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Quantum-size effects in the continuum states of semiconductor quantum wells

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We present theoretical results bearing on the energy position and spatial localization of the low-lying "barrierlike" states (i.e., states which are not bound in the narrow well) in semiconductor separate confinement heterostructures. We show that under most circumstances these states are less localized than classically expected. However, when a virtual bound state of the narrow well occurs near the onset of the narrow-well continuum or when a state has just been bound by this well, the quantum-well-projected density of states of the system is much larger than in nonresonant situations. This points out the possible influence of the virtual bound states in the mechanism of carrier capture by the quantum well.

It is now well established that lasing action is easier in separate confinement heterostructures (SCH) than in the conventional double heterostructure lasers.[1-3] This effect has been attributed to the quasi-two-dimensional density of states associated with the bound states of the quantum well (QW) between which laser action occurs. Efficient carrier collection by the QW is also frequently invoked. The mechanism of such carrier capture through optical-phonon emission has been theoretically studied by Shichijo *et al.*[4] and Tang *et al.*[5] neglecting, however, the quantum aspect of the carrier motion along the growth axis. Recently, we pointed out[6] that semiconductor QW's, like the idealized ones,[7,8] display pronounced quantum effects for both the discrete and the continuum spectra. These effects manifest themselves through an oscillatory behavior upon the carrier energy of the transmission coefficient T across the QW. Neglecting band-structure effects (effective mass mismatch, intervalley couplings, band nonparabolicity, etc.) $T(\epsilon)$ is given for a rectangular QW by[7,8]

$$T(\epsilon)=\left[1+\frac{1}{4}\left(\frac{k_w}{k_b}-\frac{k_b}{k_w}\right)^2\sin^2 k_w w\right]^{-1} , \tag{1}$$

where w is the QW thickness and k_w (k_b) are the carrier wave vectors in the well (barrier)

$$k_w^2=\frac{2m^*}{\hbar^2}(\epsilon+V_b);\quad k_b^2=\frac{2m^*\epsilon}{\hbar^2} . \tag{2}$$

In Eq. (2), m^* is the carrier effective mass and V_b the barrier height. The energy origin has been taken at the onset of the QW continuum. At $\epsilon=0$, the transmission vanishes [unless $wk_w(0)=p\pi$, where p is an integer]: the carrier is totally reflected by the QW. If however $wk_w(0)=(p+\alpha)\pi$, $\alpha \ll 1$, one sees from Eq. (1) that the transmission will steeply increase with ϵ reaching unity if $\alpha<0$ and becoming large (but <1) if $\alpha>0$. The first situation ($\alpha<0$) corresponds to the true transmission resonances which fulfill

$$wk_w(\epsilon)=p\pi . \tag{3}$$

Equation (3) is satisfied only for certain discrete energies. Transmission resonances can also be viewed as virtual bound states.[7,8] 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 levels, they decay gradually with a time constant $\hbar/\Gamma$, where Γ is the energy width of the transmission resonance. Narrow resonances exist only if $k_b/k_w \ll 1$: the closer the resonances are from the onset of the continuum, the smaller their widths.

The second situation ($0<\alpha\ll 1$) occurs when a level has just been bound by the well (binding energy $\ll V_b$). The transmission steeply increases near $\epsilon=0$ but does not reach unity. As in the case $\alpha<0$, $T(\epsilon)$ increases rapidly because the condition for constructive interferences inside the QW slab is almost fulfilled. $T(\epsilon)$ remains smaller than unity when $\alpha>0$ since, by increasing ϵ, the states move away from resonance where an integer number of carrier wavelength should fit to $2w$. On the contrary, if $\alpha<0$, the states move towards the resonance with increase in ϵ and $T(\epsilon)$ reaches unity at some. In summary, the carrier transmission across a QW vanishes at the onset of the QW continuum but can be large near $\epsilon=0$, either when a virtual bound state has just popped out of the QW ($T_{\max}=1$) or when a level has just been bound in the well ($T_{\max}<1$). A nonresonant situation occurs when $wk_w(0)=(p+\alpha)\pi$, $\alpha\sim\frac{1}{2}$. In this case, near $\epsilon=0$, $T(\epsilon)$ remains very small and the carrier repulsion by the QW is larger.

