Resonant carrier capture by semiconductor quantum wells

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We present the results of a quantum-mechanical calculation of τ, the average capture time of a carrier by a quantum well. The capture is induced by the emission of longitudinal optical phonons. The time τ displays strong oscillations versus the well thickness. These oscillations are associated with the binding of a new state by the well and with the occurrence of a quantum-well virtual bound state within one LO phonon energy from the edge of the quantum-well continuum. Holes are calculated to be more efficiently captured than electrons.

Semiconductor quantum wells are known to efficiently collect carriers. This may be one of the reasons for the improved performance of quantum-well lasers over conventional double-heterostructure lasers.[1] Recently, time-resolved cathodoluminescence[2] and photoluminescence experiments[3] have been interpreted in terms of carrier capture times as short as 0.1 (Ref. 2) or 50 ps.[3] The energy relaxation within bound quantum-well (QW) states has already been discussed[4,5] as well as the giant capture cross sections of traps in bulk materials.[6] However, to our knowledge, the only existing theory of carrier capture by a QW is due to Shichijo *et al.*[7] and Tang *et al.*[8] These authors have performed a classical calculation of the LO phonon-scattering-limited carrier mean free path 1_p in bulk GaAs and have concluded that, if the GaAs well thickness L of a GaAs-$Ga_{1-x}Al_xAs$ structure was larger than 1_p, the carrier collection would be efficient.

In this Brief Report we report the results of a quantum-mechanical calculation of the average time τ for a carrier energetically located within one LO phonon energy ($\hbar\omega_{LO}$) of the edge of the QW continuum to be captured by the well. The allowance of the quantum aspects of the problem, i.e., of the discrete nature of the QW bound states as well as of the intricacies of the QW continuum states lead to results which are markedly different from the classical analysis.[7,8] The capture time τ is an oscillating function of the well width L. The oscillations originate either from the binding of a new bound state by the QW or by the existence of a QW virtual bound state situated within $\hbar\omega_{LO}$ of the QW continuum edge.

We consider a QW structure which consists in a semiconductor layer (thickness L) clad between two thick semiconductor layers which act as potential barriers. The total thickness of the structure is $\mathscr{L}$ and $\mathscr{L} >> L$. $\mathscr{L}$ is a macroscopic quantity ($\mathscr{L} \approx 1$ μm), whereas L is of the order of 100 Å. We denote by z the growth axis of the structure. We will neglect any band-structure effects: The carrier has a constant effective mass m^* throughout the whole structure and its dispersion relations in each layer are taken as parabolic and isotropic upon the wave vector $\mathbf{k}$. The energy zero is taken at the onset of the QW continuum. Thus, assuming flat band conditions, the potential energy is constant inside the well ($-V_b$) and in the barriers (0). The QW structure has a finite number $\mathscr{N}$ of bound states of negative energies:

$$\mathscr{N} = 1 + \text{int}(2m^* V_b L^2/\pi^2\hbar^2) ,$$

where int(x) denotes the integer part of x. In addition to these bound states, virtual bound states (or, equivalently, transmission resonances) of positive energies occur in the QW continuum.[9] Compared with other continuum states, they correspond to an accumulation of the integrated probability of finding the particle in the well and, in this respect, act like true bound states.[10] The transmission resonances are narrower when their energies approach zero. At the continuum edge, they match with the true QW bound states. In addition to the z motion, the carrier is free to move in the layer plane. The in-plane wave vector will be denoted by $\mathbf{k}_\perp = (k_x, k_y)$. Thus, a QW bound state will be labeled by $|n\mathbf{k}_\perp\rangle$, where $n (n = 1, 2, \ldots)$ is the index of the bound level associated with the carrier z motion. The wave functions of the QW continuum states along the z axis are linear combinations of plane waves, either in the well (wave vector k_w) or in the barrier (wave vector k_b). These wave functions are normalized over the length $\mathscr{L}$ of the structure. In the layer plane the wave functions are plane waves (wave vector $\mathbf{k}_\perp$). The QW continuum states will be labeled $|k_b, \mathbf{k}_\perp\rangle$. For a given energy and a given $\mathbf{k}_\perp$, there exist two degenerate continuum states $|k_b, \mathbf{k}_\perp\rangle$ which correspond to a carrier moving along the z axis either from the left to the right or vice versa. It will be convenient to use the symmetric $|S, k_b, \mathbf{k}_\perp\rangle$ or antisymmetric $|A, k_b, \mathbf{k}_\perp\rangle$ combinations of these two states. When the nth QW bound state [parity $(-1)^{n+1}$] has popped in the continuum to become a transmission resonance and when this resonance is narrow enough, the virtual bound state largely retains the parity property of the original bound state. If n is odd (even bound states) the symmetric combination of continuum states $|S, k_b, \mathbf{k}_\perp\rangle$ displays an enhanced probability of being in the well. Instead, the antisymmetric combination $|A, k_b, \mathbf{k}_\perp\rangle$ is repelled by the well and consequently corresponds to a very small integrated probability of finding the carrier in the well.

