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Confined LO phonon limited free carrier absorption in quantum well wires

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Abstract. The theory of free-carrier absorption is given for quantum well wire for the case where the carriers are scattered by confined longitudinal-optical (LO) phonons and the radiation field is polarized along the length of the wire. Both the multisubband structure and confined phonon modes are considered together. The free carrier absorption coefficients are calculated taking into account all possible LO phonon modes as well as all possible electron intersubband transitions. The results show that the absorption coefficient decreases with increasing the photon frequency and decreases with temperature. It was found that in quantum wire the electron-optic phonon interaction give a greater contribution to the absorption than the electron-confined LO phonon interaction. The results are interpreted in terms of confined LO phonons-assisted transitions between size quantized subbands.

Keywords: quantum well wires, confined longitudinal-optical, free-carrier absorption.

1. Introduction

With the developments in epitaxial techniques, it is possible to fabricate quasi-one-dimensional (Q1D) semiconductor quantum well wires (QWWs) of various geometries. The motion of electrons in such semiconducting structures is confined and leads to size quantization effects which play an important role in determining their optical and electronic properties. Owing to the limited number of available final states during a scattering process, these structures will exhibit high mobilities [1] and are potentially important for high-speed device applications. Scattering mechanisms due to various processes have been studied theoretically and experimentally [2-8].

Free-carrier absorption (FCA) [9-12], which occurs concurrently with intersubband absorption, greatly distorts the absorption spectra, especially in the long-wavelength regions [13], since the free-carrier absorption coefficients are proportional to the carrier density and, roughly, to the square of the wavelength of the involved photons. Moreover, the FCA effect often hides the peak position of intersubband absorption spectra, which means the peak absorption wavelength (transition energy of the intersubband absorption) cannot be obtained solely from experi-mental absorption spectra [10, 13]. Therefore, to design a practical infrared detector with a specific peak absorption wavelength, it is necessary to distinguish between intersubband absorption and free-carrier absorption.

FCA is also very important in certain other devices, especially in long-wavelength semiconductor lasers. In semiconductor lasers, the refractive index change includes an anomalous dispersion component and the free-carrier component due to the plasma effect (free-carrier absorption) [14]. Therefore, the FCA can give rise to a change in carrier-induced refractive index, which affects the characteristics of semiconductor lasers (particularly long-wavelength lasers), such as spectral linewidth and wavelength chirping [14]. It has been reported that FCA in the case of quantum well lasers increases the linewidth enhancement factor by about 40 % [15]. For carriers confined in a quantum wells, the FCA is practically important for determining the optical absorption. Scattering-assisted absorption by free electrons and holes in the active quantum wells then usually determines the internal loss in optically pumped laser devices with undoped claddings. Even in electrically pumped devices, assisted FCA can dominate if the lasing mode is optically confined primarily to the active region, as in the interband cascade lasers [16].

FCA in diode optical cladding layers consisting of superlattice injectors [17] can also be significant.

Since FCA is one of the powerful means to understand the scattering mechanisms of carriers, it has been studied in QWWs, theoretically, for the case absorption assisted by acoustic [18], acoustic and optical phonons [19], piezoelectric coupling, acoustic and optical phonons [20], interface-roughness [21] and alloy-disorder [22]. However, confined longitudinal-optical (LO) phonon scattering is an important scattering mechanism in QWWs and some quantum-mechanical studies have been performed [23-27].

In this paper, we present the theory of FCA for the Q1D electron gas in QWW structures when carriers are scattered by confined LO phonons. We consider the FCA for the cases where the radiation field is polarized along the length of the wire. Absorption coefficient will be calculated for the examples of GaAs QWWs.

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 L_z and L_y the cross sectional dimensions along the z and y directions, respectively, and with L the wire length 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

$$E_{kjl} = E_k + E_j + E_l = \frac{\hbar^2 k^2}{2m^*} + j^2 E_a^0 + l^2 E_b^0 ,$$

$$E_a^0 = \frac{\pi^2 \hbar^2}{2m^* L_y^2} , \quad E_b^0 = \frac{\pi^2 \hbar^2}{2m^* L_z^2} , \quad j, l = 1, 2, 3, \ldots, \qquad (1)$$

$$\Psi_{kjl} = \left[2 / \left(L_y L_z L \right)^{1/2} \right] \sin\left(\pi\, j\, y / L_y \right) \times$$
$$\times \sin\left(\pi\, l\, z / L_z \right) \exp\left(i\, kx \right). \qquad (2)$$