Suppose now that a carrier has been injected deep inside the QW continuum ($\epsilon\sim V_b$). It will quickly (10^{-12}–10^{-13} s) relax its energy by emitting optical phonons (intracontinuum transitions). High-energy transmission resonances are very broad ($k_b/k_w\sim 1$) and in practice negligible; $T(\epsilon)\sim 1$ for any ϵ. The direct carrier capture by the QW (continuum $\rightarrow$ bound-states transitions) is very unlikely since it would require a very large change of the carrier wave vector in the layer plane to ensure energy conservation within the energy of an optical phonon $\hbar\omega_{\mathrm{LO}}$. The fast LO phonon emission lasts until the carrier energy is within $\hbar\omega_{\mathrm{LO}}$ from the edge of the QW continuum. A subsequent phonon emission, leading to the carrier capture, requires the carrier to shrink its delocalized wave function down to w to end up in a QW bound-state wave function. The matrix element of the electron-phonon interaction will be much smaller for the capture than the one corresponding to intracontinuum transitions. Hence, the edge of the QW continuum may act like a bottleneck for the energy relaxation. We believe the capture process can be more efficient if, within $\hbar\omega_{\mathrm{LO}}$ of the continuum edge, there exists a virtual bound state or if a QW level is marginally bound. Actual QW lasers are made from SCH or graded-index SCH (GRINSCH). Here, we focus our attention on SCH.

We model the SCH as follows (Fig. 1). A QW of thickness w and barrier height V_b is inserted at the center of a

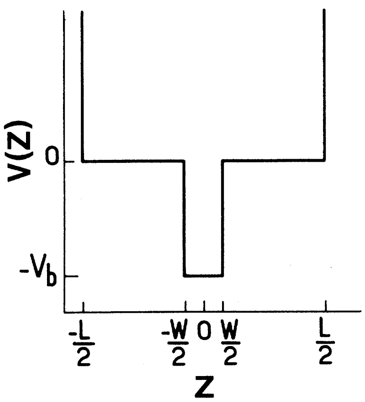

FIG. 1. Conduction-band profile of an idealized SCH. The potential energy is assumed to be infinite for $|z| > L/2$.

large well which we assume for convenience to be of infinite height ($z = \pm L/2$). The total thickness of the structure is L. We take the energy zero at the bottom of the large well and discuss the "barrierlike" states of positive energies. Since the cladding barriers are impenetrable, all the states are discrete. Neglecting band-structure effects, z and (x,y) motions separate. Energy levels and wave functions for the z motion are denoted by ϵ_n and $\chi_n(z)$, respectively. The free motion in the layer plane (wave vector $\vec{k}$) adds the kinetic energy term $\hbar^2k^2/2m^*$ to ϵ_n. Eigenstates are even or odd in z due to the mirror symmetry with respect to the center of the structure. The integrated probability of finding the carrier in the small well while being in the state χ_n is

$$P_n = 2\int_0^{w/2} \chi_n^2(z)\,dz \quad . \tag{4}$$

We define the QW-projected density of states (DOS) $\rho(E)$ as the number of states per unit energy whose total energy is between E and $E+dE$, each of the state being weighted by the probability of finding the carrier in the small well:

$$\rho(E) = 2\sum_{n\vec{k}} P_n \delta\left[E - \epsilon_n - \frac{\hbar^2k^2}{2m^*}\right] = \rho_0 \sum_n P_n Y(E-\epsilon_n) \quad , \tag{5}$$