We are interested in calculating the transition probability per unit time $W(k_b, \mathbf{k}_\perp)$ that a carrier in the initial state $|k_b, \mathbf{k}_\perp\rangle$ emits a LO phonon and becomes captured by the well. We assume that the electron-phonon coupling is described by the Fröhlich Hamiltonian. To the Born approximation $W(k_b, \mathbf{k}_\perp)$ is given by

$$W(k_b,\mathbf{k}_\perp)=\frac{2\pi}{\hbar}\sum_{\substack{n,\mathbf{k}'_\perp,\mathbf{q}\\ A,S}} |\langle X,k_b,\mathbf{k}_\perp,1_\mathbf{q}|H_{e-\mathrm{ph}}|n,\mathbf{k}'_\perp,0_\mathbf{q}\rangle|^2\delta\left[\frac{\hbar^2}{2m^*}(k_b^2+k_\perp^2)-\hbar\omega_{\mathrm{LO}}+V_b-\epsilon_n-\frac{\hbar^2k_\perp'^2}{2m^*}\right] , \quad (1)$$

where $\mathbf{q}$ is the three-dimensional phonon wave vector, ϵ_n the confinement energy of the nth bound state ($0\leq\epsilon_n\leq V_b$), and where $|X,k_b,\mathbf{k}_\perp\rangle$, where $X=A$ or S, denote the symmetric or antisymmetric combinations of continuum states of barrier wave vector k_b ($k_b>0$). In Eq. (1), the dispersion of the LO phonons has been neglected as well as the difference between the $\hbar\omega_{\mathrm{LO}}$'s in the well and in the barrier. We shall denote by τ the average capture time of the carrier. τ^{-1} is defined as the average of $W(k_b,\mathbf{k}_\perp)$ over all the continuum states weighted by a distribution function $f(k_b,k_\perp)$. We have considered a steady-state situation: f is constant for all continuum states with energy smaller than $\hbar\omega_{\mathrm{LO}}$ and vanishes elsewhere. To facilitate the discussion τ^{-1} will be written as $\tau_A^{-1}+\tau_S^{-1}$,, where τ_A, τ_S, respectively, correspond to initial continuum states which are either odd or even with respect to $z=0$, the center of the QW slab.

Before discussing the L dependence of τ_A, τ_S, we want to stress that τ_A, τ_S are proportional to the total structure thickness $\mathcal{L}$(as long as $L\ll\mathcal{L}$). This is not surprising insofar as the initial states are delocalized over $\mathcal{L}$, whereas all the final states are essentially localized over L. For multiple quantum-well structures consisting in p QW's τ_A, τ_S would be proportional to $\mathcal{L}/p$ if the captures by different wells are incoherent and if $pL\ll\mathcal{L}$.

Figures 1(a) and 1(b) present the calculated results for τ_S^{-1}, τ_A^{-1} vs L keeping $\hbar\omega_{\mathrm{LO}}$, V_b, m_e^*, and $\mathcal{L}$ fixed (36 meV, 0.3 eV, $0.067m_0$, and 1 μm, respectively). In these curves, the normalizing constant of the distribution function f has been taken equal to

$$\frac{3\pi^2}{\mathcal{L}S}\left[\frac{\hbar}{2m_e^*\omega_{\mathrm{LO}}}\right]^{3/2} ,$$

where S is the sample area. Our normalization is exact at $L=0$ but becomes only approximate if $L\neq0$; we consider, however, the resulting errors as small since $L\ll\mathcal{L}$.

The most striking features of the results shown in Figs. 1(a) and 1(b) are the pronounced oscillations displayed by τ_A^{-1} and τ_S^{-1} vs L. These oscillations, of quantum origin, are closely linked to the existence of QW bound and virtual bound states. Those labeled 1, 2, 3, . . ., show up irrespective of the parity of the initial state, whereas those labeled R_{2j+1}, $j\geq0$ are seen only in τ_s^{-1} and those labeled R_{2j+2}, $j\geq0$ are only seen in τ_A^{-1}. The first kind of oscillations ($n=1,2,\ldots$) corresponds to discrete bound states entering into the well and, by increasing L, becoming more tightly bound to finally move outside of the reach ($\sim\hbar\omega_{\mathrm{LO}}$) of any continuum state which would allow a capture event with zero $\mathbf{k}_\perp$, $\mathbf{k}'_\perp$. The second kind of capture resonances (R_{2j+1}, R_{2j+2}) is associated with the drop of QW virtual bound states within $\hbar\omega_{\mathrm{LO}}$ of the continuum edge. As these states are narrow enough, they largely retain the parity property of the QW state into which they will transform at larger L. Consequently, a virtual bound state of even n will sizably enhance τ_A^{-1} but will not affect τ_S^{-1} and vice versa if n is odd.

