Turk J Phys
26 (2002) , 369 – 374.

Free-Carrier Absorption in Quantum Well Structures for Alloy-Disorder Scattering

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Received 11.10.2001

Abstract

A free-carrier absorption theory is given for quantum wells structures in III-V semiconducting materials, for the case when the carriers a scattered by alloy-disorder. It is found that absorption coefficients due to alloy-disorder and to phonons are of the same order. Results are shown 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. We also found that absorption in quantum wells structures is enhanced by going to quantum wells of smaller thickness over its value in the bulk III-V semiconducting materials.

1. Introduction

Developments in molecular beam epitaxy and modulation doping technique have made it possible to produce high quality heterojunctions and quantum wells involving binary and ternary compound semiconductors. However, among the thing that have yet to be fully understood are the varous scattering mechanisms, important among which, in ternaries, is alloy-disorder scattering [1-4]. Alloy-disorder scattering in quantum wells (QWs) and superlattice system has been the subject of many theoretical investigation [5-9]. Free–carries absorption (FCA) is one of the powerful means to understand the scattering mechanisms of carriers. The theory of FCA in semiconducting QWs has been studied via 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 in QWs 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. Absorption coefficient will be calculated for the examples of InGAs QWs.

2. Formalism

Assuming the usual effective mass approximation for conduction band, the energy eigenfunctions and eigenvalues for electrons in an infinite QW can be written as

$$E_{k,n} = E_k + E_n = \frac{\hbar^2 k^2}{2m*} + n^2 E^0, \quad E_0 = \frac{\pi^2 \hbar^2}{2m*d^2}\ ,\ n = 1, 2, 3, ...$$

$$\Psi_{k,n} = \left(\frac{2}{\Omega}\right)^{1/2} \exp\left(i\,\overrightarrow{k}\,\overrightarrow{r}\right) \sin\left(\frac{n\pi z}{d}\right) \tag{1}$$

Here, d is the thickness of the layer, $\overrightarrow{k} = \{k_x, k_y\}$ and $\overrightarrow{r} = \{x, y\}$are wave vector and position vector in the plane of the layer, Ω_0 is the volume of the crystal, n is the subband number 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 pertubation theory, the matrix element connecting the initial and final states for an optical transition in a QW is given by

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

where $k'n'$ and $k''m$ are wave vector and subband index for initial and intermediate state, respectively, $\hbar\Omega$ is the photon energy, H_R is the interaction Hamiltonian between the electrons and the radiation field V_i is the alloy-disorder scattering potential.

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

$$< k'n'|H_R|kn >= -\frac{e\hbar}{m*} \left(\frac{2\pi\hbar n_0}{\in \Omega\Omega_0} \right)^{1/2} \left(\overrightarrow{\varepsilon}\overrightarrow{K} \right) \delta_{nn'}\delta_{k_x k_x}\delta_{k_y k_{y'}}. \quad (3)$$

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

We assume that the alloy-disorder scattering potential under 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]:

$$\begin{aligned} &V_i\left(r_i, z_i\right) = \sum_{q_{11}} 2\pi\Delta E \frac{r_z J_1(r_z q_{11})}{q_{11}} \exp\left[i\overrightarrow{q}_{11}\left(\overrightarrow{r} - \overrightarrow{r}_i\right)\right], \\ &r_z^2 = r_0^2 - \left(z - z_i\right)^2 \end{aligned} \quad (4)$$

where J_1 is the Bessel function of first order 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

$$< k'n'|V_i|kn >= \frac{2}{d} \exp\left(-iq_{II}r_i\right) \delta_{k,k'+q_{II}}\ \Lambda nn'\left(z_i\right), \quad (5)$$

where

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

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

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

where $F_{nn'} = \int_{-d/2}^{d/2} dz_i \left|\Lambda_{nn'}\left(z_i\right)\right|^2$, 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 radiation field polarized in the plane of the layer is finally given by

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

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

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

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

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

used in E_g.(7), we obtain the following for the FCA coefficient in the QW structure:

$$\begin{aligned} \alpha = \quad & \frac{64\pi^2 e^2 r_0^6 \left(\Delta \mathrm{E}\right)^2 n_e N_0 x\,(1-x)\, K_B T}{9 \in^{1/2} \hbar^4 d c \Omega^3 \gamma} \sum_{n=1}^{\infty} \sum_{n'=1}^{N_f} \left(1 + \frac{1}{2}\delta nn'\right) \\ & e^{-\frac{n^2 E_0}{K_B T}} \left[1 + \frac{\hbar\Omega - \left(n'^2 - n^2\right) E_0}{2 K_B T}\right] \left(1 - \exp\left(-\frac{\hbar\Omega}{K_B T}\right)\right) \end{aligned} \quad (9)$$

where N_f is the largest integer equal to or less than $\left(n^2 + \frac{\hbar\Omega}{E_0}\right)^{\frac{1}{2}}$. Here, n_e is the carrier density per unit volume.

