Calculation of carrier capture time of a quantum well in graded-index separate-confinement heterostructures

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The electron capture time into the quantum well of a graded-index separate-confinement heterostructure laser has been calculated at 77 and 300 K. The results (at 77 K) show oscillations between several picoseconds and several tens of picoseconds with increasing quantum-well thickness, qualitatively similar to the behavior in simple separate-confinement structures. Quantitatively, the difference in capture times for optimal structures of each kind does not explain the lower threshold of the graded-index structure.

I. INTRODUCTION

Recent experimental works[1–4] have demonstrated the high performances of quantum-well lasers. Nevertheless, all the physical mechanisms accounting for the quality of these lasers are not yet well understood. One of the reasons may be the efficient capture of carriers by the quantum wells. Shichijo *et al.*[5] and Tang *et al.*[6] studied the problem within a classical framework by considering the LO phonon scattering. More recently, Brum *et al.*[7] studied the quantum effects of the carrier capture by semiconductor quantum wells. They reported strong oscillations of the capture time as a function of the well width. These resonances originate from the binding of a new bound state by the quantum well. Göbel *et al.*[8] and Miyoshi *et al.*[9] performed time-resolved photoluminescence experiments and obtained carrier capture times of 0.05 and 2 ns, respectively. Christen *et al.*,[10] using time-resolved cathodoluminescence, obtained 0.1 ps. More recently, Mishima *et al.*[11] observed strong dependence of the excitation intensity dependence of photoluminescence by the quantum-well length. Their results were interpreted in terms of the carrier trapping efficiency under resonant and off-resonant conditions.

We present here a calculation of the LO-phonon–assisted capture time by a quantum well of the carriers confined in the optical cavity of a graded-index separate-confinement heterostructure (GRINSCH) laser and discuss to what extent the results can help to explain the improved performances observed in GRINSCH (low threshold current).

II. CALCULATION OF THE CAPTURE TIME

We consider a GRINSCH structure as the one shown in Fig. 1. In the effective mass approximation, the envelope function of a state is $\Psi(\mathbf{r})=\exp(i\mathbf{K}\cdot\mathbf{r})\xi_n(z)$, where $\mathbf{K}$ is a wave vector describing the motion parallel to the epitaxial layers, n the subband index. At high temperature, in high quality samples, the interaction with polar optical phonons prevails over any other scattering process. The probability for an electron of the barrier in the $(n,\mathbf{K})$ state to be scattered into the well state $(n',\mathbf{K}')$ by a phonon of momentum $(\mathbf{Q},q_z)$ ($\mathbf{Q}$ is the component of momentum parallel to the layers), was first computed by Price:[12]

$$S^{\pm}(n,\mathbf{K}\xrightarrow{\mathbf{Q}}n',\mathbf{K}')=\frac{2\pi g^2\Omega}{\hbar A}\left(n_q+\tfrac{1}{2}\pm\tfrac{1}{2}\right)\frac{f_{nn'}(Q)}{2Q}\times\delta_{\mathbf{K}',\mathbf{K}\mp\mathbf{Q}}\delta(E_{n'\mathbf{K}'}-E_{n\mathbf{K}}\pm\hbar\omega_{\mathrm{LO}})\ , \tag{1}$$

where

$$S^{\pm}(n,\mathbf{K}\xrightarrow{\mathbf{Q}}n',\mathbf{K}')=\sum_q S^{\pm}_{\text{Fröhlich}}(n,\mathbf{K}\xrightarrow{\mathbf{Q},q_z}n',\mathbf{K}')\ , \tag{2}$$

$$f_{nn'}(Q)=\int_{-\infty}^{+\infty}dz\int_{-\infty}^{+\infty}dz'\,\xi_n(z)\xi_{n'}(z)\xi_n(z')\xi_{n'}(z')\times e^{-Q|z-z'|}\ , \tag{3}$$

