Capture of carriers by quantum wells via optical-phonon deformation potential

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A calculation is reported for the probability of electron capture by a single quantum well that takes into account the quasi-two-dimensional electron system in the quantum well. The influence of continuum resonances, which are localized in the vicinity of the quantum well at energies above the barrier, were considered in the calculations. The scattering rate by optical-phonon deformation potentials as function of the incident electron energy and the well width are discussed.

Keywords: Electron capture rate; quantum well; optical-phonon deformation potential

En este trabajo se calcula la probabilidad de captura de un electrón por un pozo cuántico, la cual considera la biodimensionalidad del sistema electrónico en el pozo cuántico. La influencia de los estados resonantes para energías electrónicas mayores que la energía del pozo. Se presenta un análisis de la razón de dispersión de electrones vía fonones en la aproximación del potencial de deformación como función del ancho del pozo cuántico.

Descriptores: Probabilidad de captura electrónica; pozo cuántico, interacción electrón-fonón vía potencial de deformación.

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1. Introduction

Band gap engineering of semiconductor quantum well (QW) heterostructures provides the possibility of controlling the electronic and optical properties varying the layer thickness and material compositions. Several non-conventional structures have been proposed and realized for both, investigate peculiar aspects of the confined carrier physics and improving the performance of the QW devices. The mechanism of carrier capture by a QW is of fundamental importance to improve the performance of QW lasers and infrared photodetectors [1].

The carrier capture times have received special theoretical attention because the quantum mechanical aspects of the system play an important role in the capture process. Kozyrev and Shik [2] have shown that when the carrier energy is low, the probability of carrier capture by a QW and emission of an optical phonon exhibits a number of resonances as a function of the thickness well. These resonances are associated with the appearance of new states in the QW. Similar results were predicted by Brum and Bastard [3] where the fastest carrier capture process is due to the scattering by longitudinal optical (LO) phonons through the Frölich interaction.

Bradt *et al*. [4] extended the previous theories to a numerical analysis of the electron capture by a QW with the participation of the quasi-bound 2D states, which are localized in the vicinity of the QW at energies above the barrier. They calculated the rates of capture assisted by both emission and absorption of optical phonons by an electron with arbitrary positive initial energy, as well as elastic impurity and acoustic phonon scattering.

Optimization of the operating characteristics of semiconductor multiple quantum well lasers with respect to the confinement layers has been performed both experimentally and theoretically [5 - 7]. As a result graded-index-separate-confined heterostructure (GRINSCH) lasers are well known to exhibit a lower threshold current density than conventional separate-confinement multiple quantum well lasers. This performance improvement has been attributed to higher carrier capture efficiency in GRINCH lasers. Numerical calculations of electron capture times in GRINCH structures with finite electron density have been calculated for electron-electron and electron-polar optical phonon scattering as a function of the well thickness [8 - 11]. In addition, oscillations in the carrier capture rate as a function of the well thickness have been observed experimentally [12 - 13]. The capture times were obtained with femtosecond resolution using pump and probe measurements under resonant excitations conditions.

In this paper, the electron capture is treated as the transition from three-dimensional states to the truly bound two-dimensional states in a QW with energy below the barrier. An analytic expression for the carrier capture time via electron-LO phonon interaction is obtained. The capture time is based in the emission of optical phonons via the electron-optical phonon deformation interaction, which dominates in diamond-type crystals. Also, we obtain the dependency of the overall capture time on the well width.

2. Carrier capture time

We consider a single rectangular quantum well with a potential defined as

$$V(z) = \begin{cases} -V_0, & |z| \leq a, \\ 0, & \text{otherwise.} \end{cases} \tag{1}$$

We assume the difference between the electron effective mass in the well and the barriers to be small and set the effective mass m to be constant over the whole space. As usual, we separate the electron motion parallel to the interface, which we call the $x-y$ plane, from the motion in the di-

rection perpendicular to the interface, which we denote by z-direction. Parallel to the interface, the carrier is free to move in the layer plane. The in-plane solution of the Schrödinger equation yields plane wave eigenstates which are label by quantum numbers k_x and k_y. Normal to the interface, the carrier motion is quantized and the eigenstates are two types: bound states which can be distinguished by a discrete quantum numbers n and delocalized states with a continuos quantum number ξ_z. The solutions of the Schrödinger equation for this problem are well known and are given in Ref. [14]. The QW structure has a finite number of bound states of negative energies. In addition to these bound states, virtual bound states (or equivalently, transmission resonances) of positive energies occur in the QW continuum. The transmission resonances are narrower when their energies approach to zero.