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. $\frac{E_2 - E_1}{K_B T} = \frac{3E_0}{K_B T} >> 1$and $\frac{E_2 - E_1}{\hbar\Omega} = \frac{3E_0}{\hbar\Omega} >> 1$) we can assume $n = n' = 1$. The expression for α in this case to then reduces to

$$\alpha = \frac{32\ \pi^2 e^2 r_0^6 \left(\Delta E\right)^2 n_e N_0 x\,(1-x)\ K_B T}{3 \in^{\frac{1}{2}} \hbar^4 c d \Omega^3} \left(1 - e^{-\frac{\hbar\Omega}{K_B T}}\right) \left(1 + \frac{\hbar\Omega}{2 K_B T}\right). \quad (10)$$

For comparison, the FCA in a nondegenerate bulk semiconductor when electron-alloy-disorder scattering is dominant, is [20]

$$\alpha_{bulk} = \frac{32\sqrt{2}\pi^{1/2} m^{*1/2} n_e r_0^6 \left(\Delta \mathrm{E}\right)^2 \mathrm{N}_0 x\,(1-x)}{27\hbar^3 \left(k_B T\right)^{1/2} c\Omega \in^{1/2}} \sinh\left(\hbar\Omega / 2K_B T\right) K_2\left(\hbar\Omega / 2K_B T\right) \quad (11)$$

In the limit $\hbar\Omega$¿¿$\mathrm{K_B T}$ the ratio of the FCA in QW to that in the bulk for electron-alloy-disorder scattering takes the particularly simple form

$$\frac{\alpha}{\alpha_{bulk}} = \frac{9\pi\hbar^{1/2}}{\sqrt{2} d \Omega^{1/2} m^{*1/2}}. \quad (12)$$

3. Results and Discussion

We have evaluated, the above expressions for α at 300K in $In_{0.53}Ga_{047}As$-InP QW_s using the following parameters [7]: d=10 nm; m*=0.042m$_0$; ΔE=0.53eV; $r_0 = \sqrt{3}a/4$; $N_0 = 4/a^3$; *a=0.587nm* with α the lattice constant, and $n_e = 10^{17}cm^{-3}$

The results are presented in Figure 1 as a function of photon frequency. Curve 2 refers to the alloy disorder and curves 1 and 3 refer to confined and bulk phonon modes [15]. The frequency range is chosen such that the 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 the FCA coefficients are of the same order due to alloy-disorder and phonons.

In Figure 2 , we plot the FCA coefficient α in InGaAs QW with $d = 10$ 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

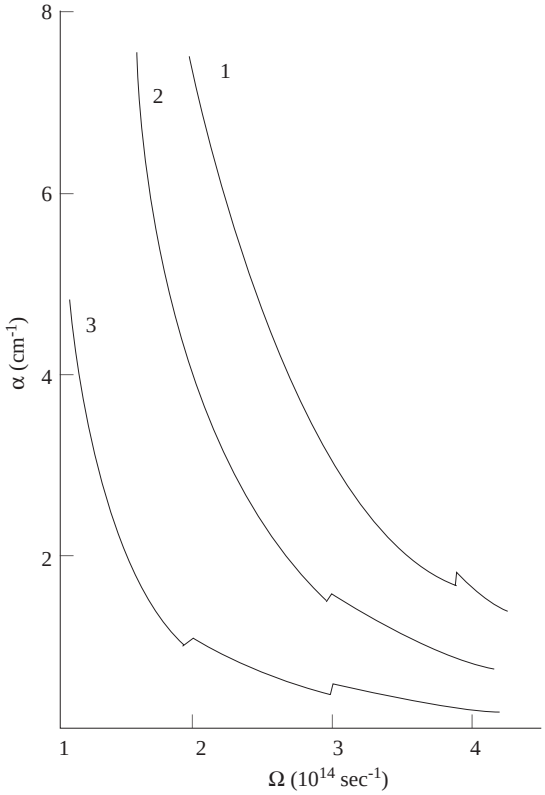

Figure 1. FCA coefficient in InGaAs QW due to alloy disorder scattering as a function of the photon frequency for T=300 K (2). Curves 1 and 3 correspond to the FCA for GaAs/GaAlAs QWs when the carrier are scattered by confined and bulk phonons (Ref. [15]), respectively.

