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Free-carrier absorption in semiconducting quantum wells for alloy-disorder scattering

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Abstract

A theory of free-carrier absorption (FCA) is given for quantum well (QW) structures from III–V semiconducting materials when electrons are scattered by alloy disorder. It is found that absorption coefficients due to alloy disorder and to phonons are of the same order. The obtained results are compared with those of the quantum theory of FCA in a bulk semiconductor and it is found that the absorption coefficient decreases with increasing photon frequency and increases with increasing temperature. It is also shown that the absorption coefficient increases with decreasing layer thickness. In addition, it was found that in QW structures the electron–alloy-disorder interaction gives a greater contribution to the absorption than the electron–acoustic and piezoelectric phonon interaction.

1. Introduction

The developments in the molecular beam epitaxy (MBE) and modulation doping technique have produced high-quality heterojunctions and quantum wells (QWs) involving binary and ternary compound semiconductors. An important scattering mechanism in ternaries is the alloy-disorder scattering [1–4]. In ternary structures, free-carrier absorption (FCA) is affected by alloy scattering, which is an intrinsic process arising from the random distribution of the alloy atoms on the available lattice points. Alloy-disorder scattering in QWs and superlattices has been the subject of many theoretical investigations [5–9]. FCA is one of the powerful means to understand the scattering mechanisms of carriers. The theory of FCA in semiconducting QWs was studied considering the absorption assisted by acoustic [10] and polar optical [11–14] phonon scattering including the effects of phonon confinement [15], piezoelectric coupling [16], ionized impurities [17], interface roughness [18] and electron–electron scattering [19].

In this paper we present the theory of FCA for the two-dimensional 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 in the plane of the layer. The absorption

coefficient will be calculated for the examples of InGAs QWs. We shall also consider in detail the applicability of the standard semiclassical approximation to these QW structures.

2. Formalism

2.1. Theory of FCA

We consider a QW of an alloy denoted by the symbol $A_{1-x}B_xC$. Assuming the usual effective-mass approximation for the conduction band, the energy eigenfunctions and eigenvalues for electrons in an infinite QW can be written as

$$E_{k,n} = E_k + E_n = \frac{\hbar^2 k^2}{2m^*} + n^2 E_0, \quad E_0 = \frac{\pi^2 \hbar^2}{2m^* d^2}, \quad n = 1, 2, 3, \dots$$

$$\Psi_{k,n} = \left(\frac{2}{\Omega_0}\right)^{1/2} \exp(i\vec{k}\vec{r}) \sin\left(\frac{n\pi z}{d}\right). \quad (1)$$

Here d is the thickness of the layer, $\vec{k} = \{k_x, k_y\}$ and $\vec{r} = \{x, y\}$ are the wavevector and position vector in the plane of the layer, Ω_0 is the volume of the crystal, n is the number of the subband and z is the coordinate perpendicular to the plane of the layer.

The FCA coefficient when alloy-disorder 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 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 is given by

$$\langle k'n' | M | kn \rangle = \sum_{k''m} \left[\frac{\langle k'n' | H_R | k''m \rangle \langle k''m | V_i | kn \rangle}{E_{nk} - E_{mk''}} + \frac{\langle k'n' | V_i | k''m \rangle \langle k''m | H_R | kn \rangle}{E_{nk} - E_{mk''} + \hbar\Omega} \right] \quad (2)$$

where kn , $k'n'$ and $k''m$ are the wavevector and subband indices 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 and V_i is the alloy-disorder scattering potential.

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

$$\langle k'n' | H_R | kn \rangle = -\frac{e\hbar}{m^*} \left(\frac{2\pi\hbar n_0}{\epsilon\Omega\Omega_0} \right)^{1/2} (\vec{\epsilon}\vec{k}) \delta_{nn'} \delta_{k_x k_x'} \delta_{k_y k_y'}. \quad (3)$$

Here ϵ is the dielectric constant of the material, n_0 is the number of photons in the radiation field and $\vec{\epsilon}$ is the polarization vector of the radiation field.

