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Properties of electrons and excitons in graded quantum wells of $Ga_{1-x}Al_xAs$ in an electric field

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Abstract. Using the method of series expansion, sub-bands of electrons and holes, electron–hole overlap functions and binding energies of excitons are calculated for the graded quantum well of $Ga_{1-x}Al_xAs$ with a $Ga_{0.66}Al_{0.34}As$ barrier in the electric field F between 0 and ± 9 (10^4 V cm^{-1}). The width of the well is 200 Å, and the electric field is perpendicular to the material layers. The calculations reveal that the behaviour of electrons and excitons in this well is very different from that in square quantum wells and is useful for some device applications.

The advances in crystal growth techniques such as molecular beam expitaxy (MBE) and metal–organic chemical vapour deposition (MOCVD) has made possible the growth of GaAs – $Ga_{1-x}Al_xAs$ systems with very precisely controlled thicknesses of players and concentration x of aluminium. Among the systems, the square quantum wells (SQW) have frequently been studied by a number of techniques. Recently, Capasso *et al* [1] drew attention to some interesting application of graded-gap structures such as sawtooth superlattices. The electronic structure of the graded-gap systems without an applied electric field has been studied by several authors [2–4]. In order to achieve high device performances, such as a high on/off ratio and a low operation voltage, a small decrease of the oscillator strength of a ground-state exciton and a large Stark shift of excitons by an external electric field, Polland *et al* [5], Nishi and Hiroshima [6] and Zhu *et al* [7] have proposed a graded quantum well (GQW) structure, where the conduction- and valence-band edges vary linearly along the growth direction in the well layer, and have studied sub-bands and excitons in GQW in an electric field. Hiroshima and Nishi [8] have calculated the exciton states associated with the lowest electron and heavy-(light-) hole sub-bands. However, they have not studied the exciton states associated with higher electron and hole sub-bands in a GQW under an electric field. In this paper, we study not only the properties of electrons and holes in different sub-bands but also those of the exciton states associated with different electron and hole sub-bands in a GQW under an electric field. A novel method is used to calculate the quantum levels and wavefunctions of electrons and holes. The method is suitable not only for a linear GQW, mentioned above, but also for the other kinds of GQW. Calculated results reveal that the behaviour of electrons and excitons in GQW in an electric field is very different from that in SQW, and that it is useful for some device applications.

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Assuming that the GQW are of the form

$$V(Z) = \begin{cases} V_0 & |Z| \geqslant L/2 \\ V_0 R(Z/L + \frac{1}{2})^n & |Z| < L/2 \end{cases} \qquad (0 \leqslant R \leqslant 1, n = 1, 2, 3, \ldots) \tag{1}$$

we take the effective Hamiltonian of a particle, with charge q and mass m_Z, under an electric field F in the Z direction as follows:

$$H_Z = H_{Z0} + H'_Z \tag{2}$$

where

$$H_{Z0} = -\frac{\hbar^2}{2m_Z}\frac{d^2}{dZ^2} + V(Z) - \theta(L/2 - |Z|)qFZ - \theta(|Z| - L/2)\,\mathrm{sgn}(Z)qFL/2 \tag{3}$$

and

$$H'_Z = \theta(|Z| - L/2)[-qFZ + \mathrm{sgn}(Z)qFL/2]. \tag{4}$$

$\theta(x)$ is a step function, V_0 and L are the height and width of the GQW respectively. Here the theoretical calculation is different from those which several other authors have performed [9–12]. We solve exactly the Schrödinger-like equation of an electron ($q = -e < 0$) and a hole ($q = e > 0$) corresponding to H_{Z0} of (3). Under the bound-state assumption, the H'_Z of (4) is treated as a perturbation to H_{Z0}.

