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Free-carrier absorption in semiconducting quantum well wires for alloy-disorder scattering

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Abstract

A theory of free-carrier absorption is given for quasi-one-dimensional ternary semiconducting structures when the carriers are scattered by alloy disorder 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 area of the cross-section of the wire. It is found that the absorption coefficient increases with decreasing transverse dimension of the quantum wire. The results obtained are compared with those from the quantum theory of free-carrier absorption in quasi-two-dimensional structures. In addition, it was found that in quantum wire the electron–alloy-disorder interaction gives a greater contribution to the absorption than the electron–acoustic phonon interaction.

1. Introduction

Recently there has been growing interest in the study of properties of ultrathin semiconducting wires, also called quantum well (QW) wires, with submicron dimensions. Electrons in a semiconductor quantum wire can be viewed as a quasi-one-dimensional (Q1D) electron gas. There are Q1D structures where carriers are confined to move along the length of the wire and the motion is quantized in the transverse directions. The 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 QWs, the free-carrier absorption (FCA) is practically important for determining the optical absorption. In QW structures, apart from the direct interband and intersubband optical transitions, optical absorption can also take place via indirect intrasubband optical transitions in which carriers absorb or emit a photon with the simultaneous scattering of carriers from phonons or other imperfections. 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 claddings.

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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 cladding layers consisting of superlattice injectors [3] can also be significant. Since FCA is one of the most powerful means for understanding the scattering mechanisms of carriers, it has been studied in Q2D structures, theoretically, 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], and electron–electron [13] and alloy-disorder scattering [14]. FCA has been studied theoretically in Q1D structures only (to our knowledge) for the cases where the carriers are scattered by acoustic [15] or acoustic and optical phonons [16]. However, alloy-disorder scattering is an important scattering mechanism when the confining QW consists of ternary semiconductor. Alloy-disorder scattering in ternary compound semiconductors and QW structures has been the subject of many theoretical and experimental investigations [17–28]. In its conventional theory, the constituent pairs of type A and type B atoms are assumed to be distributed randomly within the volume of the crystal.

In this paper we present the theory of FCA for the Q1D electron gas in QW structures of ternary alloys when carriers are scattered by alloy disorder. We consider the FCA for the cases where the radiation field is polarized along the length of the wire. The absorption coefficient will be calculated for the example of $Ga_{0.47}In_{0.53}As$ QW wires. We shall also consider in detail the applicability of the standard semiclassical approximation to these QW wires.

2. Formalism

We consider a QW of an alloy denoted by the symbol $A_{1-x}B_xC$. 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 a and b the cross-sectional dimensions along the x- and y-directions, respectively, and with L the wire length along the z-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

$$\begin{aligned} &E_{knl} = E_k + E_n + E_l = \frac{\hbar^2 k^2}{2m^*} + n^2 E_a^0 + l^2 E_b^0 \\ &E_a^0 = \frac{\pi^2\hbar^2}{2m^* a^2}, \qquad E_b^0 = \frac{\pi^2\hbar^2}{2m^* b^2} \qquad n, l = 1, 2, 3, \ldots \\ &\Psi_{knl} = [2/(abL)^{\frac{1}{2}}] \sin(\pi n x/a) \sin(\pi l y/b) \exp(\mathrm{i}kz). \end{aligned} \tag{1}$$

The FCA coefficient when alloy-disorder scattering is dominant can be related to the scattering rate for free carriers making an intraband transition from a given initial state with the simultaneous scattering of carriers by alloy disorder 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

$$\begin{aligned} \langle k'n'l'|M|knl\rangle = \sum_{k''n''l''} \Bigg[&\frac{\langle k'n'l'|H_R|k''n''l''\rangle\langle k''n''l''|H_{dis}|knl\rangle}{E_{knl} - E_{k''n''l''}} \\ &+ \frac{\langle k'n'l'|H_R|k''n''l''\rangle\langle k''n''l''|H_{dis}|knl\rangle}{E_{knl} - E_{k''n''l''} + \hbar\Omega} \Bigg] \end{aligned} \tag{2}$$

where knl, $k'n'l'$ and $k''n''l''$ are the wavevector and subband indices for the initial, final, and intermediate states, respectively, $\hbar\Omega$ is the photon energy, H_R is the interaction Hamiltonian for the electrons and the radiation field, H_{dis} is the alloy-disorder scattering potential.

