coefficient in a GaAs quantum wire due to boundary roughness scattering as a function of the photon frequency for $T = 300$ K (3). Curves 1 and 4 correspond to the FCA for a GaAs quantum wire when the carriers are scattered by polar optical and acoustic phonons [16]. Curve 2 corresponds 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.

reasonable approximation in the limit of $k_B T \gg \hbar\Omega$ for non-degenerate statistics. In this limit the absorption coefficient of equation (9) can be rewritten as

$$\alpha^{sc} = \frac{3\pi^{11/2} e^2 \hbar^2 n_e \Lambda \Delta^2}{\sqrt{2} c \Omega^2 \in^{1/2} m^{*5/2} W^6 (k_B T)^{1/2}}. \tag{13}$$

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 300 K 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 figures 1–4.

In figure 1, we plot the FCA coefficient α_{BR}^{1D} as a function of the photon energy $\hbar\Omega$. Curves 1 and 4 refer to polar optic and acoustic phonon modes [16] and curves 2 and 3 to alloy disorder

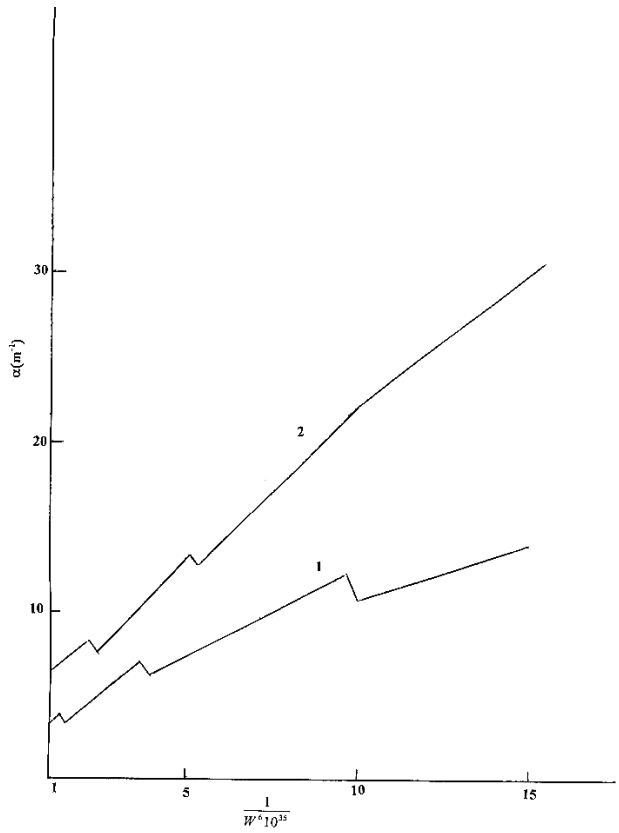

Figure 2. The FCA coefficient is shown as a function of $1/W^6$. Curve 1 is for the wavelength $\lambda = 3\ \mu$m and curve 2 is for $\lambda = 5\ \mu$m.

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 a 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 figure 2, we plot the FCA coefficient α_{alloy}^{1D} in a GaAs quantum wire as a function of the width of the wire. The absorption coefficient shows the oscillatory behaviour 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 the width of the wire 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 present numerical results for a quantum wire. As the wavelength decreases more and more oscillations are observed and the absorption coefficient increases linearly with $\alpha_{BR} \propto 1/W^6$.

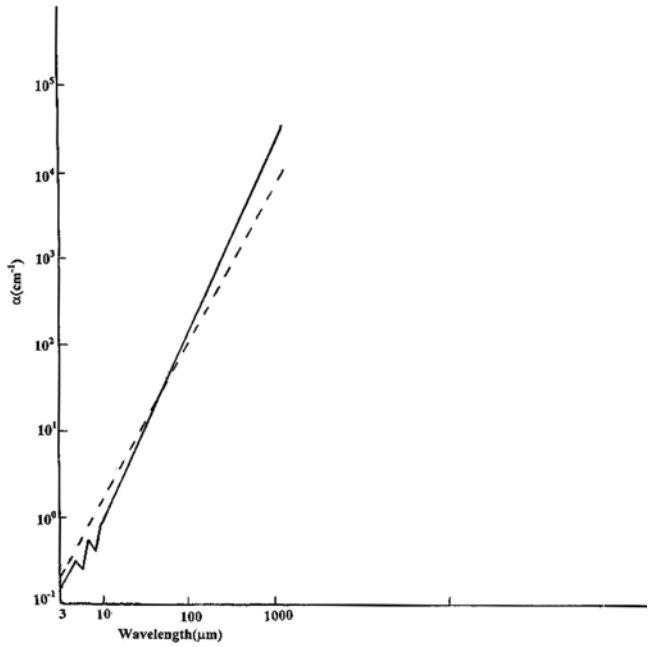

Figure 3. Boundary roughness-assisted quantum (full curve) and semiclassical (dashed curve) FCA coefficients as a function of wavelength in a GaAs quantum wire.

