FREE-CARRIED ABSORPTION IN QUANTUM WELL STRUCTURES FOR ALLOY-DISORDER SCATTERING

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A theory of free-carrier absorption is given for quantum well structures from III – V semiconducting materials when carriers are scattered by alloy-disorder. It is found that the absorption coefficients due to alloy-disorder and to phonons are of the same order. The results show that the absorption coefficient decreases with increasing the photon frequency and increases with temperature. It is also shown that the absorption coefficient increases with decreasing the layer thickness.

Introduction

The developments in the molecular beam epitaxy and modulation doping technique have produced high quality heterojunctions and quantum wells involving binary and ternary compound semiconductors. An important scattering mechanism in ternaries is the alloy-desorder scattering [1 – 4]. Alloy-disorder scattering in quantum wells (QWs) and a superlattice has been the subject of many theoretical investigations [5 – 9]. Free-carrier absorption (FCA) is one of the powerful means to understand the scattering mechanisms of carriers. The theory of FCA in a semiconducting QW was studied considering the case where absorption is assisted by acoustic [10] and polar optical [11 – 14] phonon scatterings 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 a layer. The absorption coefficient will be calculated for InGaAs QWs.

Formalism

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

$$E_{k,n} = E_k + E_n = \frac{\hbar^2 k^2}{2m^*} + n^2 E^2,$$

$$E_0 = \frac{\pi^2 \hbar^2}{2m^* d^2},\ n = 1, 2, 3,\ldots,$$

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

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

When the alloy-disorder scattering is dominant, the FCA coefficient 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

$$\langle k'n' \mid M \mid kn \rangle =$$

$$= \sum_{k'' m} \left[\frac{\langle k'n' \mid H_R \mid k'' m \rangle \langle k'' m \mid V_i \mid kn \rangle}{E_{nk} - E_{mk''}} + \right.$$

$$\left. + \frac{\langle k'n' \mid V_i \mid k'' m \rangle \langle k'' m \mid H_R \mid kn \rangle}{E_{nk} - E_{mk''} + \hbar\Omega} \right], \quad (2)$$

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

The matrix elements of the electron-photon interaction Hamiltonian are

$$\langle k'n' \mid H_R \mid kn \rangle =$$

$$= -\frac{e\hbar}{m^*} \left(\frac{2\pi\hbar n_0}{\hat{U}\Omega\,\Omega_0}\right)^{1/2} (\vec{\varepsilon}\vec{k})\, \delta nn'\, \delta k_x k_x\, \delta k_y k_y . \quad (3)$$

Here, $\hat{U}$ is the dielectric constant of the material, n_0 is the number of photons in the radiation field, $\vec{\varepsilon}$ is the polarization vector of the radiation field.

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 the site (r_i, z_i) may be expanded in the following two-dimensional Fourier series [7, 8]:

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

$$r_z^2 = r_0^2 - (z - z_i)^2, \tag{4}$$

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

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

where

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

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

$$W_{kn, k'n'} = \frac{16\pi^2 e^2 n_0 N_0 x (1-x) |\vec{k}' - \vec{k}|^2}{\hat{U} m^{*2} \Omega^3 \Omega_0^2 d} \times$$

$$\times F_{nn'} \delta(E_{n'k'} - E_{nk} - \hbar\Omega), \tag{6}$$

where $F_{nn'} = \int_{-d/2}^{d/2} dz_i |\Lambda_{nn'}(z_i)|^2$. N_0 is the number of alloy sites per unit volume.

The absorption coefficient is calculated by summing over all ocupied initial states and unoccupied final states. The coefficient FCA for a quasi-two-dimensional electron gas for the radiation field polarized in the plane of the layer is finally given by

$$\alpha = \frac{4e^2 m^* N_0 x (1-x)}{\pi \hbar^6 d^3 c \hat{U}^{1/2} \Omega^3} \sum_{n=1}^{\infty} \sum_{n'=1}^{N_f} \int\int (f_{kn} - f_{k'n'}) \times$$

$$\times F_{nn'}(E_{k'} + E_k) \delta(E_{k'n'} - E_{kn} - \hbar\Omega)\, dE_k\, dE_{k'}. \tag{7}$$

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

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

$$\gamma = \sum_n \exp\left(-\frac{E_n}{K_B T}\right), \tag{8}$$

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

$$\alpha = \frac{64\pi^2 e^2 r_0^6 (\Delta E)^2 n_e N_0 x (1-x) K_B T}{9\hat{U}^{1/2} \hbar^4 dc \Omega^3 \gamma} \times$$

$$\times \sum_{n=1}^{\infty} \sum_{n'=1}^{N_f} (1 + \frac{1}{2}\delta nn') \exp\left(-\frac{n^2 E_0}{K_B T}\right) \times$$

$$\times \left[1 + \frac{\hbar\Omega - (n'^2 - n^2) E_0}{2K_B T}\right]\left(1 - \exp\left(-\frac{\hbar\Omega}{K_B T}\right)\right), \tag{9}$$

where N_f is the largest integer equal to or less than $\left(n^2 + \frac{\hbar\Omega}{E_0}\right)^{1/2}$. Here, n_e is the concentration of electrons.