where $Y(x)$ is the step function [$Y(x)=1$ if $x>0$, $Y(x)=0$ if $x<0$] and $\rho_0 = m^*S/\pi\hbar^2$ is the two-dimensional DOS, S being the sample area. $\rho(E)$ emphasizes the carrier localization in the small well. We believe it is more appropriate than the conventional DOS [obtained by deleting P_n in Eq. (5)] to ascertain which continuum states are more efficient in a capture event (the final state of the carrier is essentially localized over w). Figure 2 shows the energy dependence of $\rho(E)$ for increasing w keeping V_b and L constant ($V_b = 195$ meV, $L = 3000$ Å) and taking $m^* = 0.067m_0$. These values correspond roughly to the conduction-band parameters of a GaAs-$Ga_{0.82}Al_{0.18}As$ SCH. The classical regime (not shown in Fig. 2) occurs at large E ($E \sim V_b$) where the narrow well is a small perturbation for the large well states. In that case, $P_n \sim w/L$ and $\rho(E)$ becomes proportional to the conventional DOS. It is evident on Fig. 2 that the low-energy barrierlike states behave completely differently.

(i) $\rho(E)$ is much smaller than its classical limit (w/L per step on Fig. 2). This is reminiscent of the carrier repulsion by the narrow QW when L is infinite [$T(0)=0$] and implies incidentally that $\rho(E)$ does not behave like $E^{1/2}$ near the onset of the continuum.

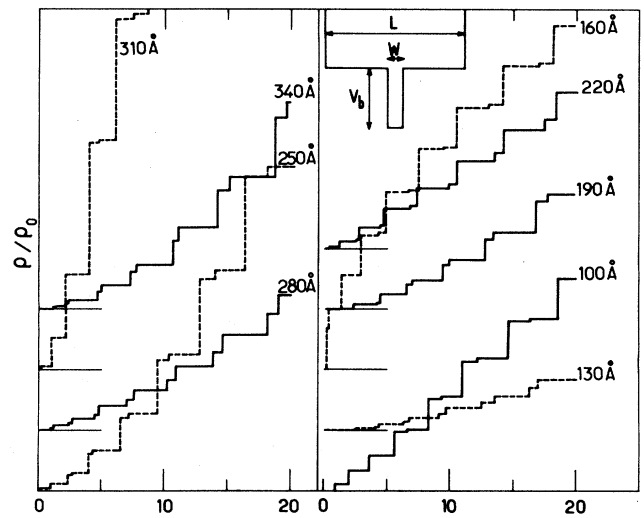

FIG. 2. Quantum-well projected density of states (in units of ρ_0) of an idealized SCH vs energy E. L and V_b are kept constant (0.3 μm and 195 meV, respectively) while w varies. Curves corresponding to different w are displaced vertically and are alternatively drawn in solid and broken lines. ρ/ρ_0 (linear scale) varies by 0.05 between two horizontal divisions.

(ii) For some w, $\rho(E)$ is much larger and increases faster with E than found for wells of adjacent w (compare, for instance, $\rho(E)$ for $w = 160$ Å with the ρ's calculated for $w = 130$ Å and $w = 190$ Å.) These enhanced $\rho(E)$ occur whenever $wk_w(E=0) = (p+\alpha)\pi$, $|\alpha| << 1$, i.e., when a level has just become bound ($\alpha > 0$) or has become a virtual bound state of the small well ($\alpha < 0$). In the specific case of $w = 160$ Å, the fourth QW bound state[9] (E_4) has just entered in the well ($\alpha \sim 0.045$) whereas for $w = 310$ Å, E_7 forms a resonance near 6.7 meV from the edge. For $w = 130$ Å and $w = 190$ Å, the whole investigated energy range corresponds to a nonresonant situation [$wk_w(\epsilon) \sim 2.5\pi$ and $wk_w(\epsilon) \sim 3.7\pi$, respectively]. Correspondingly, the ρ's are very small.

(iii) In the resonant situation, there exists a strong asymmetry between the heights of the steps associated with even or odd levels. For $w = 160$ Å, the odd states have a much larger probability density to be localized in the well: inside the QW, they closely resemble the odd E_4 QW bound state. On the other hand, it is impossible for even levels to fit the shape of the E_4 state within the well. They are accordingly heavily repelled by the small QW and their contribution to $\rho(E)$ is then very small. In the nonresonant situation, the even and odd contributions display less asymmetry.