We consider the virtual-crystal potential to be perfectly periodic as it is composed of the composition-weighted potentials due to the A and B atoms. We assume that the alloy-disorder scattering potential under the virtual-crystal approximation is a spherically symmetric square well of height ΔE and radius r_0 . The potential at site (r_i, z_i) may be expanded in the following two-dimensional Fourier series [7, 8]:

$$V_i(r_i, z_i) = \sum_{q_{\parallel}} 2\pi \Delta E \frac{r_z J_1(r_z q_{\parallel})}{q_{\parallel}} \exp[i\vec{q}_{\parallel}(\vec{r} - \vec{r}_i)] \quad r_z^2 = r_0^2 - (z - z_i)^2 \quad (4)$$

where J_1 is the first-order Bessel function of the first kind. Using this form of the potential, the matrix element for transition from a state kn to another state $k'n'$ may be expressed as

$$\langle k'n' | V_i | kn \rangle = \frac{2}{d} \exp(-iq_{\parallel} r_i) \delta_{k, k'+q_{\parallel}} \Lambda_{nn'}(z_i) \quad (5)$$

where

$$\Lambda_{nn'}(z_i) = \int_{z_i-r_0}^{z_i+r_0} dz 2\pi \Delta E \frac{r_z J_1(r_z q_{11})}{q_{11}} \sin \frac{n\pi z}{d} \sin \frac{n'\pi z}{d}.$$

Now considering all the alloy sites to be randomly distributed in the ratio $x : (1-x)$, one may write for the scattering rate from the initial state to the final state

$$W_{kn,k'n'} = \frac{16\pi^2 e^2 n_0 N_0 x(1-x) |\vec{k}' - \vec{k}|^2}{\epsilon m^* \Omega^3 \Omega_0^2 d} F_{nn'} \delta(E_{n'k'} - E_{nk} - \hbar\Omega) \quad (6)$$

where

$$F_{nn'} = \int_{-d/2}^{d/2} dz_i |\Lambda_{nn'}(z_i)|^2$$

and N_0 is the number of alloy sites per unit volume.

The absorption coefficient is calculated by summing over all occupied initial states and unoccupied final states. The absorption coefficient for a radiation field polarized in the plane of the layer is finally given by

$$\alpha = \frac{4e^2 m^* N_0 x(1-x)}{\pi \hbar^6 d^3 c \epsilon^{1/2} \Omega^3} \sum_{n=1}^{\infty} \sum_{n'=1}^{N_f} \int \int (f_{kn} - f_{k'n'}) F_{nn'}(E_{k'} + E_k) \times \delta(E_{k'n'} - E_{kn} - \hbar\Omega) dE_k dE_{k'}. \quad (7)$$

The integral over final states can be eliminated using the energy-conserving delta function. In order to evaluate $F_{nn'}$, it is assumed that $q_{\parallel} r_z \ll 1$, so that $J_1(x) \approx \frac{x}{2}$, and also that the variations of the sine terms in the range $z_i - r_0 \leq z < z_i + r_0$ are negligible. We may then put $z = z_i$ in the arguments and take the terms outside the integral, thus obtaining a factor $\frac{4}{3} r_0^3$ after integration. The z_i integration is then performed analytically to give

$$F_{nn'} = \left(\frac{4}{3} \pi r_0^3 \Delta E \right)^2 \frac{d}{4} \left(1 + \frac{1}{2} \delta_{nn'} \right).$$

When the distribution function for a quasi-two-dimensional nondegenerate electron gas

$$f_{nk} = \left(\frac{2\pi \hbar^2 n_e d}{m^* k_B T \gamma} \right) \exp\left(-\frac{E_n}{k_B T}\right) \exp\left(-\frac{E_K}{k_B T}\right), \quad \gamma = \sum_n \exp\left(-\frac{E_n}{k_B T}\right) \quad (8)$$

is used in equation (7), we obtain for the FCA coefficient in a QW structure

$$\alpha = \frac{64\pi^2 e^2 r_0^6 (\Delta E)^2 n_e N_0 x(1-x) k_B T}{9\epsilon^{1/2} \hbar^4 d c \Omega^3 \gamma} \sum_{n=1}^{\infty} \sum_{n'=1}^{N_f} \left(1 + \frac{1}{2} \delta_{nn'} \right) e^{-\frac{n^2 E_0}{k_B T}} \times \left[1 + \frac{\hbar\Omega - (n'^2 - n^2) E_0}{2k_B T} \right] \left(1 - \exp\left(-\frac{\hbar\Omega}{k_B T}\right) \right) \quad (9)$$

where N_f is the largest integer equal to or less than $(n^2 + \frac{\hbar\Omega}{E_0})^{\frac{1}{2}}$.

Here n_e is the concentration of the electrons.