$$g^2=e^2\hbar\omega_{\mathrm{LO}}/(2\Omega)(1/\epsilon_\infty-1/\epsilon_0)\ , \tag{4}$$

$$n_q=1/(e^{\hbar\omega/kT}-1)\ , \tag{5}$$

where A and Ω are the area and volume of the sample, respectively. ϵ_∞ and ϵ_0 are the dielectric permittivity at very high and very low frequencies. The sign + (respectively, −) is for the emission (absorption) of a LO phonon. The total particle flow from the barrier to the well can then be obtained by summing over all initial (barrier) states and all final (well) states:

$$J^{\pm}=\sum_{n(\text{barrier})}\sum_{n'(\text{well})}\int d^2K\,\rho(n,\mathbf{K})f_b(E_n,\mathbf{K})\int d^2K'\,\rho(n',\mathbf{K}')[1-f_w(E_{n'},\mathbf{K}')]\int d^2Q\,\rho(Q)S^{\pm}(n,\mathbf{K}\xrightarrow{\mathbf{Q}}n',\mathbf{K}')\ , \tag{6}$$

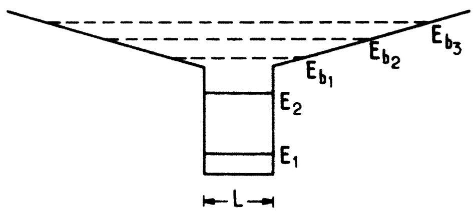

FIG. 1. GRINSCH potential profile for the conduction band. The dimensions are not to scale.

$\rho(n,\mathbf{K})$, $\rho(n',\mathbf{K}')$, and $\rho(\mathbf{Q})$ being the density of modes, $f_b(n,\mathbf{K})$ and $f_w(n',\mathbf{K}')$, the occupation probability, respectively, in the barrier and in the well. As the total number of carriers in the barrier is given by

$$N=\sum_n \int d^2K\,\rho(n,\mathbf{K})f_b(E_n,\mathbf{K})\ , \tag{7}$$

the average time for a carrier to be trapped by the well is $\tau_c=N/J$, where $J=J^+ + J^-$.

The complete calculation and formula are given in Appendix A. Note that in formula (6), we somewhat arbitrarily consider as a "well state" any state whose subband minimum is under the potential energy at the beginning of the confining barrier, even if a carrier in such a state has a non-negligible probability of being outside the well, especially for shallow levels. Symmetrically, we count as "barrier states" the first subband above the well which is sometimes almost localized in the well, owing to the funnel shape of the energy profile. This leads to some artifacts in the results, as mentioned below.

III. RESULTS

We consider the injected electrons as thermalized in the confining layers with a Boltzmann distribution (this point is discussed in Appendix A). The electron effective mass used is $0.07m_0$, where m_0 is the free-electron mass. In Fig. 2 we plot the electron capture time τ_c versus the quantum-well (QW) width L. The conduction-band discontinuity at the abrupt interface, ΔE_c is 150 meV (corresponding to an Al concentration of about 0.2). The barrier is graded resulting in a built in electric field of 0.1 meV/Å [Fig. 2(a)]. Finally, all the calculations were performed for a carrier temperature of 77 K [Fig. 2(a)] or 300 K [Fig. 2(b)]. In Fig. 2(a) we have also plotted (dashed line) the results[7] for a QW with horizontal barrier [equivalent to a separated confined structure (SCH)] with the same parameters (electron effective mass of $0.07m_0$, $x=0.2$, $T=77$ K) and a total thickness structure of 1 μm.

For the GRINSCH, starting from very narrow wells, we first see a decrease of the τ_c as the (unique) bound state gets deeper into the well. It reaches its minimum value when it is separated from the lowest barrier state E_{b1} by about $\hbar\omega_{\rm LO}$ ($\sim$36 meV). Beyond this point, the energy difference of the two levels increases, allowing only processes involving final states with $k_\perp \neq 0$, and the capture becomes less efficient. In competition with this effect is the better confinement of E_{b1} in a wide well, which favors a lot the capture (better overlap) and causes τ_c to decrease again.