It is interesting to note that, in the quantum size limit and 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 $\frac{E_2 - E_1}{\hbar\Omega} = \frac{3E_0}{\hbar\Omega} \gg 1$),

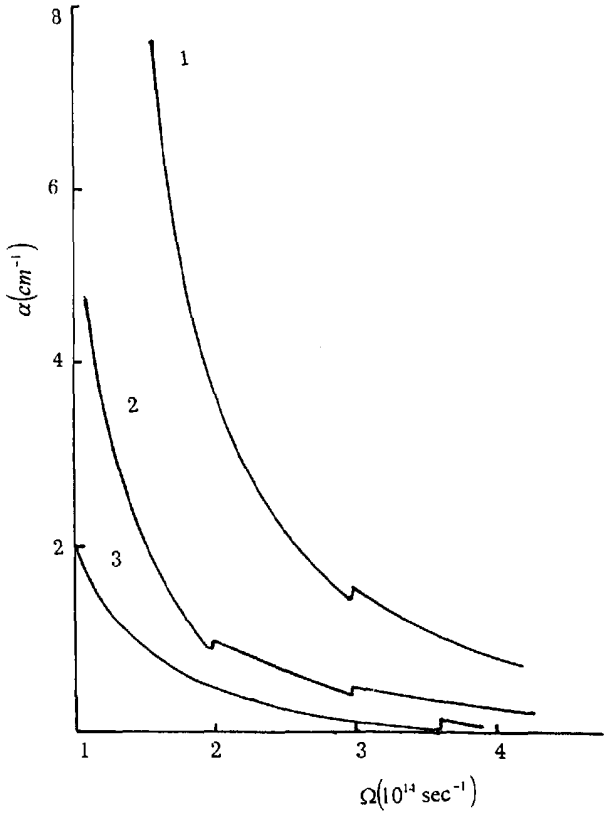

Fig. 1. FCA coefficient in GaAlAs QW due to alloy disorder scattering as a function of the photon frequency for $T = 300$ K (*3*). Curves *1* and *2* correspond to the FCA for GaAs/GaAlAs Qws when carriers are scattered by confined and bulk phonons [15], respectively. In all three cases, the bulk density of electrons is the same, $n_e = 10^{17}$ cm^{-3}

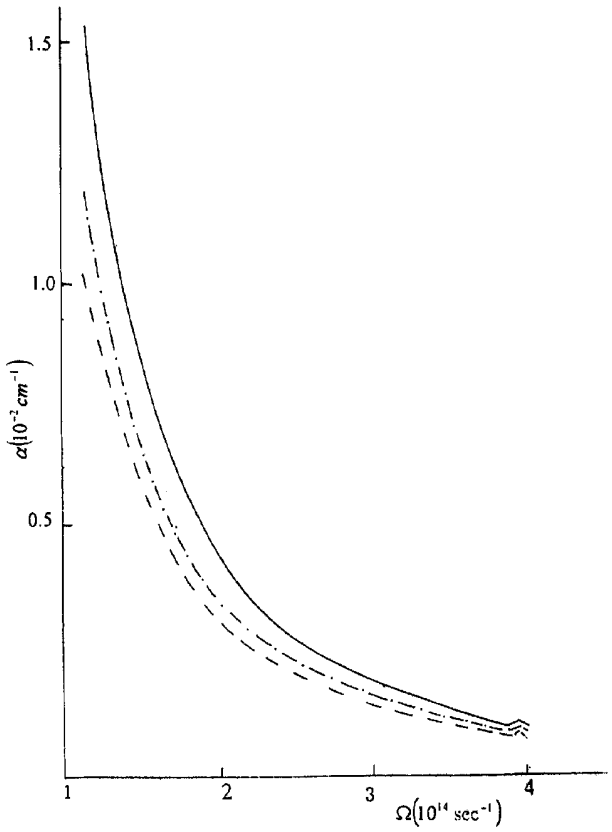

Fig. 2. FCA coefficient in the $Ga_{0.47}$ $In_{0.53}As$ QW structure for alloy-disorder scattering as a function of the photon frequency; $d = 10$ nm. We have chosen $T = 300$ K (solid curve), $T = 77$ K (dash-dotted) and $T = 20$ K (dashed). In all three cases, the bulk density of electrons is the same, $n_e = 10^{15}$ cm^{-3}