For comparison, the FCA in a nondegenerate bulk semiconductor is [3]

$$\alpha_B = \frac{4\sqrt{2} e^2 N_0 x(1-x) V^2 m^{*\frac{1}{2}} n_e (k_B T)^{\frac{1}{2}}}{3\epsilon^{\frac{1}{2}} c \hbar^2 (\hbar\Omega)^2} (1 - e^{-\frac{\hbar\Omega}{k_B T}}) \times e^{\frac{\hbar\Omega}{2k_B T}} x \left\{ \frac{3}{2} W_{-\frac{1}{2}, \frac{3}{2}} \left(\frac{\hbar\Omega}{k_B T} \right) + W_{\frac{1}{2}, \frac{3}{2}} \left(\frac{\hbar\Omega}{k_B T} \right) \right\} \quad (10)$$

where V is the matrix element of the difference between the atomic potentials of the component semiconducting alloys and $W_{\mu, K}(Z)$ is the Whittaker function. In the quantum limit, in which

only the $n_i = 1$ (ground) quantum level is occupied, the ratio of the FCA in a quasi-two-dimensional QW system to that in the bulk

$$\frac{\alpha}{\alpha_B} = \frac{6\sqrt{2}(k_B T)^{\frac{1}{2}}}{\Omega^{\frac{5}{2}} d m^{*\frac{1}{2}}} e^{-\frac{\hbar\Omega}{2k_B T}} \frac{\sum_{n=1}^{N_f} \left(1 + \frac{1}{2}\delta_{1,n}\right) \left(1 + \frac{\hbar\Omega - (n^2-1)E_0}{2k_B T}\right)}{\left\{\frac{3}{2}W_{-\frac{1}{2}, \frac{3}{2}}\left(\frac{\hbar\Omega}{k_B T}\right) + W_{\frac{1}{2}, \frac{3}{2}}\left(\frac{\hbar\Omega}{k_B T}\right)\right\}} \quad (11)$$

where we have used $V^2 = \left(\frac{2}{3}\pi r_0^3 (\Delta E)\right)^2$.

The ratio of the FCA coefficient for a QW structure to that in a bulk semiconductor of the same material, α/α_B given by equation (11), is shown as a function of photon frequency. The FCA coefficient becomes an oscillatory function of both the QW thickness and the photon frequency in QW structure.

2.2. Connection with semiclassical formalism

It is interesting to note that in the quantum size limit, in a temperature range where the inter-subband transitions are not allowed due to the energy differences between the subbands being very large (i.e. $\frac{E_2-E_1}{k_B T} = \frac{3E_0}{k_B T} \gg 1$ and $\frac{E_2-E_1}{\hbar\Omega} = \frac{3E_0}{\hbar\Omega} \gg 1$) we can assume $n = n' = 1$. The expression for α reduces in this case to

$$\alpha = \frac{32\pi^2 e^2 r_0^6 (\Delta E)^2 n_e N_0 x (1-x) k_B T}{3\epsilon^{\frac{1}{2}} \hbar^4 c d \Omega^3} \left(1 - e^{-\frac{\hbar\Omega}{k_B T}}\right) \left(1 + \frac{\hbar\Omega}{2k_B T}\right). \quad (12)$$

In the limit of very long wavelengths, the absorption coefficient is known to reduce to the semiclassical form [20], which scales as λ^2 . The semiclassical expression becomes a reasonable approximation in the limit of $k_B T \gg \hbar\Omega$ for nondegenerate statistics. In this limit the absorption coefficient of equation (12) can be rewritten:

$$\alpha^{sc} = \frac{32\pi^2 e^2 r_0^6 (\Delta E)^2 n_e N_0 x (1-x)}{3\epsilon^{\frac{1}{2}} \hbar^3 c d \Omega^2}. \quad (13)$$

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 :

$$\alpha^{sc} = \frac{e^3 n_e}{\epsilon^{1/2} c d^2 m^{*2} \Omega^2 \mu}. \quad (14)$$

Here we do this using the quasi-two-dimensional electron mobility due to scattering by alloy disorder [6, 8]

$$\mu = \frac{3e\hbar^3}{32(\pi m^* r_0^3 \Delta E)^2 N_0 dx (1-x)}. \quad (15)$$

3. Results and discussion

We have obtained general expressions for the FCA coefficients for QWs when the carriers are scattered by alloy disorder. The FCA coefficient is expressed as a function of $\hbar\Omega$ and also depends on d and T . On the basis of expressions obtained we have constructed figures 1–3. As a numerical example, we consider the FCA in GaInAs and GaAlAs QWs for alloy-disorder scattering. The relevant values of physical parameters are taken to be [7] $\Delta E = 0.53$ eV, $r_0 = \sqrt{3}a/4$ and $N_0 = 4/a^3$, where a is the lattice constant.