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

$$\langle k'n'l'|H_R|knl\rangle = -\frac{e\hbar}{m^*}\left(\frac{2\pi\hbar n_0}{V\Omega\epsilon}\right)^{\frac{1}{2}}(\varepsilon K)\delta_{kk'}\delta_{nn'}\delta_{ll'} \tag{3}$$

when the radiation field is polarized along the wire. Here ϵ 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.

When the confining QW consists of a ternary semiconductor (such as $Ga_{1-x}In_xAs$), in the virtual crystal approximation, alloy-disorder scattering potential has the form [21, 27, 28]

$$H_{dis} = \delta V\left\{(1-x)\sum_{r_{\rm In}} Y_{\Omega_0}(r-r_{\rm In}) - x\sum_{r_{\rm Ga}} Y_{\Omega_0}(r-r_{\rm Ga})\right\}, \tag{4}$$

where $Y_{\Omega_0}(r_a - r_b) = 1/\Omega_0$ when r_a and r_b are inside the same unit cell and vanish elsewhere, and the summations run over all the unit cells; Ω_0 is the volume of the unit cell. Using this form of the potential, the matrix element for transition from a state knl to another state $k'n'l'$ may be expressed as

$$\langle k'n'l'|H_{dis}|knl\rangle = \delta V\left[\frac{\Omega_0}{V}x(1-x)\left(1+\frac{1}{2}\delta_{nn'}\right)\left(1+\frac{1}{2}\delta_{ll'}\right)\right]^{\frac{1}{2}}. \tag{5}$$

From equations (2), (3), and (5), the scattering rate for the electron–alloy-disorder interaction and the electron–photon interaction can be obtained as

$$\begin{aligned} W_{knl,k'n'l'} = {} & \frac{4\pi^2e^2n_0(\delta V)^2\Omega_0x(1-x)}{m^{*2}\Omega^3\epsilon V^2}\sum_{n'l'}\left(1+\frac{1}{2}\delta_{nn'}\right) \\ & \times\left(1+\frac{1}{2}\delta_{ll'}\right)|k'-k|^2\delta(E_{k'n'l'}-E_{knl}-\hbar\Omega). \end{aligned} \tag{6}$$

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

$$\begin{aligned} \alpha^{1D}_{alloy} = {} & \frac{2\pi e^2(\delta V)^2\Omega_0x(1-x)}{\hbar^4\Omega^3\epsilon^{\frac{1}{2}}(ab)^2c}\sum_{nl}\sum_{n'l'}\left(1+\frac{1}{2}\delta_{nn'}\right)\left(1+\frac{1}{2}\delta_{ll'}\right) \\ & \times\iint\frac{(E_{k'}+E_k)}{\sqrt{E_{k'}}\sqrt{E_k}}(f_{knl}-f_{knl})\delta(E_{k'n'l'}-E_{knl}-\hbar\Omega)\,{\rm d}E_{k'}\,{\rm d}E_k. \end{aligned} \tag{7}$$

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

$$\begin{aligned} f_{knl} = {} & \frac{(2\pi)^{\frac{1}{2}}\hbar n_eab}{\gamma\delta(m^*k_BT)^{\frac{1}{2}}}\exp\left[\frac{n^2E_n^0+l^2E_n^0}{k_BT}\right]\exp\left(-\frac{\hbar^2k^2}{2m^*k_BT}\right) \\ \gamma = {} & \sum_n\exp\left(-\frac{n^2E_n^0}{k_BT}\right), \qquad \delta = \sum_l\exp\left(-\frac{l^2E_l^0}{k_BT}\right) \end{aligned} \tag{8}$$

where n_e is the concentration of the electrons. Using equation (8) in (7) we obtain the FCA coefficient in the Q1D structure:

$$\begin{aligned} \alpha^{1D}_{alloy} = {} & \frac{2^{\frac{5}{2}}\pi^{\frac{3}{2}}e^2(\delta V)^2\Omega_0x(1-x)n_e(k_BT)^{\frac{1}{2}}}{c\hbar^3\Omega^3\epsilon^{\frac{1}{2}}abm^{*\frac{3}{2}}\gamma\delta}\left(1-\exp\left(-\frac{\hbar\Omega}{k_BT}\right)\right) \\ & \times\sum_{nl}\sum_{n'l'}(1+\tfrac{1}{2}\delta_{nn'})(1+\tfrac{1}{2}\delta_{ll'}) \end{aligned}$$

where

$$Z = \frac{\hbar\Omega - E_n^0(n'^2 - n^2) - E_l^0(l'^2 - l^2)}{2k_BT} \exp\left[-\frac{n^2E_n^0 + l^2E_l^0}{k_BT}\right] Z\exp(Z)K_1(Z). \tag{9}$$