Another feature apparent in Fig. 2 is the size quantization associated with the large well. Actually broadening effects will smooth the $\rho(E)$ curves. Nevertheless, the high quality of the present SCH's may be sufficient to observe this size quantization. We present in Fig. 3 $\rho(E)$ curves obtained by varying L while keeping V_b and w constant (195 meV and 155 Å, respectively). For $w = 155$ Å, E_4 has become a resonance located at ~ 6.7 meV from the edge. One sees in Fig. 3 the strong increase of ρ/ρ_0 near that energy. The symmetry-induced repulsion is also clearly apparent for all

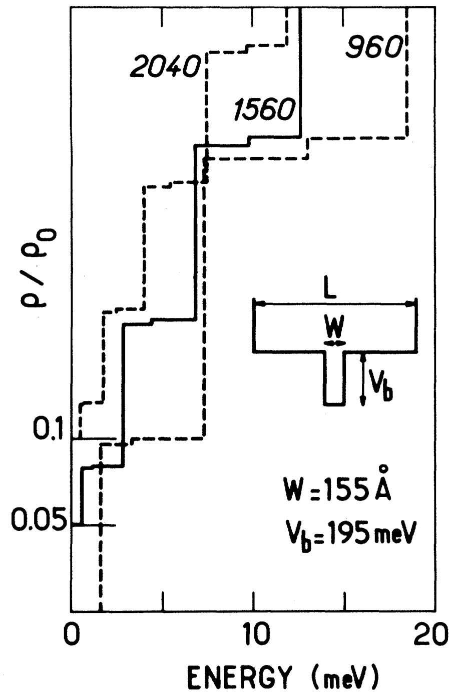

FIG. 3. Quantum-well-projected density of states (in units of ρ_0) of an idealized SCH vs energy E. w and V_b are kept constant (155 Å and 195 meV, respectively) while L varies. Curves corresponding to different L are displaced vertically and are alternatively drawn in solid and broken lines. ρ/ρ_0 (linear scale) varies by 0.05 between two horizontal divisions.

L: large steps occur only for odd levels. Note again that the energy levels are not dominated by the large well (they do not vary like n^2/L^2).

Lasing action in very narrow wells ($w \lesssim 30$ Å) is known[1] to be more difficult than in larger wells ($w \sim 150$ Å). Difficulties in growing good interfaces may be an explanation.[10,11] Shichijo *et al.*[4] has applied Fermi's "age theory" to predict that carrier collection will be inefficient in narrow wells. If we link the easy carrier capture to the condition $wk_w(0) = (p+\alpha)\pi$, $\alpha << 1$, we deduce the carrier capture will become difficult when the last virtual bound level (E_2 for electrons) will have moved beyond $\hbar\omega_{\rm LO}$ from the bottom of the large well (all the low-energy barrierlike states being then repelled by the small QW). For the parameters we used $V_b = 195$ meV, $m^* = 0.067m_0$, $\hbar\omega_{\rm LO} = 37$ meV; this corresponds to $w \lesssim 50$ Å. Heavy holes ($V_b = 34.4$ meV, $m^* = 0.048m_0$) will not be collected if $w \lesssim 33$ Å.

In summary, we have discussed the low-lying barrierlike states in semiconductor QW and SCH. We have shown that their behavior is strongly influenced by constructive or destructive interferences in the narrow QW. We have also shown that each time a level (bound or virtually bound) is near the onset of the small well continuum, the QW-projected DOS is much larger than in other (nonresonant) situations. The calculations have neglected band-structure effects and assumed impenetrable confining barriers in the SCH. These two assumptions can be relaxed. This will change the numbers but in no case alter the qualitative features of the analysis. GRINSCH structures appear to be more efficient carrier collectors than SCH.[1] Preliminary results indicate that actual GRINSCH (equivalent electric field $\sim 10^6$ V/m) considerably increase the localization of the low-lying barrierlike states in the narrow well, therefore enhancing the carrier collection. Detailed results on these GRINSCH structures will be reported elsewhere.

We have suggested that the virtual bound levels may be efficient relays in the carrier capture because, in many respects, they behave like true bound levels. A complete theory of the energy relaxation, accounting for the complicated nature of the QW continuum states, is however, necessary to prove or disprove the correctness of our suggestion.

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