In the regions $Z \leqslant -L/2$ and $Z \geqslant L/2$, the solution of the equation

$$H_{Z0}\psi = E_Z\psi \tag{5}$$

are respectively

$$\psi^{\mathrm{I}}(Z) = A\exp(K_1 Z) \tag{6}$$

and

$$\psi^{\mathrm{III}}(Z) = D\exp(-K_3 Z) \tag{7}$$

where

$$K_1 = [2m_Z(V_0 - E_Z + qFL/2)]^{1/2}/\hbar^2 \tag{8}$$

$$K_3 = [2m_Z(V_0 - E_Z - qFL/2)]^{1/2}/\hbar^2 \tag{9}$$

and A, D are constants. In the region $|Z| < L/2$, expanding $\psi^{\mathrm{II}}(Z)$ as a uniformly covergent Taylor series and substituting it into (5), we get the solution as follows:

$$\psi^{\mathrm{II}}(Z) = B\sum_{K=0}^{\infty} b_K Z^K + C\sum_{K=0}^{\infty} c_K Z^K \tag{10}$$

where B and C are constants; b_K and c_K are the coefficients of the series solution which can be determined by the recurrence relations. Using the connection conditions of the wavefunction at $Z = -L/2$ and $Z = L/2$, we can obtain the equation of the eigen-energy of an electron or a hole. It should be pointed out that the effective mass has been assumed to be spatially independent in the Hamiltonian and the connection conditions. In order to get sub-band energies and wavefunctions, we have solved the eigen-energy equation and calculated the perturbation correction numerically.

The Hamiltonian of excitons in a quantum well in the presence of an electric field is written as (Greene *et al* [13]):

$$H = H_{eZ} + H_{hZ} + \frac{P_x^2 + P_y^2}{2M} + \frac{p_x^2 + p_y^2}{2\mu} - \frac{e^2}{\varepsilon r}. \tag{11}$$

Here H_{eZ} (H_{hZ}) is the H_Z of (2) with the mass m_Z and charge q replaced by electron mass m_{eZ} (hole mass m_{hZ}) and charge $-e$ (e). The third and fourth terms of (11) represent, respectively, the kinetic operators of the motion of the centre of mass and the relative motion of an exciton in the xy plane, which is parallel to the material layers. The electron–hole Coulomb interaction is described by the last term of (11). Based on the above sub-band calculation, the variational calculation of an exciton can be performed numerically.

Sub-bands of electrons and holes, electron–hole overlap functions and binding energies of excitons have been calculated for the GQW ($L = 200$ Å) with a $Ga_{0.66}Al_{0.34}As$ barrier with $R = 1$ and $n = 1$ in an electric field F between 0 and ± 9 (10^4 V cm^{-1}). Here the total band-gap mismatch is $\Delta E_g = 1.115x + 0.37x^2$ (eV) (Lee *et al* [14]), where x is the aluminium concentration in $Ga_{1-x}Al_xAs$. The mismatch is divided between the conduction and valence bands into $Q_e\Delta E_g$ and $Q_h\Delta E_g$. The band offset parameters Q_e and Q_h are taken to be 0.6 and 0.4, respectively. Electron and heavy-hole effective masses in the Z direction are taken to be, respectively, $m_{eZ} = 0.067m_0$ and $m_{hZ} = 0.34m_0$ (m_0 is the free electron mass). The μ in the kinetic operators of the relative motion of heavy-hole excitons in the xy plane is equal to $0.04m_0$.

The first three hole and electron quantum levels in the GQW with $R = 1$ and $n = 1$ and $F = 0$ are equal to 27.95, 63.37, 92.30 (meV), and 68.66, 147.61, 211.44 (meV), respectively. The wavefunctions are very different from those in SQW. They are either symmetric or antisymmetric in SQW which is not the case in GQW. Both electron and hole wavefunctions ae localised in the left side of the GQW. It is worthwhile to point out that the wavefunctions of holes in GQW without electric fields are more localised in the left side of the GQW than those of the electrons with the same number of sub-bands. When a positive electric field is applied, the holes and the electrons move, respectively, in the Z and $-Z$ directions in both GQW and SQW. If the direction of the electric field is changed, they move in the opposite directions. The squares of the wavefunctions are symmetric under a reversal of the direction of the electric field in SQW. However, in GQW a reversal of the direction of the electric field changes the squares of the wavefunctions a great deal.