Starting at $L=0$, τ_A^{-1} and τ_S^{-1} are very small. This is because only a single continuum state can recombine with the single $n=1$ QW bound state of vanishing binding energy. When L increases the $n=1$ QW bound state deepens in the well and thus the number of initial states available for capture increases as well as the number of final states; τ_A^{-1} and τ_S^{-1} both increase. When $V_B-\epsilon_1$ comes to exceed $\hbar\omega_{\mathrm{LO}}$ it is no longer possible to have efficient quasi-one-dimensional capture events which are characterized by zero initial and final $\mathbf{k}_\perp$'s. Accordingly, τ_A^{-1} and τ_S^{-1} decrease. τ_A^{-1} stops

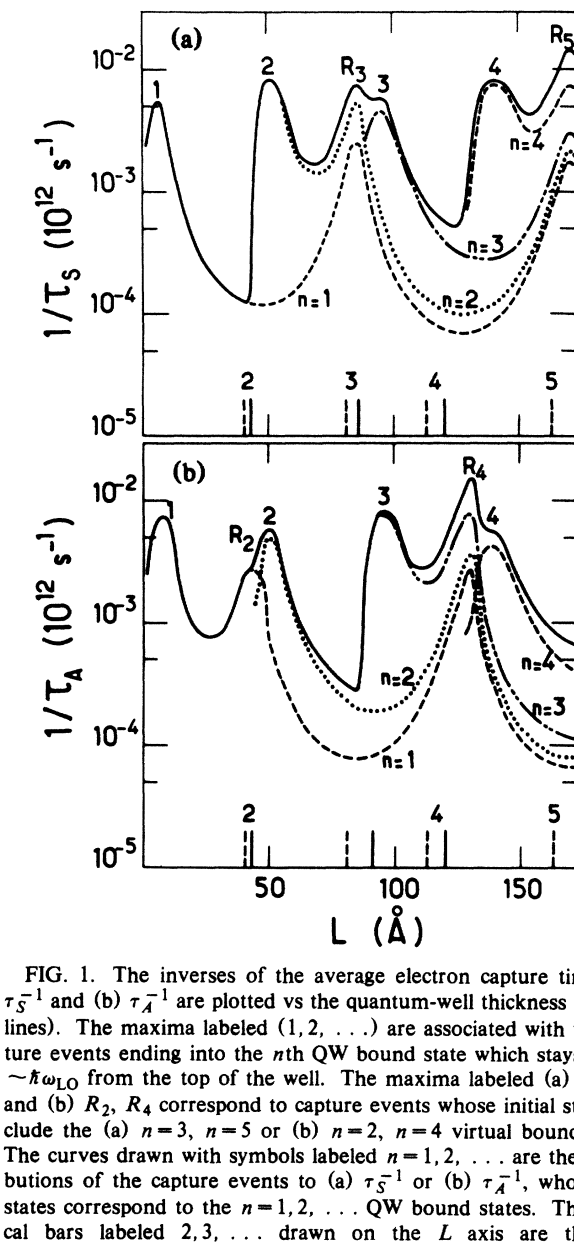

FIG. 1. The inverses of the average electron capture times (a) τ_S^{-1} and (b) τ_A^{-1} are plotted vs the quantum-well thickness L (solid lines). The maxima labeled (1, 2, . . .) are associated with the capture events ending into the nth QW bound state which stays within $\sim\hbar\omega_{\mathrm{LO}}$ from the top of the well. The maxima labeled (a) R_3, R_5 and (b) R_2, R_4 correspond to capture events whose initial states include the (a) $n=3$, $n=5$ or (b) $n=2$, $n=4$ virtual bound states. The curves drawn with symbols labeled $n=1,2,\ldots$ are the contributions of the capture events to (a) τ_S^{-1} or (b) τ_A^{-1}, whose final states correspond to the $n=1,2,\ldots$ QW bound states. The vertical bars labeled 2, 3, . . . drawn on the L axis are the QW thicknesses beyond which the nth QW virtual bound state stays within $\hbar\omega_{\mathrm{LO}}$ of the continuum edge (dashed bars) and beyond which this nth state has become a true QW bound state (solid bars).