The semiclassical (with a λ^2 wavelength dependence) absorption coefficient (equation (13)) and quantum FCA coefficient (8) in the intermediate wavelength range are plotted in figure 3. The quantum absorption coefficient is seen to converge to the semiclassical value as the wavelength increases beyond 100 μm. For shorter wavelengths, the quantum FCA coefficient is significantly lower than semiclassical result. These results are directly analogous to the distinct regimes in the wavelength dependence of the quasi-two-dimensional [12] and bulk FCA coefficients [29].

In figure 4 we plot the temperature dependence of the ratio $\alpha_{BR}^{1D}/\alpha_{ac}^{1D}$ and $\alpha_{BR}^{1D}/\alpha_{alloy}^{1D}$ for various transverse dimensions of the wire. In these structures, as is well known, the FCA coefficient due to phonon [15, 16] and alloy-disorder scattering [17] increases with decreasing cross-sectional area of the wire. Since the absorption coefficient due to boundary roughness scattering increases with decreasing transverse dimensions of the thin wire as a function of $1/W^6$, we expect boundary roughness scattering to dominate the scattering of the carriers in thinner wires.

With increasing temperature, scattering by boundary roughness and alloy disorder diminishes so the scattering rate should be smaller than that at lower temperatures. Thus, one should expect the FCA coefficient due to boundary roughness and alloy disorder to become much higher as the temperature is lowered.

With decreasing temperature, scattering by phonons diminishes so the scattering rate should be smaller than that at higher temperatures. Therefore the FCA coefficient due to phonons becomes much smaller as the temperature is lowered.

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

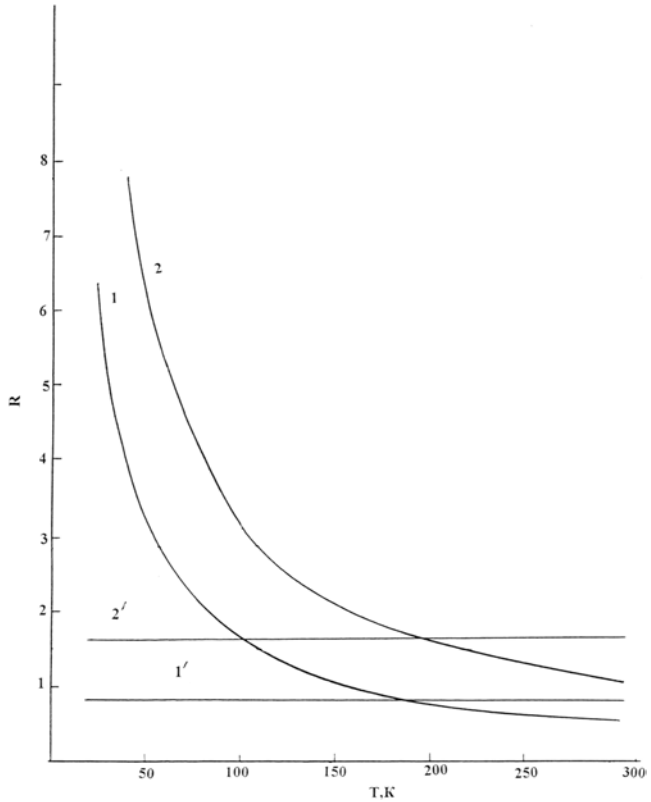

Figure 4. In the quantum limit, the ratio of the FCA coefficient α_{BR} to the $\alpha_{ac}(1,2)$ and $\alpha_{alloy}(1',2')$ FCA coefficient is shown as a function of the temperature for various transverse dimensions of the wire. We have chosen: $1, 1' W = 100$ Å and $2, 2' W = 80$ Å.

on the width of the wire and photon frequency. The oscillatory behaviour is explained in terms of boundary roughness transitions between quantized 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 and temperature 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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