We are interested in calculating the transition probability per unit time $w(k_x, k_y, \xi_z)$ that the carrier in the initial state (k_x, k_y, ξ_z) emits an optical phonon and becomes captured by the well into a final state with quantum numbers (k'_x, k'_y, ξ_n). In general, the scattering rates for emission or absorption of a phonon with energy $\hbar\omega_q$ and momentum $\hbar\mathbf{q}$, within Fermi golden rule are given by

$$w = \frac{2\pi}{\hbar}\left|\left\langle k'_x, k'_y, \xi_n \left|H_{e-p}\right| k_x, k_y, \xi_z\right\rangle\right|^2 \times\delta(\varepsilon_f - \varepsilon_i + \hbar\omega_q), \quad (2)$$

where

$$\varepsilon_i = (\hbar^2/2m)(k_x^2 + k_y^2 + k_z^2)$$

and

$$\varepsilon_f = \hbar^2/2m(k'^2_x + k'^2_y) + \varepsilon_n$$

correspond to the initial and final electron energy above and in the QW. Here H_{e-p} is the electron-phonon interaction Hamiltonian.

The phonons, which usually dominate the scattering probability, are long-wavelength optical phonons. The long-wavelength optical phonons set up a short–range potential in the crystal, which shifts the electronic band states. In polar semiconductors, the longitudinal optical phonons are also accompanied by a long–range macroscopic electric field that produces additional scattering. This long-range polar-optical interaction potential is strictly additive to the short-range potential and its coupling constants are well established. It will not be considered in this paper. The non-polar optical phonon electron interaction dominates in diamond-type crystals, particular in *n-Ge*, and in the total (non-polar plus polar) optical phonon scattering rates for holes in *p-Ge*, *p-Si* , $p-$type III-V and II-VI semiconductors. The shifts of the band states per unit ionic displacement associated with a long-wavelength optical phonon are called deformation potentials. The theory of the optical-phonon deformation potentials in tetrahedral semiconductors has been extensively investigated by Potz and Vogl [15].

Therefore, in general, the electron-phonon interaction H_{e-p} consists of a long-range contributions. In polar crystals, the long-range part of H_{e-p} gives rise to the polar optical Frölich intrarction. Here we will concerned solely with the short-range part of H_{e-p}, *i.e.*, the optical deformation-potential interaction. It dominates in diamond-type crystals and in most diamond or zinc-blende semiconductors [15]. In the one-electron approximation;

$$H_{e-p} = M_q e^{-iq\cdot r} b_r^+ + cc,$$

where M_q is the electron-phonon coupling and b_q^+ is the phonon creation operator, the probability w by the emission of a phonon is given by

$$w = \frac{2\pi}{\hbar}(N_q + 1)\left|M_q\right|^2 \left|\int \xi_n^* e^{-iq_z z}\xi_{k_z} dz\right|^2 \times\delta_{\mathrm{k'}_\perp, \mathrm{k}_\perp - \mathrm{q}_\perp}\delta(\varepsilon_n + \frac{\hbar^2}{2m}k'^2_\perp - \varepsilon_i + \hbar\omega_q). \quad (3)$$

Here

$$N_q = \left[\exp\left(\frac{\hbar\omega_q}{k_B T}\right) - 1\right]^{-1}$$

is the phonon occupation factor and T is the lattice temperature. In the long-wavelength optical-phonon the two sublattices vibrate rigidly against each other. In the deformation potential coupling to optical phonons at long-wavelength limit, the dispersion relation of phonons is constant, *i.e.*, $\omega_q = \omega_0$ and for a non-degenerate band state M_q is given by [16]

$$M_q = D\left(\frac{\hbar}{2\rho V\omega_q}\right)^{1/2},$$

where D is the optical deformation potential constant. Under this approximation, the total electron capture rate per unit time, *i.e.* the electron lifetime $\tau^{-1} = \sum_{n,k'_\perp,q} w(n, k'_\perp, q)$, is given by

$$\frac{1}{\tau} = \frac{mM_0^2(N_0+1)}{4\pi^2\hbar^2\rho\omega_0}\sum_n \int \left|\xi_{k_z}(z)\right|^2\left|\xi_n(z)\right|^2 dz \times \int \frac{2q_\perp dq_\perp}{\sqrt{4k_\perp^2 q_\perp^2 - (q_\perp^2 - k_z^2 + \frac{2m}{\hbar^2}\left[\varepsilon_n + \hbar\omega_0\right])^2}}. \quad (4)$$