decreasing when the $n=2$ virtual bound state comes within $\hbar\omega_{LO}$ of the continuum edge. For this L and onward, the capture events associated with odd continuum states are enhanced due to the increasing probability of finding the particle in the quantum well. On the other hand, τ_S^{-1} keeps decreasing since all the even continuum states are repelled by the well, inhibiting the capture. At still larger L, the $n=2$ virtual bound state becomes a true bound state and the scenario at $L=0$ is repeated (irrespective of the parity of the initial states). However, there now exists two kinds of final states which are, respectively, associated with the $n=1$, $n=2$ QW bound states. Both $n=1$ and $n=2$ contributions decrease (when $V_b-\epsilon_2 \gtrsim \hbar\omega_{LO}$), until the $n=3$ virtual bound state comes within $\hbar\omega_{LO}$ of the continuum edge. Since $n=3$ is the reminiscence of an even bound state τ_S^{-1} is markedly enhanced, whereas τ_A^{-1} keeps decreasing. Then the $n=3$ level becomes bound by the QW and the whole cycle starts again.

Figure 2 presents a comparison between the L dependences of the electron and hole capture times τ_e, τ_h. For the holes, we took $m_h^*=0.45m_0$, $V_b=0.2$ eV; otherwise, the

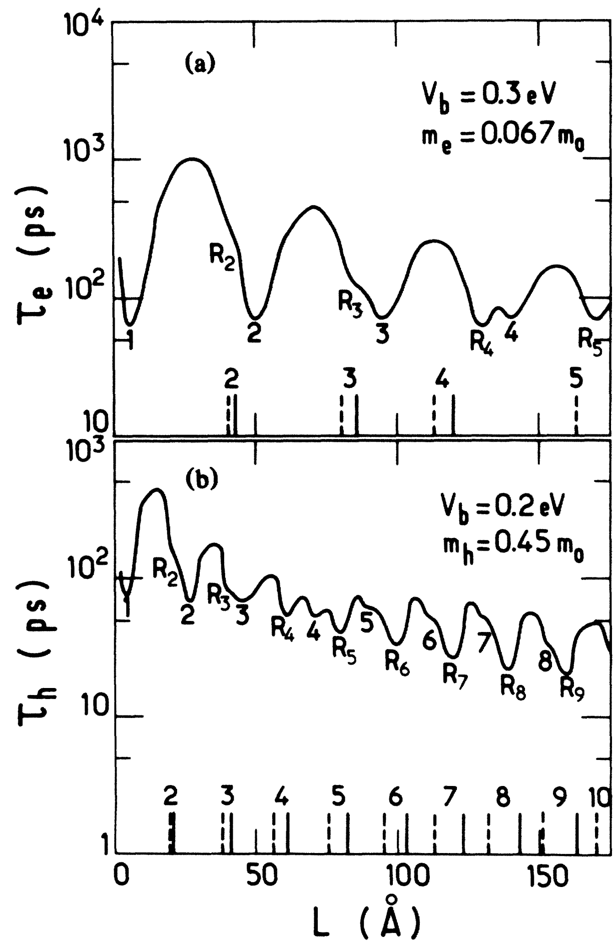

FIG. 2. The average capture times for electrons and holes τ_e, τ_h (in ps) are plotted vs the QW thickness L. The minima labeled $n=1,2,\ldots$ correspond to capture events ending into the nth QW bound state which stays within $\sim\hbar\omega_{LO}$ of the top of the well. The minima labeled $R_2,R_3,\ldots$ correspond to capture events whose initial states include the $n=2,3,\ldots$ QW virtual bound state. The dashed and solid vertical bars drawn on the L axis have the same meaning as in Figs. 1(a) and 1(b).

same parameters as used in Figs. 1(a) and 1(b). Clearly, τ_e, τ_h vary with L in the same qualitative way, exhibiting oscillations versus the well width. Quantitatively, however, the holes are found four times more rapidly captured than the electrons. We attribute this fact, which may be of importance for the understanding of QW based devices, to the larger density of final states for holes in the capture events.

In addition, it can be seen in Fig. 2(b) that the amplitudes of the τ_h oscillations are smaller than those of τ_e. Indeed, beyond $L \sim 30$ Å, τ_h is rather smoothly varying. We believe the latter feature evidences the transition from a truly quantum regime, where the QW binds few levels and where τ oscillates strongly, to a quasiclassical regime, where the QW binds so many levels that they form a quasicontinuum, in such a way that the binding of a new QW state little affects the total number of available final states for the capture events. Note that in the quasiclassical regime, the analysis of Shichijo *et al.*[7] is likely to become correct.