In figure 1, we plot the FCA coefficient α as a function of the photon frequency Ω in Ga_{0.9}Al_{0.1}As QWs for $n_e = 10^{17}$ cm⁻³ at $T = 300$ K. Curve 3 refers to alloy disorder and curves 1 and 2 to confined and bulk phonon modes [15]. The frequency range is chosen such

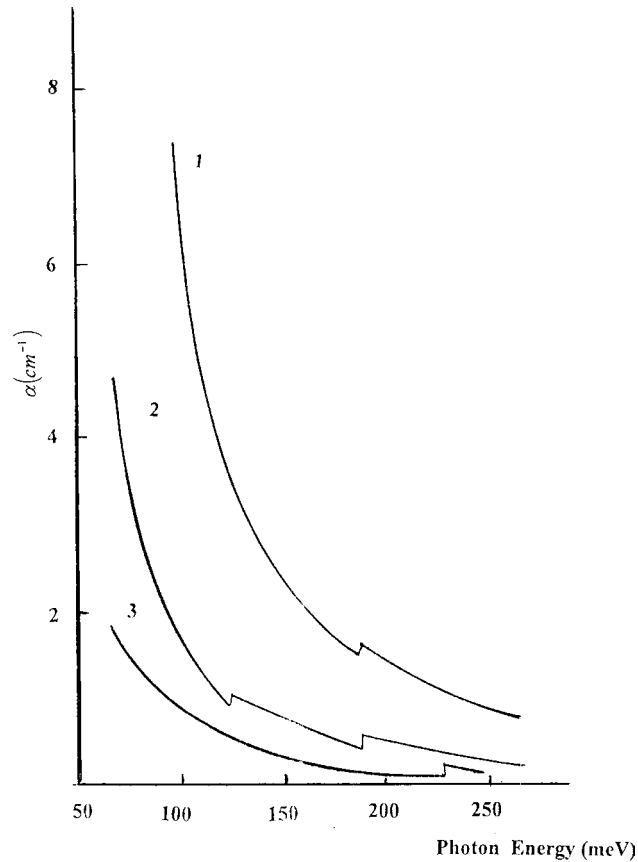


Figure 1. FCA coefficient in a $\text{Ga}_{0.9}\text{Al}_{0.1}\text{As}$ QW due to alloy-disorder scattering as a function of the photon frequency for $T = 300\text{ K}$ (3). Curves 1 and 2 correspond to the FCA for GaAs/GaAlAs QWs when the carriers are scattered by confined and bulk phonons (see [15]), respectively. In the three cases the bulk density of electrons is the same, $n_e = 10^{17}\text{ cm}^{-3}$, and $d = 10\text{ nm}$.

that only the two lowest subbands are involved in the transitions. It is shown that α decreases monotonically with increasing photon frequency. It can also be seen that FCA coefficients due to alloy disorder and to bulk and confined LO phonons are of the same order.

In figure 2, we plot the FCA coefficient α in a GaInAs QW with $d = 10\text{ nm}$ as a function of the photon frequency for various temperatures. It is shown that α decreases monotonically with increasing photon frequency and increases with increasing temperature. The kinks in the curves indicate alloy-disorder-assisted transition between the subbands. The enhancement of the absorption coefficient associated with scattering to higher subbands also holds for other scattering mechanisms [10–14]. Curve 1 refers to alloy disorder and curves 2 and 3 to piezoelectric and acoustic phonons scattering respectively. It is shown that in QW structures the electron–alloy-disorder scattering contribution to the absorption still dominates over that due to the electron–acoustic and piezoelectric phonon scattering contribution.