$K_1(Z)$ is the modified Bessel function of the second kind. This expression can be compared with the following expression for the FCA in a nondegenerate Q1D electron gas when acoustic phonon scattering via the deformation potential dominates [15]:

$$\alpha_{ac}^{1D} = \frac{2^{\frac{7}{2}}\sqrt{\pi}n_e e^2 E_d^2 (k_BT)^{\frac{3}{2}}}{\epsilon^{\frac{1}{2}} c\rho v_s^2 m^{*\frac{1}{2}} ab\gamma\delta} \frac{[1 - \exp(-\frac{\hbar\Omega}{k_BT})]}{(\hbar\Omega)^3} \times \sum_{nl}\sum_{n'l'}\left(1 + \frac{1}{2}\delta_{nn'}\right)\left(1 + \frac{1}{2}\delta l_{ll'}\right) \exp\left[-\frac{n^2E_n^0 + l^2E_l^0}{k_BT}\right] Z\exp(Z)K_1(Z) \tag{10}$$

where ρ is the density of the semiconductor, v_s is the velocity of sound, and E_d is the deformation potential. That the variations of the coefficients with photon frequency Ω are identical may be seen from (9) and (10). The identical nature of variation for the two scattering processes may be explained by examining the matrix elements for scattering. The ratio $\alpha_{alloy}^{1D}/\alpha_{ac}^{1D}$ is

$$\frac{\alpha_{alloy}^{1D}}{\alpha_{ac}^{1D}} = \frac{\pi(\delta V)^2\Omega_0 x(1-x)\rho v_s^2}{2E_d^2 k_BT}. \tag{11}$$

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

It is interesting to note that in the quantum size limit, in the temperature range where the intersubband transitions are not allowed due to the energy differences between the subbands being very large (i.e. $E_a/k_BT > 1$, $E_l/k_BT > 1$, and $E_a > \hbar\Omega$, $E_b > \hbar\Omega$), we can assume $n = n' = l = l' = 1$. The expression for α_{alloy}^{1D} reduces in this case to

$$\alpha_{alloy}^{1D} = \frac{9\pi^{\frac{3}{2}}e^2(\delta V)^2\Omega_0 x(1-x)}{\sqrt{2\epsilon m^* k_BT}abc\hbar^2\Omega^2} \exp\left(\frac{\hbar\Omega}{2k_BT}\right)\left(1 - \exp\left(-\frac{\hbar\Omega}{2k_BT}\right)\right) K_1\left(\frac{\hbar\Omega}{2k_BT}\right). \tag{12}$$

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 reasonable approximation in the limit of $k_BT \gg \hbar\Omega$ for nondegenerate statistics. In this limit the absorption coefficient of equation (12) can be rewritten as

$$\alpha^{sc} = \frac{9\pi^{\frac{3}{2}}e^2(\delta V)^2\Omega_0 x(1-x)n_e}{\sqrt{2\epsilon m^* k_BT}abc\hbar^2\Omega^2}. \tag{13}$$

In this paper, we shall refer to the quantity α^{sc} given by equation (13) as the semiclassical absorption coefficient. It displays the widely assumed quadratic dependence on the wavelength of the light. Then α^{sc} can be expressed in terms of mobility μ:

$$\alpha^{sc} = \frac{4\pi e^3 n_e}{\epsilon^{\frac{1}{2}} m^{*2} c\Omega^2 \mu}. \tag{14}$$

Here we do this using the Q1D electron mobility due to scattering by alloy disorder [26]:

$$\mu = \frac{4\sqrt{2k_BT}eab\hbar^2}{9\sqrt{\pi}m^{*\frac{3}{2}}(\delta V)^2\Omega_0 x(1-x)} \tag{15}$$