In arriving at Eq. (4) the Parseval theorem has been used, *i.e.*

$$\int f(s)g^*(s)ds = \int F(t)G^*(t)dt,$$

and the integral over $\mathrm{q}_\perp$ obeys the energy conservation condition

$$\left|\frac{q_\perp^2 - k_z^2 + \frac{2m}{\hbar^2}\left[\varepsilon_n + \hbar\omega_0\right]}{2k_\perp q_\perp}\right| \leq 1 \quad (5)$$

and the result is π. The integral over z is straightforward, and its is given by

$$\int |\xi_{kz}(z)|^2 |\xi_n(z)|^2 dz = \frac{T(\varepsilon_i)}{4} \left(\frac{cs^2 qa}{\frac{cs^2 qa}{\kappa} + a + (-1)^{n+1} \frac{\sin 2qa}{2q}} \right) \left\{ \frac{2aq + (-1)^{n+1} \sin 2qa}{q\, cs^2 qa} \left(1 + \frac{k_z^2}{q'^2}\right) \right.$$
$$+ \frac{k_0^2}{q'^2} \left[\frac{\sin 4q'a}{2q' cs^2 qa} + (-1)^{n+1} \frac{q \sin 2qa \cos^2 2q'a - (q' \cos 2qa \sin 4q'a)/2}{(q^2 - q'^2) cs^2 qa} \right]$$
$$\left. + \left[\frac{(q'^2 + k_z^2) k_0^2 \kappa \sin^2 2q'a + q' k_0^2 k_z^2 \sin 4q'a}{(q^2 - q'^2) k_z^2 q'^2} + \left(1 + \frac{k_0^4 \sin^2 2q'a}{4 k_z^2 q'^2}\right) \right] \right\}, \quad (6)$$

where csx is cosx if the final state of the electron is even or sinx if the final state of the same one is odd. The variables

$$q^2 = \frac{2m}{\hbar^2} (V_0 - |\varepsilon_n|), \quad k_0^2 = \frac{2m}{\hbar^2} V_0, \text{ and } \quad \kappa^2 = \frac{2m}{\hbar^2} |\varepsilon_n|$$

stand for electron bound states in the QW, while the parameters for the unbounded states are defined as:

$$k_z^2 = \frac{2m\varepsilon_i}{\hbar^2} \cos^2 \theta, \quad k_\perp^2 = \frac{2m\varepsilon_i}{\hbar^2} sin^2\theta$$
$$\text{and } q'^2 = \frac{2m}{\hbar^2} (\varepsilon_i + V_0),$$

where θ represents the incidence angle of the electron on the well, understood among the axis z and the electron wave-vector k. Here L is a normalization constant which for typical quantum well lasers devices, $L \sim 1\mu m$. It is worth noting that the electron life time is proportional to the transmission coefficient $T(\varepsilon)$ across the QW of thickness a and it is given as

$$T(\varepsilon) = \left[1 + \frac{1}{4} \left(\frac{q'}{k_z} - \frac{k_z}{q'} \right) sin^2 2q'a \right]^{-1}. \quad (7)$$

An analysis of Eq (7) is given in any standard book of quantum mechanics. In the limit of the electron energy $(\varepsilon/V_0) << 1$, Eq. (6) reduces to

$$\int |\xi_{kz}(z)|^2 |\xi_n(z)|^2 dz = \frac{k_z^2}{4k_z^2 + k_0^2 sin^2 2k_0 a} \frac{1}{\frac{cs^2 qa}{\kappa} + a + (-1)^{n+1} \frac{sin2qa}{2q}} \left\{ 2a + \frac{(-1)^{n+1} sin2qa}{q} \right.$$
$$\left. + \frac{sin4k_0 a}{2k_0} - (-1)^{n+1} \frac{q sin2qa \cos^2 2k_0 a - (k_0 \cos 2qa sin4k_0 a)/2}{\kappa^2} \right\}, \quad (8)$$

which is similar to that obtained by Kosytev and Shik in Ref. 2.

3. Results and discussion

We perform numerical calculations for AlGaAs/GaAs/AlGaAs single quantum well of depth V_0= 300 meV, neglecting the difference between the effective electron mass of the well and the barriers and using the material constants of GaAs.