The calculated energy shifts of electrons and holes due to the electric field are shown in figure 1. For conduction-band electrons, the GQW become sharper or flatter if the electric field is increased in Z or $-Z$ direction respectively, and for valence-band holes, the opposite occurs. Therefore, the absolute variation of the electron sub-band energies due to a positive field is larger than that due to a negative field. It is a different story for the hole sub-band energies. For valence-band holes, the absolute variation due to a positive field is smaller than that due to a negative field. Since the effective mass of a hole is larger than that of an electron, the absolute variations of the states with $1_h = 1$, 2 under $-F$ and F are larger than those of the states with $1_e = 1, 2$ under F and $-F$. In figures 1(a) and 1(b) it is easily seen that the energy shifts of electron and hole sub-bands are not symmetric about $F = 0$. For $1_e = 1_h$, the differences between the absolute variations of the electron and hole sub-bands in the positive field are smaller than those in the negative field. It should be noted that the energy difference between the first two electron states is increased if the field is increased in the Z direction, and it is decreased if the field is increased in the $-Z$ direction. This is quite different from the situation for SQW.

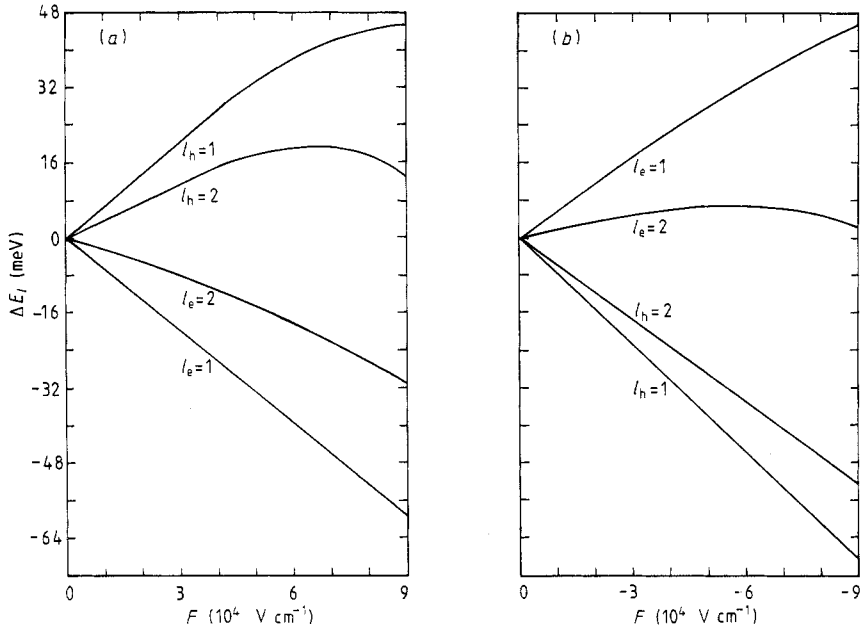

Figure 1. Energy shifts ΔE_i (meV) of first two heavy-hole and electron sub-bands in the GQW of $L = 200$ Å, $R = 1$ and $n = 1$ with a $Ga_{0.66}Al_{0.34}As$ barrier defined in the text. The energy shifts are plotted against (*a*) the positive electric field (10^4 V cm^{-1}) and (*b*) the negative electric field (10^4 V cm^{-1}). The same GQW is taken in the following figures.