we can assume $n = n' = 1$. In this case, the expression for α reduces to

$$\alpha = \frac{32\,\pi^2 e^2 r_0^6 (\Delta E)^2 n_e N_0 x (1-x) K_B T}{3\,\hat{U}^{1/2} \hbar^4 cd\,\Omega^3} \times$$

$$\left(1 - \exp\left(-\frac{\hbar\Omega}{K_B T}\right)\right)\left(1 + \frac{\hbar\Omega}{K_B T}\right). \qquad (10)$$

Results and Discussion

We have obtained the 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 the expressions obtained, we have constructed Figs. 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, $r_0 = \sqrt{3}\,a/4$; $N_0 = 4/a^3$; where a is the lattice constant.

In Fig. 1, we plot the FCA coefficient α as a function of the photon frequency Ω in GaAlAs QWs for $n_e = 10^{17}$ cm^{-3} at $T = 300$ K. Curve *3* refers to alloy-disorder and curves *1* and *2* to the confined and bulk phonon modes [15]. The frequency range is chosen to be such that only two lowest subbands are involved in transitions. It is shown that α decreases monotonically with increasing the photon frequency. It can also be seen that the FCA coefficients due to alloy-disorder and to bulk and confined LO phonons are of the same order.

In Fig. 2, we plot the FCA coefficient α in GaInAs QW with $d = 10$ nm as a function of the photon frequency for various temperatures. It is shown that α decreases monotonically with increasing the photon frequency and increases with temperature. The kinks in the curves indicate the alloy-disorder-assisted transition between subbands. The enhancement of the

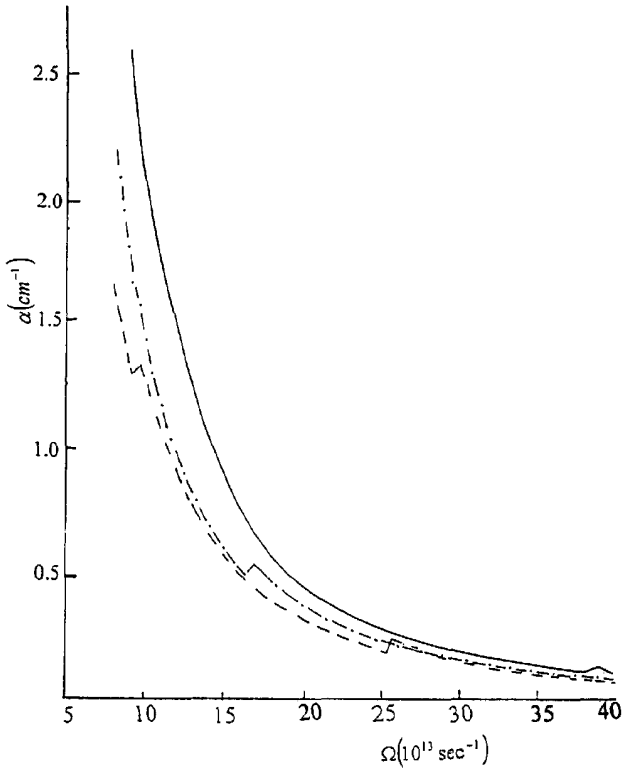

Fig. 3. FCA coefficient in the $Ga_{0.47}$ $In_{0.53}As$ QW structure for alloy-disorder scattering as a function of the photon frequency with $T = 300$ K. We have chosen $d = 10$ nm (solid curve), 15 (dash-dotted) and 20 (dashed). In all three cases, the bulk density of electrons is the same, $n_e = 10^{17}$ cm^{-3}

absorption coefficient associated with scattering to higher subbands also holds for other scattering mechanisms [10 – 14].

In Fig. 3, we plot the FCA coefficient α as a function of the photon frequency in InGaAs QW with the temperature $T = 300$ K. As in Fig. 3, the inflection points correspond to the connection of new intersubband transitions. Fig. 3 shows that the FCA coefficient increases 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 QW thickness 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 a QW thickness such that $\hbar\Omega < 3E_0$, the absorption process depends just upon the rate, at which the free-carriers are scattered by alloy-disorder. It was predicted in [20,21] that the relaxation rate due to alloy-disorder scattering in QW structures increases with decrease of the 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 the QW thickness, the threshold, at which the alloy-disorder-assisted transition can take place to the first excited subband, will be shifted to higher frequencies as the QW thickness decreases.

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