The results of the numerical calculations of the capture rates are presented in Fig. 1 as function of the carrier incident energy for two different incident angles. We choose the width of well $2a$ = *100Å*, the lattice temperature T= 300 K, the energy phonon $\hbar\omega_0 = 36meV$, the density ρ = 5.310 g/cm^3 and the optical deformation potential *D = 3.54 10^{8}eV/cm.*

In Fig. 1 we show the capture rate $1/\tau$ for emission of optical phonons as function of the incident electron energy for three bounded states in the QW as shown in Fig. 2. As can be seen, the scattering rate by non-polar phonon scattering is linear at electron energy close to the bottom of the QW (low energy) which is in agreement with the result obtained by Lent and Porod [16]. However at high electron energy, the capture rate presents an oscillatory structure at some resonant energy. This oscillatory behavior of the capture rate at energies higher than the AlGaAs band gap, is very likely due to the existence of the quasibound states above the QW.

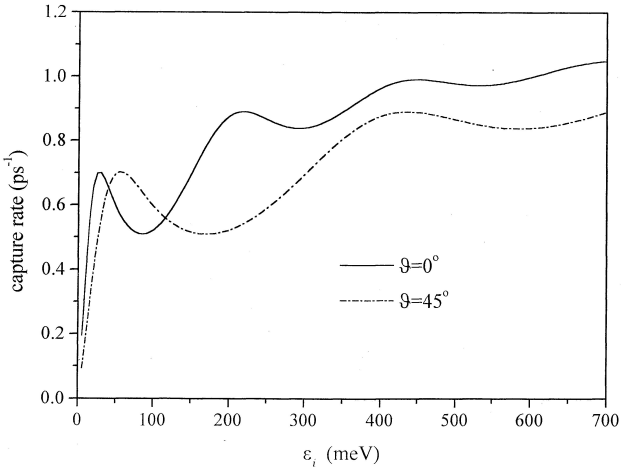

FIGURE 1. Capture rates, $1/\tau$ as a function of the initial electron energy due to the emission of non-polar optical phonons. Full curve correspond to the electron motion parallel to the quantum well growth axis ($\theta = 0$) and the dashed curve to $\theta = \pi/4$.

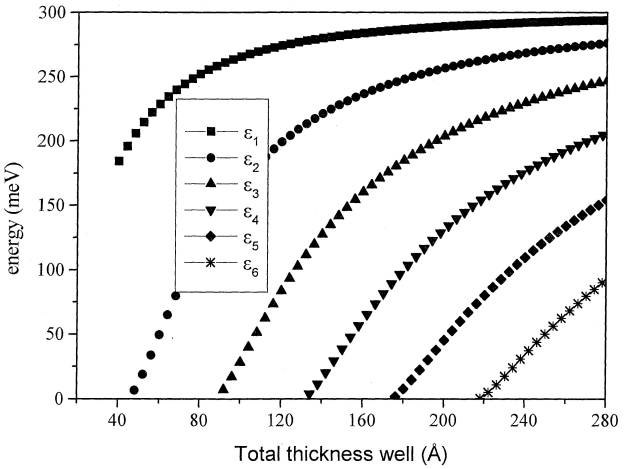

FIGURE 2. Absolute value of the electron energy (bound states) in the QW as a function of the thickness of the well

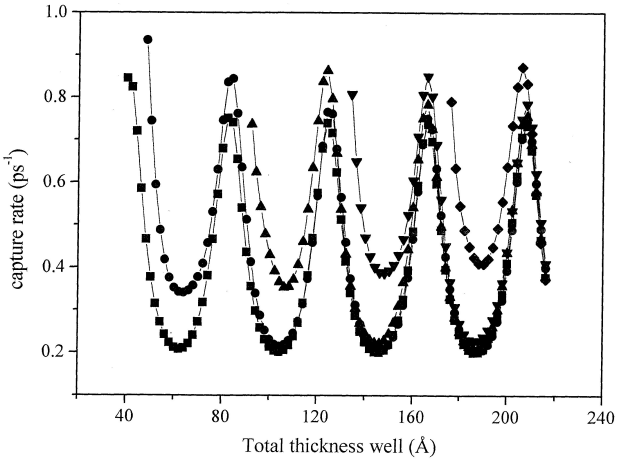

FIGURE 3. Partial contributions to the total capture rates due to the emission of non-polar optical phonon for different electron final states as a function of the width of the well at $\theta = 0$. The initial electron energy $\varepsilon_i = 25meV$.Different symbols stand for bound states in the QW: $\varepsilon_1; \circ \quad \varepsilon_2; \triangle \quad \varepsilon_3; \bigtriangledown \quad \varepsilon_4; \diamond \quad \varepsilon_5$.