This drop stops when E_{b2} becomes the second bound state ($L\sim 70$ Å). Although the appearance of a new bound state should favor the carrier capture, the latter is in fact hampered by the loss of a well localized quasicontinuum state. Furthermore, the separation between initial and final levels is much lower than $\hbar\omega_{\rm LO}$, allowing only capture from high transverse momentum initial states. The net result is an abrupt increase of the capture time. If we keep increasing L, τ_c decreases again and the whole cycle is repeated. It is important to observe that the abrupt variation of τ_c when the well accepts a new bound state is not a real physical effect. This variation has its origin in our definition of bound and barrier states and of their occupation. In fact, when the topmost bound state is near the top of the QW (or the bottom barrier state is localized in the well), a more complex situation occurs and the abrupt variation should be smoothed. Our model cannot describe this situation and more sophisticated calculations would have to be performed, either by Monte-Carlo simulations or by refining the model, e.g., by considering three populations in interaction (the well states, E_{b1}, and

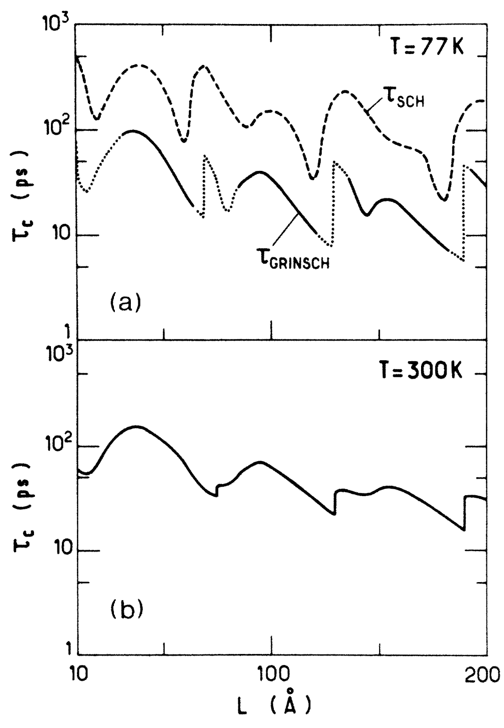

FIG. 2. Electron capture times τ_c versus the quantum-well thickness L for a GRINSCH [(a), solid and dotted lines] and a SCH [(a), dashed line] for an electron temperature of 77 K and for a GRINSCH (b) at 300 K. The parameters used are as follows: electron effective mass of $0.07m_0$, $\Delta E_c=150$ meV, $F=0.1$ meV/Å (for the GRINSCH) and a total structure length of 1 μm (for the SCH). The dotted parts of the GRINSCH curve in (a) correspond to L values for which either the topmost bound state has a probability smaller than 60% to be found in the well or the first barrier state has a probability larger than 30% to be found in the well.

the barrier states other than E_{b1}). To give an idea of the limits of validity of the calculations we have drawn in dotted line on Fig. 2(a) the part of the curve for which the topmost bound state has a probability lower than 60% in the well or the first barrier state is more than 30% in the well.

We have included in our calculations the contribution to the capture into all the bound states. However, as for the QW with a horizontal barrier,[7] only the topmost bound state is important. The SCH results (dashed line) show almost the same structures. However, we cannot compare directly the GRINSCH and SCH capture time since the last is directly proportional to the total structure length and it is not obvious what is the equivalent value which should be taken for a determined value of F for the GRINSCH.

The results obtained at 300 K with the same parameters [Fig. 2(b)] show similar structures. The oscillations are weaker since we have more populated levels. Also, the capture is a little slower since the more effective levels for the capture (smaller energy) are less populated than for a temperature of 77 K.

We do not show a computation we made for $T=77$ K and $F=0.08$ meV/Å (all the other parameters being the same) since the resulting curve appears to be almost parallel to that of Fig. 2(a).