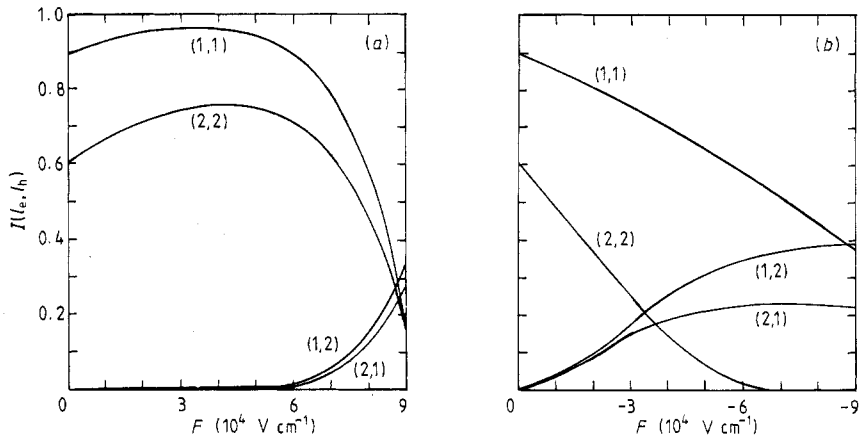

Figure 2. Electron–heavy-hole overlap functions, associated with the l_eth electron and l_hth hole sub-bands, plotted against (*a*) the positive electric field (10^4 V cm^{-1}) and (*b*) the negative electric field (10^4 V cm^{-1}).

In figure 2 and figure 3 we have plotted the electron–hole overlap functions and the exciton binding energies, respectively. As seen, they are also dependent on the direction of the electric field. It should be noted that the overlap functions and the binding energies, associated with an equal number of electron and hole sub-bands, are slightly

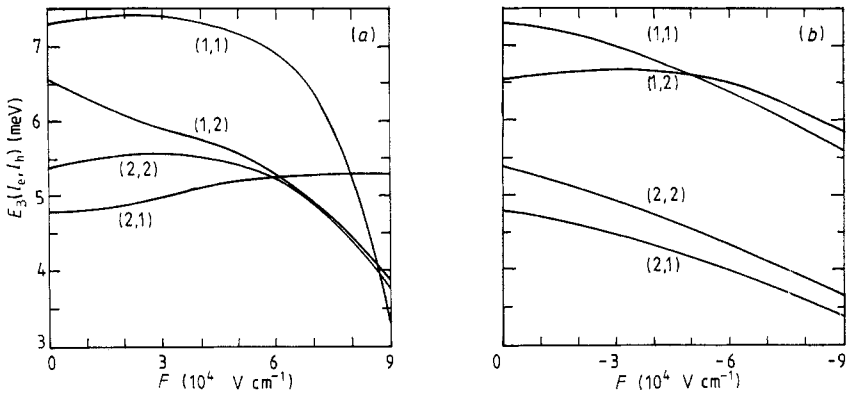

Figure 3. Binding energies $\Delta E_B(l_e, l_h)$ (meV) of excitons, associated with the l_eth electron and l_hth hole sub-bands, plotted against (*a*) the positive electric field (10^4 V cm^{-1}) and (*b*) the negative electric field (10^4 V cm^{-1}).