The ratio of the FCA coefficient for a QW structure to that in a bulk semiconductor of the same material, α/α_β , given by equation (11), is shown as a function of photon frequency for various thickness QWs in figure 3. As in figure 1 the inflection points correspond to the connection of new intersubband transitions. Figure 3 shows the FCA coefficient is enhanced

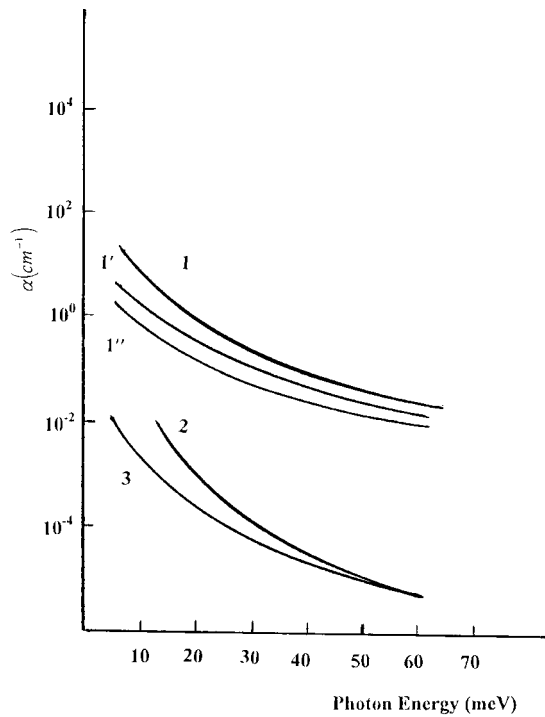


Figure 2. The FCA coefficient in a $\text{Ga}_{0.47}\text{In}_{0.53}\text{As}$ QW structure for alloy-disorder scattering as a function of the photon frequency for $d = 10$ nm. We have chosen $T = 300$ K (1), $T = 77$ K (1') and $T = 20$ K (1''). Curves 2 and 3 (see [16]) correspond to the FCA GaAs films when the carriers are scattered by piezoelectric and acoustic phonons respectively. In the three cases the bulk density of electrons is the same, $n_e = 1.73 \times 10^{15} \text{ cm}^{-3}$.

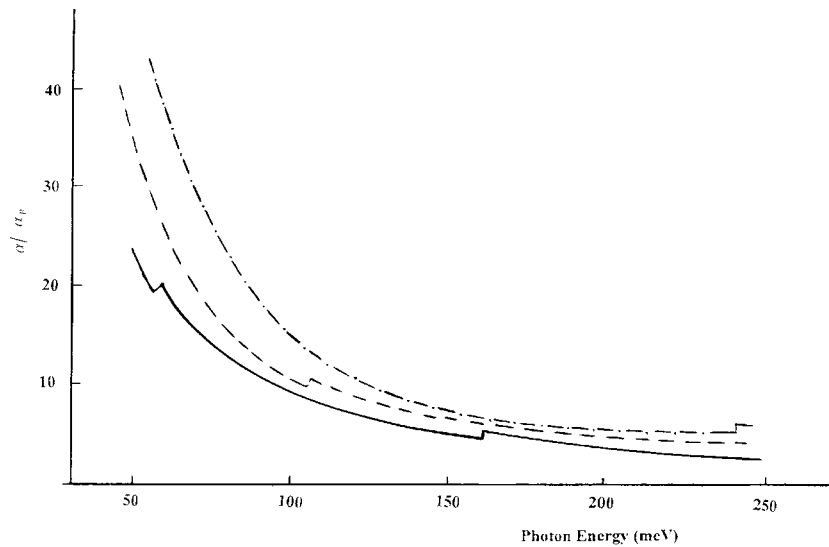


Figure 3. The ratio of the FCA in a quasi-two-dimensional QW structure to its value in the bulk shown as a function of photon frequency for alloy-disorder scattering for various thicknesses of QW using the parameters characteristic of $\text{Ga}_{0.47}\text{In}_{0.53}\text{As}$. We have chosen $d = 10$ nm (— · —), 15 nm (---) and 20 nm (—).

as the QW thickness decreases. Also, as the QW thickness decreases, the location of the first inflection point in the absorption is shifted to higher photon frequencies. As the thickness of the QW decreases the separation between adjacent subbands increases, and when $\hbar\Omega < 3E_0$ the alloy-disorder-assisted transitions can only take place to states in the same subband. For thickness QW such that $\hbar\Omega < 3E_0$, the absorption process depends just upon the rate at which the free carriers are scattered by the alloy disorder. It was predicted in [21, 22] that the relaxation rate due to alloy-disorder scattering in QW structures increases with decrease of QW thickness. This increase in the scattering rate explains the increase in the FCA coefficient predicted in our present numerical results for a QW structure. Also, because of the increase in E_0 with decreasing QW thickness, the threshold at which an alloy-disorder-assisted transition can take place to the first excited subband will be shifted to higher frequency as the QW thickness decreases.

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