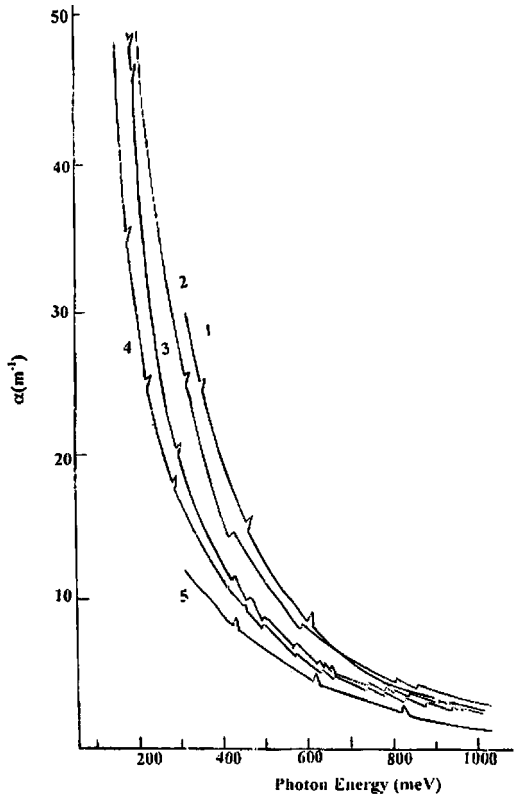

Figure 1. The FCA coefficient in a quantum wire is shown as function of the photon frequency for the case of alloy-disorder scattering for various transverse dimensions of the wire. Curves 1 and 5 correspond to the FCA for GaAs quantum wire when the carriers are scattered by polar optical and acoustic phonons (see [16]) for $a = b = 10^{-6}$ cm. We have chosen: (1) $a = b = 10^{-6}$ cm; (2) $a = 2 \times 10^{-6}$ cm; $b = 10^{-6}$ cm; (3) $a = b = 2 \times 10^{-6}$ cm.

For comparison, in the quantum limit, the FCA in a nondegenerate Q2D electron gas when electron–alloy-disorder scattering is dominant is [14]

$$\alpha_{alloy}^{2D} = \frac{9\pi^2 e^2 \Omega_0 (\delta V)^2 n_e x(1-x) k_B T}{8\epsilon^{\frac{1}{2}} \hbar^4 c d \Omega^3} \left[1 - \exp\left(-\frac{\hbar\Omega}{k_B T}\right)\right]\left(1 + \frac{\hbar\Omega}{2k_B T}\right). \tag{16}$$

Here d is the thickness of the layer. In the quantum limit, the ratio of the FCA in a Q1D system to that in the Q2D system:

$$\frac{\alpha_{alloy}^{1D}}{\alpha_{alloy}^{2D}} = \frac{4\sqrt{2}\mathrm{e}^{\frac{\hbar\Omega}{k_B T}}(1 - \mathrm{e}^{\frac{-\hbar\Omega}{2k_B T}}) K(\frac{\hbar\Omega}{2k_B T}) \hbar^2 \Omega d}{\sqrt{\pi} a b m^{*\frac{1}{2}} (k_B T)^{\frac{3}{2}} (1 - \mathrm{e}^{\frac{\hbar\Omega}{k_B T}})(1 + \frac{\hbar\Omega}{2k_B T})}. \tag{17}$$

This ratio takes a particularly simple form in the limit $(\hbar\Omega / k_B T) \gg 1$:

$$\frac{\alpha_{alloy}^{1D}}{\alpha_{alloy}^{2D}} = \frac{2\sqrt{2}\hbar^{\frac{3}{2}} \rho^{\frac{1}{2}} d}{a b m^{*\frac{1}{2}} (1 + \frac{\hbar\Omega}{2k_B T}) k_B T}. \tag{18}$$

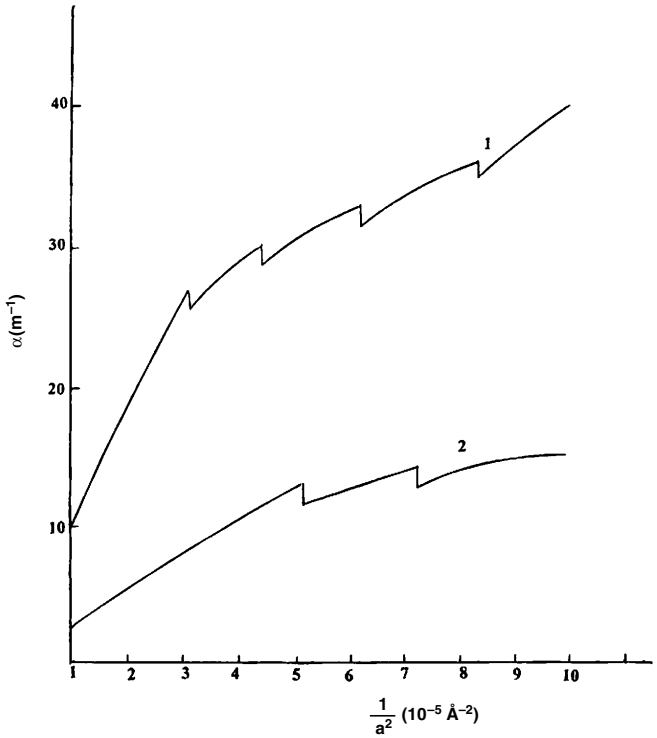

Figure 2. The FCA coefficient is shown as a function of the reciprocal of the cross-section of the QW wire, $1/a^2$, at 300 K. Curve 1 is for the wavelength $\lambda = 5\ \mu$m and curve 2 is for $\lambda = 3\ \mu$m.