In Fig. 3 we show the carrier capture time for a QW of 100 Å width as a function of the inverse of the quasielectric field F, all the other parameters being the same as in Fig. 2(a). We observe a rapidly decreasing τ_c for increasing F for small values of F. This is because of the increased confinement of the quasicontinuum states. For actual F values, the energy separation between the topmost bound state and the first quasicontinuum state is almost constant. The predominant effect is the increase of the confinement of the barrier state which saturates for values of F between 0.05 and 0.1 meV/Å. Other effects may appear for larger values of F, but these values do not correspond to experimental situations.

Note that in the range of current lasers (0.04 to 0.2 meV/Å), τ_c is approximatively proportional to $1/F$. As the density of states of a symmetrical triangular well also varies as $1/F$ (see, e.g., Ref. 6), this means that the injection current ($J \sim N/\tau_c$) does not depend strongly on the slope F. This result is very similar to what happens in rectangular SCH where both τ_c and N are about proportional to the width of the optical confinement layer.

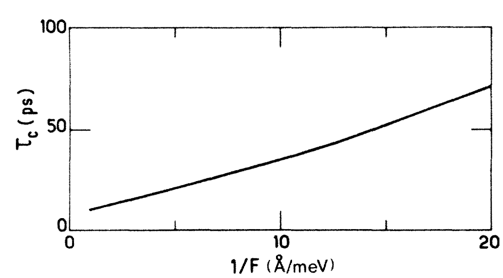

FIG. 3. Electron capture time versus the inverse of the quasielectric field of a GRINSCH with a quantum-well thickness of 100 Å. All the other parameters are the same as those in Fig. 2(a).

IV. CONCLUSIONS

We have calculated the carrier capture time by a QW in a GRINSCH structure. Strong oscillations were observed as a function of L, whose amplitude decreases at high temperature. These oscillations have similar origin as those reported for the quantum well with a horizontal barrier. The GRINSCH structure presents new aspects for the carrier capture time because of the confinement of the quasicontinuum states. Unlike its dependence on the well width, the capture time does not vary very much with the geometry of the confinement layers (slope for a GRINSCH).

Furthermore, it can be seen from simple rate equations that the populations in the barrier N and the well n_0 are given approximately by $N=t_c n_0/t_w$ and $I=n_0(1+t_c/t_b)/t_w$ in the stationary case. Here, I is the injected current, t_c the capture time, t_b the lifetime of a carrier in the barrier (by radiative or nonradiative recombination), and t_w the lifetime in the well. As the threshold for positive gain depends directly on n_0 and on the optical confinement factor, a laser with a given optical confinement is the better the lower t_c/t_b. However, this effect is rather weak so the capture time is not a crucial parameter for the optimization of the laser threshold current. For that purpose the optical confinement factor and the relation between the number of carriers in the well and the Fermi level[13] are much more relevant.

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APPENDIX A: CALCULATION FOR A GRINSCH AND A SCH

The quantities $\rho(n,\mathbf{K})$,$\rho(n',\mathbf{K})$ and $\rho(\mathbf{Q})$ are equal to

$$\rho(n,\mathbf{K})=\rho(n',\mathbf{K})=A/(2\pi^2)\ , \tag{A1}$$

$$\rho(\mathbf{Q})=A/(4\pi^2)\ . \tag{A2}$$

We use a parabolic band approximation

$$E_{n\mathbf{K}}=E_n^0+\hbar^2K^2/(2m)\ , \tag{A3}$$

$$E_{n'\mathbf{K}'}=E_{n'}^0+\hbar^2(K')^2/(2m)\ . \tag{A4}$$

Noting that

$$\delta(E_{n'\mathbf{K}'}\pm\hbar\omega_{\mathrm{LO}}-E_{n\mathbf{K}})=(m/\hbar^2Q)\delta((m/\hbar^2Q)(E_{n'}^0\pm\hbar\omega_{\mathrm{LO}}-E_n^0)+Q/2\mp\mathbf{K}\cdot\mathbf{Q}/Q) \tag{A5}$$