The FCA coefficient α, which is related to the quantum-mechanical transition probabilities in which the carriers absorb or emit a photon with the simultaneous scattering of the carriers from phonons, is given by

$$\alpha = \frac{\varepsilon_0^{1/2}}{n_0 c} \sum_i W_i f_i . \qquad (3)$$

Here ε_0 is the static dielectric constant of material, n_0 is the number of photons in the radiation field and f_i is the free carrier distribution function. The sum is over all the possible initial states i of the system. The transition probabilities W_i can be calculated using the standard second-order Born golden rule approximation:

$$W_i = \frac{2\pi}{\hbar} \sum_{fq} \Big[\left| \langle f | M_+ | i \rangle \right|^2 \delta\left(E_f - E_i - \hbar\Omega - \hbar\omega_q \right) +$$
$$+ \left| \langle f | M_- | i \rangle \right|^2 \delta\left(E_f - E_i - \hbar\Omega + \hbar\omega_q \right) \Big]. \qquad (4)$$

Here E_i and E_f are the initial and final state energies, respectively, of electrons, $\hbar\Omega$ is the photon energy, $\hbar\omega_q$ is the phonon energy, and $\langle f | M_\pm | i \rangle$ are the transition matrix elements from the initial state to the final state for the interaction between electrons, photons and phonons. This transition matrix element can be represented by

$$\langle f | M_\pm | i \rangle = \sum_\alpha \left(\frac{\langle f | H_R | \alpha \rangle \langle \alpha | H_{LO} | i \rangle}{E_i - E_\alpha \mp \hbar\omega_q} + \right.$$
$$\left. + \frac{\langle f | H_{LO} | \alpha \rangle \langle \alpha | H_R | i \rangle}{E_i - E_\alpha - \hbar\Omega} \right), \qquad (5)$$

where H_R is the interaction Hamiltonian between the electrons and the radiation field, H_{LO} is the scattering potential due to the electron-phonon interaction.

The interaction Hamiltonian with the radiation field is

$$H_R = -\frac{e}{m^*} \left(\frac{2\pi\hbar n_0}{V \Omega \varepsilon_0} \right)^{1/2} \left(\varepsilon P \right), \qquad (6)$$

where ε is the polarization vector of the radiation field, V is the volume of the crystal, and P is the electron momentum.

The interaction of electrons with the confined-LO phonon is given by [23]

$$H_{LO} = 2\alpha' \sum_{k_x} e^{i k_x x} \left\{ \sum_{m=1,3,5,\ldots} \sum_{n=1,3,5,\ldots} \frac{\cos\left(m\pi y / L_y \right) \cos\left(n\pi z / L_z \right)}{\left[k_x^2 + \left(m\pi / L_y \right)^2 + \left(n\pi / L_z \right)^2 \right]^{1/2}} \left[A_{LO}(k_x) + A_{LO}^+(-k_x) \right] + \right.$$
$$\left. + \sum_{m=1,3,5,\ldots} \sum_{n=2,4,6,\ldots} \frac{\cos\left(m\pi y / L_y \right) \sin\left(n\pi z / L_z \right)}{\left[k_x^2 + \left(m\pi / L_y \right)^2 + \left(n\pi / L_z \right)^2 \right]^{1/2}} \left[A_{LO}(k_x) + A_{LO}^+(-k_x) \right] \right. \qquad (7)$$

where $A_{LO}(k_x)$ and $A_{LO}(-k_x)$ are the annihilation and creation operators for appropriate LO-phonon modes of the QWW.

$$\alpha' = \left\{ \left(e^2 / 2\varepsilon_0 L_y L_z L \right) \hbar\omega_{LO}[1/\varepsilon_\infty - 1/\varepsilon_0] \right\}^{1/2} ,$$

where ε_∞ is the optical dielectric constant or the high-frequency dielectric constant of the material.