To our knowledge, there is no precise experimental or theoretical insights about the energy dependence of the distribution function of continuum states in semiconductor quantum wells. To obtain Figs. 1 and 2 we took an equirepartition of continuum states up to $\hbar\omega_{LO}$ for the sake of definiteness. This f roughly mimics a situation where carriers, after having been injected high in the continuum, have quickly cascaded down (through phonon-assisted intracontinuum transitions) to stay within $\hbar\omega_{LO}$ from the continuum edge without thermalizing among themselves.

To check whether the pronounced oscillations shown in Figs. 1 and 2 are independent of the assumed f, we have also investigated the τ vs L relationship when f is taken to be a Maxwell-Boltzmann distribution function, characterized by the effective temperature T^*. Such an f may result from a fast thermalization among carriers. We found that, compared with the results shown in Figs. 1 and 2, the capture times τ_e, τ_h are increased by a factor ~ 1.4–6 when T^* ranges from 100–10 K. Moreover, our calculations have demonstrated that the oscillations labeled $1,2,\ldots$, associated with the binding of a new state by the QW, show up *irrespective* of T^*. On the other hand, the oscillations labeled $R_2,R_3,\ldots$, weaken and tend to move closer from those labeled $2,3,\ldots$, in a τ vs L plot when T^* decreases. This is hardly surprising since low T^*'s (i.e., $k_BT^* \ll \hbar\omega_{LO}$, where k_B is the Boltzmann constant) exponentially cut off the continuum states which are beyond k_BT^* from the continuum edge. Thus, the virtual bound states $2,3,\ldots$ have necessarily to be within k_BT^* (instead of $\hbar\omega_{LO}$ like in Figs. 1 and 2) from the continuum edge to give rise to a capture resonance, i.e., $R_2,R_3,\ldots$ have to move closer from $2,3,\ldots$ than shown in Figs. 1 and 2, if a Boltzmann f is used instead of an equirepartition.

Our calculations have not included the thermally activated carrier escape from the QW to the continuum due to the absorption of LO phonons, a process which takes place in the same L range as the resonant capture. Thus, strictly speaking, our calculations can only be applied to low-temperature experiments where no LO phonons are present. In room-temperature operating devices, the resonant capture will be smoothed out due to the simultaneous occurrence of carrier escape. This feature may eventually be correlated with the rather smooth L dependence of lasing threshold observed by Hersee *et al.*[1] in QW lasers operating at room temperature.

There is only a single experimental result with which our calculations can reasonably be compared. Göbel *et al.*[3] have fitted their time-dependent photoluminescence experiments with a single capture time: $\tau = 50$ ps for a single GaAs-$Ga_{0.82}Al_{0.18}As$ quantum well of nominal parameter $L = 50$ Å, $\mathscr{L} = 1$ μm. Taking $V_e = 135$ meV, $V_h = 90$ meV (i.e., V_e equal to 60% of the band-gap difference between GaAs and $Ga_{1-x}Al_xAs$), $m_e = 0.074 m_0$ (to account for nonparabolicity) and $m_h = 0.45 m_0$, we have found $\tau_e = 180$ ps and $\tau_h = 45$ ps. We consider these values to be in good agreement with the experiments of Göbel *et al.*, especially in view of the uncertainties of the fitting procedure (a single τ) and of the assumption of the equirepartition of the continuum states. In any event, a more systematic study of the τ vs L dependence is required to ascertain whether our approach of the carrier capture is correct. The experiments of Christen *et al.*[2] were performed on multiple quantum wells and, thus, cannot be safely compared with our one-well theory.

In conclusion, we have presented the results of quantum-mechanical calculations of the carrier capture by idealized semiconductor quantum-well structures. We have shown that in contrast with classical calculations, the capture time exhibits marked oscillations upon the well width, which we have shown to be associated either with the binding of a new bound state by the QW or with the occurrence of a virtual bound state within $\hbar\omega_{\mathrm{LO}}$ from the continuum edge. We have found that the holes are more efficiently collected than the electrons by the QW due to the larger density of states of holes for final states. We believe that the inclusion of band-structure effects (effective-mass mismatch, band nonparabolicity, etc.) cannot qualitatively alter the conclusions of our paper which are ultimately based on the existence of two genuine QW features: the bound and virtual bound states. Finally, the pronounced oscillations of the capture time will have an impact on the design of more efficient QW devices, if the device performances are closely linked to the capture phenomena.

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