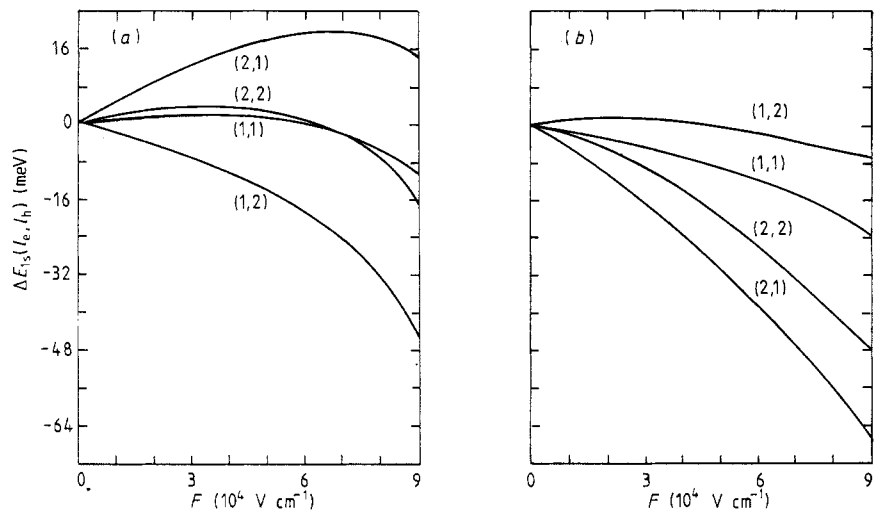

Figure 4. Energy shifts $\Delta E_{1s}(l_e, l_h)$ (meV) of heavy-hole excitons plotted against (*a*) the positive electric field (10^4 V cm^{-1}) and (*b*) the negative electric field (10^4 V cm^{-1}).

increased when the electric field is slightly increased in the Z direction. The changes are smaller in the electric field F between 0 and 6 (10^4 V cm^{-1}). When $F > 6$ (10^4 V cm^{-1}), the changes of the overlap functions and binding energies are larger. This is easily understood if one considers the wavefunctions, mentioned above, for $F = 0$ and $F > 0$. When the electric field is increased in the $-Z$ direction, the binding energies and the overlap functions, associated with an equal number of electron and hole sub-bands, decrease gradually, but the overlap functions, associated with an unequal number of electron and hole-sub-bands, increase gradually.

As seen in figure 3, the change in the binding energies is small in the present region of $\pm F$ compared with the energy shift of the sub-band energies. Thus, the energy shift of excitons mainly comes from the shifts of electron and hole sub-band energies. In figures 4(*a*) and 4(*b*), the energy shifts of the excitons in the GQW are plotted for $F > 0$

and $F < 0$, respectively. They show strong sub-band dependence. Comparing figure 4(a) with figure 4(b), we can see the strong dependence of the energy shifts on the field direction. The absolute values of the energy shifts of $\Delta E_{1s}(1, 1)$ and $\Delta E_{1s}(2, 2)$ in the negative electric field are larger than those in the positive field. As seen in figure 4(a), they are very small when the positive field F is less than $6(10^4\ \mathrm{V\ cm^{-1}})$. It is worthwhile to point out that the absolute value of $\Delta E_{1s}(2, 2)$ is larger than that of $\Delta E_{1s}(1, 1)$ for the both directions of the electric field when $|F|$ is larger. This is again different from the situation in SQW [15–17]. Based on the above discussion about changes of wavefunctions and energy shifts of sub-bands, the other energy shifts of excitons are also seen in figures 4(a) and 4(b).

So far we have discussed electrons, holes and excitons in GQW in an electric field. Based on this, we can first see that the resonant tunnelling in a GaAlAs barrier/$Ga_{1-x}Al_xAs$ GQW structure will be very different from that in the GaAlAs barrier/SQW structure, so that the current–voltage (I–V) characteristic and the derivative dI/dV of a device with GQW will be quite different from those of a device with SQW. Secondly, the effects of electric fields on the optical properties of GQW are also quite different from those for SQW. In GQW, the effects are strongly dependent on the direction of the electric field. On the basis of the properties of excitons in GQW, Miller [18] has presented an interesting possibility of blue-shift self-electro-optic effect devices, which share the potential advantages of lower loss in the transmitting state and less stringent requirements on the exciton absorption peaks. Therefore, it can be concluded that the investigation of properties of electrons and excitons in GQW in an electric field is useful for some device applications.

In conclusion, we have used the method of series expansion to obtain the energy shifts of sub-bands and excitons, the electron–hole overlap functions and the binding energies of excitons in the GQW ($R = n = 1$) in an electric field. The calculated results have revealed the behaviour of electrons and excitons in the GQW in the electric field quantitatively. It is quite different from that in SQW, and strongly dependent on the field direction. The properties of electrons and excitons in GQW are useful for some device applications. It is, therefore, interesting to extend the present work to the systematic investigation of the other kinds of GQW and properties. Finally, it is also interesting to point out that the method used here can be useful for analysing experimental results [19] and designing some devices in the future, where GQW are not linear and Airy functions cannot be used.

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