Using Eq. (3) and straightforward calculation of transition probabilities using matrix elements of H_R and H_{LO}, we obtain the following expression for the FCA coefficient in a Q1D semiconducting structure:

$$\alpha = \frac{e^4 \omega_{LO}}{4\pi^2 \varepsilon^{3/2} c\hbar^3 \Omega^3 L_y L_z} \sum_{jl} \sum_{j'l'} \int f(E_{knl}) \times$$

$$\times \left\{ N_q \left(\left[E_k - 2\sqrt{E_k(E_k+Z_+)} + (E_k+Z_+)\right] I\left(q_{+a}, L_y, L_z\right) + \right. \right.$$

$$+ \left[E_k + 2\sqrt{E_k(E_k+Z_+)} + (E_k+Z_+)\right] \times$$

$$\times I\left(q_{-a}, L_y, L_z\right) \Big) / \sqrt{E_k(E_k+Z_+)} + (N_q+1) \times$$

$$\times \frac{\left[E_k + 2\sqrt{E_k(E_k+Z_-)} + (E_k+Z_-)\right] I\left(q_{+e}, L_y, L_z\right)}{\sqrt{E_k(E_k+Z_-)}} + (N_q+1) \times$$

$$\times \frac{\left[E_k - 2\sqrt{E_k(E_k+Z_-)} + (E_k+Z_-)\right] I\left(q_{-e}, L_y, L_z\right)}{\sqrt{E_k(E_k+Z_-)}} \right\} dE_k . \quad (8)$$

Here, $Z_\pm = E_{jl} - E_{j'l'} + \hbar\Omega \pm \hbar\omega$, $q_{\pm a} = -k \pm \sqrt{Z_+ 2m}/\hbar$, $q_{\pm e} = k \pm \sqrt{Z_- 2m}/\hbar$, n_q is the number of phonons in a made of wave vector q with the Bose-Einstein distribution function. Moreover

$$I_{LO}\left(k_x, L_y, L_z\right) = \left(\frac{1}{\varepsilon_1(\infty)} - \frac{1}{\varepsilon_1(0)}\right) \frac{(2\pi)^2}{L_y L_z} \times$$

$$\times \sum_{m=1,2,3...} \sum_{n=1,2,3,...} \left\{ \frac{4P_{mn}}{\left[k_x^2 + \left(m\pi/L_y\right)^2 + \left(n\pi/L_z\right)^2\right]^{1/2}} \right\}^2$$

$$(9)$$

with

$$P_{mn} = \int_0^{L_y} dy \frac{2}{L_y} \int_0^{L_z} dz \frac{2}{L_z} \sin\left(\frac{j\pi y}{L_y}\right) \sin\left(\frac{j'\pi y}{L_y}\right) \times$$

$$\times \sin\left(\frac{l\pi z}{L_z}\right) \sin\left(\frac{l'\pi z}{L_z}\right) \sin\left(\frac{m\pi y}{L_y}\right) \sin\left(\frac{n\pi z}{L_z}\right) .$$

In the quantum limit, in which only the $j = l = 1$ ground level is occupied, the dominant contribution to the sum over phonon modes is made by the mode with $m = n = 1$, Eq. (9) may be approximated as [23]

$$I_{LO}\left(k_x, L_y, L_z\right) = \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right) \frac{(2\pi)^2}{L_y L_z} \times$$

$$\times \frac{16\left(8/3\pi\right)^4}{k^2 + \left(\pi/L_y\right)^2 + \left(\pi/L_z\right)^2} .$$

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

$$f_{kjl} = \frac{(2\pi)^{1/2} \hbar n_e a b}{\gamma \delta \left(m^* K_B T\right)^{1/2}} \exp\left[-\frac{j^2 E_a^0 + l^2 E_b^0}{K_B T}\right] \times$$

$$\times \exp\left(-\frac{\hbar^2 k^2}{2m^* K_B T}\right), \quad (10)$$

$$\gamma = \sum_j \exp\left(-\frac{j^2 E_a^0}{K_B T}\right), \qquad \delta = \sum_l \exp\left(-\frac{l^2 E_b^0}{K_B T}\right),$$

where n_e is the concentration of the electrons. Using Eq. (10) in Eq. (7) in the quantum limit we obtain the FCA coefficient

$$\alpha = \frac{3\pi^{1/2}(8/3\pi)^5 e^4 \omega_{LO} n_e}{\sqrt{2} m^{*3/2} \varepsilon_0^{3/2} \Omega^3 c L_y L_z (K_B T)^{1/2}} \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right) \times$$

$$\times \sum_{jl} \sum_{j'l''} \left\{ N_q \exp\left(\frac{Z_+}{2K_B T}\right) K_0\left(\frac{Z_+}{2K_B T}\right) + \right.$$

$$+ (N_q+1) \exp\left(\frac{Z_-}{2K_B T}\right) K_0\left(\frac{Z_-}{2K_B T}\right) -$$

$$\left. - N_q \frac{(b^2 - Z_+^2)}{(K_B T)^2} F(Z_+) - (N_q+1)\frac{(b^2 - Z_+^2)}{(K_B T)^2} F(Z_-) \right\}. \quad (11)$$