3. Results and discussion

We have obtained general expressions for the quantum wires when the carriers are scattered by alloy disorder. The FCA coefficient is expressed as a function of $\hbar\Omega$ and also depends on a, b, and T. We have evaluated, numerically, the above expressions for the FCA coefficient at 300 K and parameters characteristic of $Ga_{0.47}In_{0.53}As$, and the electron concentration $n_e = 10^{17}\,\mathrm{cm}^{-3}$. On the basis of the expressions obtained we have constructed figures 1–3.

In figure 1, we plot the FCA coefficient α^{1D}_{alloy} as a function of the photon energy $\hbar\Omega$. The curves 2, 3, and 4 refer to alloy disorder and curves 1 and 5 to polar optical and acoustic phonon modes [16]. It is shown that α^{1D}_{alloy} decreases monotonically with increasing photon energy. The kinks in the curves indicate alloy-disorder-assisted transitions between the subbands. The enhancement of the absorption coefficient associated with scattering to higher subbands also holds for other scattering mechanisms [15, 16]. It is shown that in quantum wire the electron–alloy-disorder interaction gives a greater contribution to the absorption than the electron–acoustic phonon interaction. It can also be seen that the FCA coefficients due to alloy disorder and to polar optical phonons are of the same order.

In figure 2, we plot the FCA coefficient α^{1D}_{alloy} in a $Ga_{0.47}In_{0.53}As$ quantum wire as a function of the cross-section of the wire. The absorption coefficient shows the oscillatory behaviour as a function of $1/a^2$ whenever the photon energy is such that an alloy-disorder-assisted transition takes place to one of the higher subbands of the QW wire. It is shown that the FCA becomes considerably enhanced as the cross-sectional area of the wire decreases. It was predicted in [26] that the relaxation rate due to alloy-disorder scattering in Q1D structures

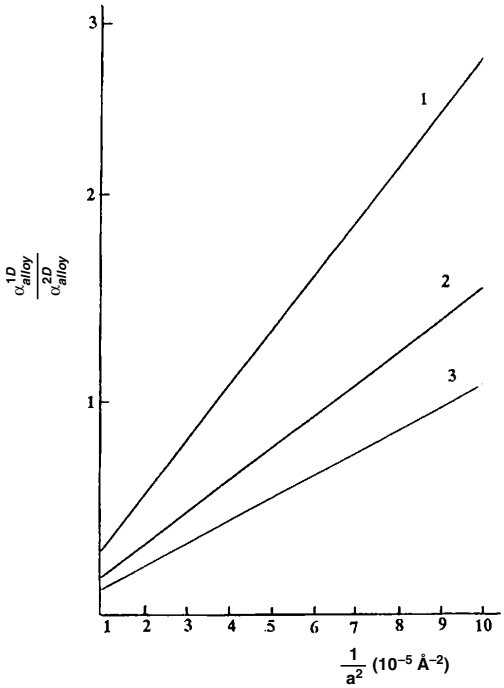

Figure 3. The ratio of the FCA coefficient in QW wire to its value in the Q2D structure is shown as a function of the reciprocal cross-section of the QW wire. Curve 1 is for the wavelength $\lambda = 10\ \mu$m, curve 2 is for the wavelength $\lambda = 5\ \mu$m, curve 3 is for the wavelength $\lambda = 3\ \mu$m.

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 QW structure. As the wavelength decreases, more and more oscillations are observed and the absorption coefficient increases linearly with a^{-2}.

In figure 3 we have plotted $\alpha^{1D}_{alloy}/\alpha^{2D}_{alloy}$ given by equation (18) as a function of the cross-section of the wire. It is shown that $\alpha^{1D}_{alloy}/\alpha^{2D}_{alloy}$ is considerably enhanced as the cross-sectional area of the wire decreases.

In conclusion, we predict that when alloy-disorder 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 cross-section on the wire and it is enhanced over its 2D value by going to wires of decreasing cross-section. The oscillatory behaviour is explained in terms of alloy-disorder transitions between quantized subbands arising from the confinement of electrons in the Q1D semiconducting structure. Similarly, as in Q2D structures, the electron–alloy-disorder 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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