$$J^{\pm}=(\mathrm{A}g^2\Omega m/4\pi^3\hbar^3)(n_q+\tfrac{1}{2}\pm\tfrac{1}{2})\sum_n\sum_{n'}\int d^2Q\,f_{nn'}(Q)/Q^2\int d^2K\,[1-f_w(E_{n',\mathbf{K}\pm\mathbf{Q}})]f_b(E_{n,\mathbf{K}})$$
$$\times\delta((m/\hbar^2Q)(E_{n'}^0\pm\hbar\omega_{\mathrm{LO}}-E_n^0)+Q/2\mp\mathbf{K}\cdot\mathbf{Q}/Q)\ . \tag{A6}$$

The sum over $\mathbf{K}$ can be split into a sum over the components parallel and perpendicular to $\mathbf{Q}$,

$$\int d^2Q\ldots=\int dQ\,2\pi Q^{-1}f_{nn'}(Q)\int dK_\perp[1-f_w(E_{n',\mathbf{K}\mp\mathbf{Q}})]f_b(E_{n,K,K=(m/\hbar^2Q)(E_n^0\pm\hbar\omega-E_n^0)+Q/2})\ . \tag{A7}$$

In the following we shall assume that f_b can be taken as a Maxwellian distribution and that f_w is much smaller than 1 (which means that there are few electrons in the conduction band). These conditions are not so good in the standard working conditions of lasers, but an accurate calculation requires a good knowledge of the position of the Fermi level in the structure which depends dramatically on all the technological and physical parameters of the laser (length of the chip, internal losses, etc.). Then the integral in Eq. (A7) can be explicitly calculated,

$$\int dK_\perp(1-f_w)f_b\simeq\int\exp[-(\hbar^2/2mkT)(K_\parallel^2+K_\perp^2)]dK_\perp=(\sqrt{2\pi mkT}/\hbar)e^{-\hbar^2K_\parallel^2/(2mkT)}\ . \tag{A8}$$

Dividing $J^{\pm}$ by the number of particles in the barrier (calculated with the same assumptions), one gets

$$1/\tau_c^{\pm}=\frac{g^2\Omega(n_q+\frac{1}{2}\pm\frac{1}{2})}{2\hbar^2\sqrt{2\pi kT/m}}\sum_{n'}\left\langle\int dQ\,Q^{-1}f_{nn'}(Q)\exp[(-\hbar^2/8mkT)(Q+B^{\pm}/Q)^2]\right\rangle_n\ , \tag{A9}$$

where

$$B^{\pm}=(2m/\hbar^2)(E_{n'}^0\pm\hbar\omega_{\mathrm{LO}}-E_n^0) \tag{A10}$$

and

$$\langle g\rangle=\sum_n e^{-E/kT}g_n\Big/\sum_n e^{-E/kT}\ . \tag{A11}$$

One can see from this formula that almost all the contribution will come from scattering into the shallowest level of the well, as the exponential factor in the last integral will become very small as soon as

$$E_{n'}^0-E_n^0\pm\hbar\omega_{\mathrm{LO}}\gg\hbar^2Q^2/2m\sim\hbar^2K^2/2m\ .$$

For a SCH, the levels are very close to each other so that one can use a continuous approximation for the integration

$$1/\tau_c^{\pm}=[g^2\Omega(n_q+\tfrac{1}{2}\pm\tfrac{1}{2})/(4\pi\hbar kT)]\sum_n\sigma_n\ , \tag{A12}$$

with

$$\sigma_n=\int d\xi\int dQ\,Q^{-1}\exp\{-(\hbar^2/8mkT)[4\xi^2+(Q+B^{\pm}/Q)^2]^2\}f_{\xi n}(Q)\ . \tag{A13}$$

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