Here, $K_n(x)$ is the modified Bessel function of the second kind of argument x and order n, and

$$b = \frac{\hbar^2 \pi^2}{2m^* L_y^2} + \frac{\hbar^2 \pi^2}{2m^* L_z^2},$$

$$F(Z_\pm) =$$

$$= \int_0^\infty \frac{e^{-x} dx}{\sqrt{x\left(x + Z_\pm/K_B T\right)\left(4bx/K_B T + (Z_\pm + b)^2/(K_B T)^2\right)}} .$$

3. Discussion

We have obtained general expressions FCA for the quantum wires when the carriers are scattered by confined LO phonons. The FCA coefficient is expressed as a function of the photon energy $(\hbar\Omega)$, cross section wire $(L_y L_z)$ and temperature T. We have evaluated, numerically, the above expressions for FCA coefficient at 300 and 77 K, and parameters characteristic of GaAs and electron concentration $n_e = 10^{17}\,\text{cm}^{-3}$, phonon energy $\hbar\omega_{LO} = 36.2\,\text{meV}$.
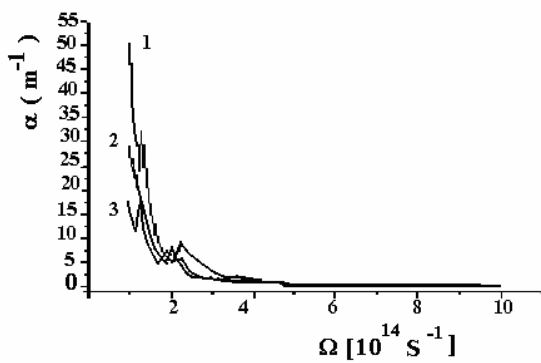
Fig. 1. FCA coefficient in the GaAs QWWs for confined LO phonon scattering as a function of the photon frequency with $T = 300$ K. We have chosen: $L_y = L_z = 10^{-6}$ cm (1); $L_y = 2 \cdot 10^{-6}$ cm, $L_z = 10^{-6}$ cm (2); $L_y = L_z = 2 \cdot 10^{-6}$ cm, $L_y = L_z = 10^{-6}$ cm, $L_y = L_z = 2 \cdot 10^{-6}$ cm, $L_y = L_z = 10^{-6}$ cm (3).
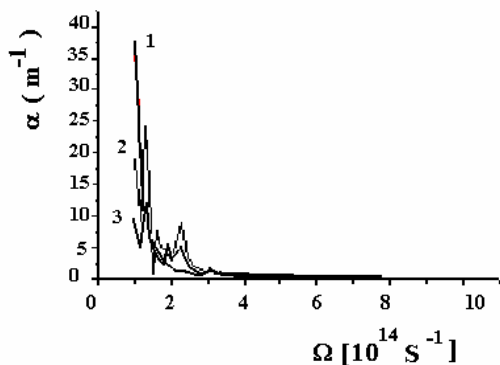

Fig. 2. FCA coefficient in the GaAs QWWs for confined LO phonon scattering as a function of the photon frequency with $T = 77$ K, the values of L_y, L_z are the same as in Fig. 1.

In Figs 1 and 2, we plot the FCA coefficient as a function of the photon frequency Ω in GaAs QWW with the temperature $T = 300$ K and 77 K. From Figs 1 and 2 it is shown that FCA coefficient decreases monotonically with increases with temperature. It is shown that FCA coefficient is an oscillatory function of the photon frequency in this case. These oscillations can be understood in terms of the subband structure, which arises because of the confinement of the carriers. When the photon energy is greater than the energy separation between the various subbands, the absorption of a photon can occur with the simultaneous emission or absorption of optical phonons in transitions to the same or to other subbands. The kinks in the curves indicate confined LO phonon-assisted transition between the subbands. There is a kink in the absorption coefficient as a function of photon frequency Ω followed by peak. The absorption coefficient is found to be considerably enhanced as the cross-sectional area of the wire decreases. It was predicted [23] that the scattering of electrons by confined LO phonons in QWWs increases

as the transverse dimensions of the wire diminish. From Fig. 1 and Ref. [19], it is shown that in quantum wire the electron-optic phonon interaction give a greater contribution to the absorption than the electron-confined LO phonon interaction.

Acknowledgements

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