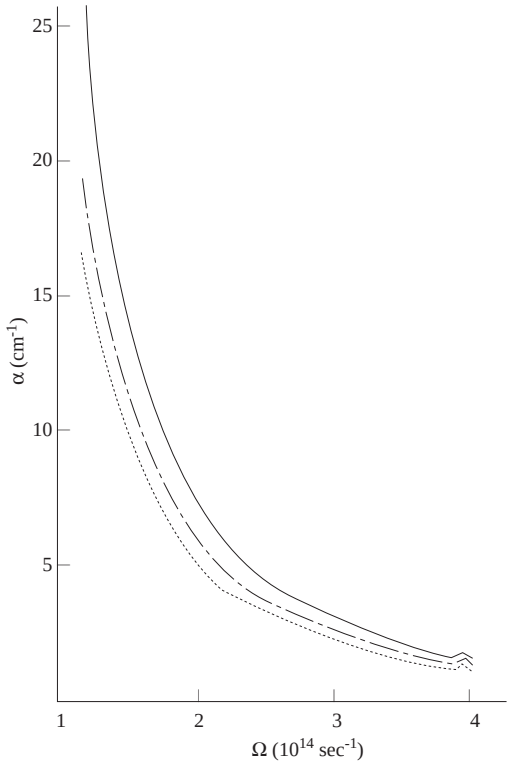

Figure 2. The FCA coefficient in InGaAs QW structure for alloy-disorder scattering as a function of the photon frequency d=10 nm. We have chosen T=300 K (—), T=77 K (- · - · -) and T=20 K (- - -).

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].

In Figure 3, we plot the FCA coefficient α as a function of the photon frequency in InGaAs QW with the temperature at T=300 K. As in Figure 3 the inflection points correspond to the connection of new intersubband transitions. From Figure 3 we see that the FCA coefficient is enhanced as the QW thickness decreases. Also, as the QW thickness decreases, the location of the first 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-carrier are scattered by the alloy-disorder.

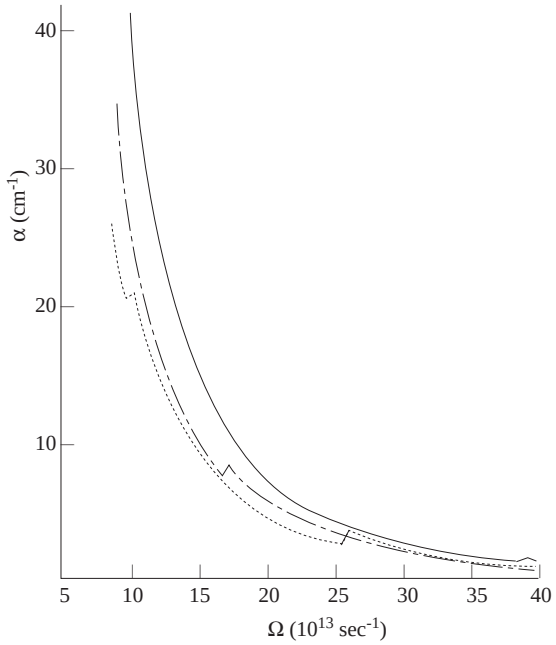

Figure 3. The FCA coefficient in InGaAs QW structure for alloy-disorder scattering as a function of the photon frequency with T=300 K. We have chosen d=10 nm (—-) , 15 nm (- · - · -) and 20 nm (- - -).

We have evaluated, numerically, the Expression (12) and found that FCA in QW structures is enhanced by going to QWs of smaller thickness over its value in the bulk semiconducting materials.

4. Acknowledgement

The author would like to thank Prof. M. I. Aliev and Prof. F. M. Gashimzade for helpful discussions.

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