This effect is due to the transmission coefficient given by Eq(7) and is similar as that which produces resonance oscillations in the transmission coefficient for plane waves passing over the well.

The dependence of the scattering rate on the angle is also specified by the dependence on the transmission coefficient Eq. (7) throughout the initial electron energy. For electrons moving parallel to the interface, , the electron capture vanishes because the electron do not cross the well, and the probability of finding the electron in the vicinity of the well is proportional to.

This transmission resonances can also be viewed as virtual bound states. These levels, like QW bound levels, correspond to an accumulation of probability for the carrier to be in the well; but unlike the true bound states, they decay gradually with a time constant, where is the energy width of the transmission resonance.

In Fig. 3, the partial carrier capture rate is plotted as function of the width of the QW for an incident electron energy 25 meV parallel to the QW growth axis. As we can see, there exist several different sets of resonances in the $1/\tau(a)$ dependence. The first set occurs when the energy of the nth level is equal to $\hbar\omega_0$ below the barrier, *i.e.* the ionization energy $E_n = \hbar\omega_0$. In this situation the electron with an incident energy ε_i above the QW can emit an optical phonon and it decays in the nth bound state in the QW and, by increasing the well width, the bound states in the QW become more tightly bound to finally move outside of the reach of any continuum state ($\approx \hbar\omega_0$) which allow a capture event. The second set of capture resonances is associated with the quasibound states with energies above the QW. As these states are narrow enough, most of the electrons occupy the resonant state, and consequently, will enhance the electron capture rates.

In Fig. 4 we have plotted the total capture rates due to the emission of optical phonon as a function of the width well for an initial electron energy equal to 25 meV. One can point out that the strength of the first set of resonances ($E_n \approx \hbar\omega_0$) remains, practically all the electrons have the same probabilities of emitting a phonon and relaxing to the bottom of the nth bound state. On the other hand, the magnitudes of the second set of peaks increase with the well width *i.e.* when the thickness increase the number of final virtual bound states available for capture increases and therefore it enhance the capture rate.

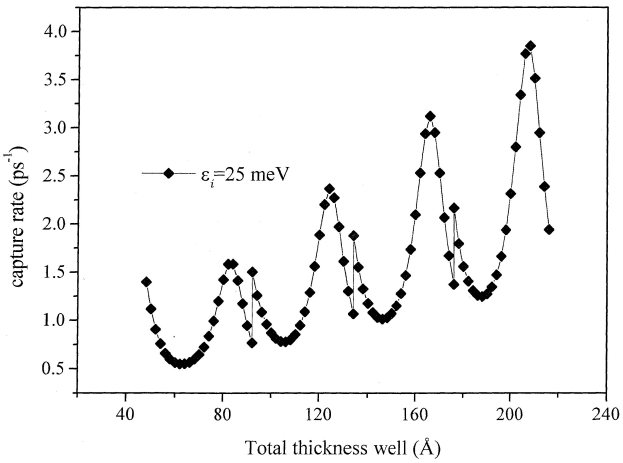

FIGURE 4. Total electron capture rate due to the emission of non-polar optical phonon versus the width of the well.

4. Conclusions

In conclusion, we have presented the results of quantum mechanical calculations of the carrier capture within the two-dimensional bound states via deformation potential optical

phonon emission. We have shown, that the capture rate exhibits marked oscillations upon the initial electron energy and the well width, which are associated either with the binding of a new bound state by the QW or with the occurrence of a quasibound state from the continuum edge.

Finally, its is important to mention that the results obtained are in agreement with those obtained by numerical analysis of the capture rate in Refs. 10 and 11 using different electron-phonon interaction potentials. According to this, it should be noted that these resonant peaks exhibited by the dependence of $1/\tau(a)$ are associated with the form of the delocalized wave function of the initial state. The electron bound in the well and the form factor of the electron-phonon interaction in Eq. (3) are not important and they only affect the overlap integral given by Eq. (7). Therefore, the dependence shown in Fig. 4 is of general validity and it applies to any inelastic scattering, including that involving polar optical phonons and at low temperature also acoustic phonons.

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