Dependence of energy shifts on the field direction in a graded $Ga_{1-x}Al_xAs$ quantum well

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We report the energy shifts in an electric field in a $Ga_{1-x}Al_xAs$ graded-gap quantum well (GGQW) and a novel method to calculate subbands. Our calculations have revealed the dependence of the energy shifts of subbands and excitons on the field direction in GGQW's. The subband dependence of energy shifts under an electric field in GGQW's is different from that in a square quantum well.

The effects of an electric field on the optical properties of quantum well (QW's) are attracting much attention.[1-6] The electric field changes the transition strength, the transition lifetime, and the intrinsic transition energy (Stark shift). The energy shift has been extensively studied both theoretically[1-4] and experimentally.[2,5,6] It can be theoretically determined by using the subband shifts of the electron and hole, which combine an exciton, and the change of its binding energy. Recently, Capasso *et al.*[7] drew attention to some interesting applications of graded-gap structures. Although the exciton energy shifts in square-quantum-well (SQW) systems have been frequently studied by several authors, no quantitative predictions are available for graded-gap structures. In this paper we report for the first time the energy shift of an exciton in a $Ga_{1-x}Al_xAs$ graded-gap quantum well (GGQW) and a novel method to calculate subbands associated with the exciton. We have solved equations of electron and hole subbands by using this method and performed variational calculations of excitons. These calculations reveal the dependence of energy shifts on the direction of an electric field in the GGQW.

Assuming that the GGQW is

$$V(z)=\begin{cases} V_0, & |z|\geq L/2 \\ V_0 R\,(z+L/2), & |z|<L/2 \end{cases} \tag{1}$$

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 unit step function; V_0 and L are the height and width of the GGQW, respectively. Here the theoretical calculation is different from the others which have been performed by several authors.[1-4] Under the bound-state assumption, we use series expansion to obtain the wave function in the region of $|z|<L/2$ and to solve exactly the Schrödinger-like equation of an electron ($q=-e<0$) and a hole ($q=e>0$) corresponding to H_{z0} of Eq. (3). The H_z' of Eq. (4) is treated as a perturbation on H_{z0}.

In the regions of $z\leq -L/2$ and $z\geq L/2$, the solutions of the equation

$$H_{z0}\psi(z)=E_z\psi(z) \tag{5}$$

are, respectively,

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

and

$$\psi^{\mathrm{II}}(z)=D\exp(-K_3 z) , \tag{7}$$

where

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

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

A and D are constants. In the region of $|z|<L/2$, expanding the $\psi^{\mathrm{II}}(z)$ in the uniformly convergent Taylor series and substituting it into Eq. (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 wave function at $z=-L/2$ and $z=L/2$, we can obtain the equation of the eigenenergy of an electron or a hole. In order to get subband energies and wave functions, we have solved the equation and calculated the perturbation correction numerically.

We treat the degenerate valence bands[8] of $Ga_{1-x}Al_xAs$ as ellipsoidal heavy- and light-hole bands for the Hamiltonian of excitons in GGQW's in the presence of an electric field. We use a variational method to calculate exciton states. The following variational wave function is chosen for 1s-type state, associated with the l_eth electron and l_hth hole subbands,

$$\Phi(z_e,z_h,\rho,\alpha)=\psi_{l_e}(z_e)\psi_{l_h}(z_h)\phi_{1s}(\rho,\alpha)\ , \tag{11}$$

where $\psi_{l_e}(z_e)$ [$\psi_{l_h}(z_h)$] is the normalized l_eth electron (l_hth hole) subband wave function, and this is obtained by using the method mentioned above. $\phi_{1s}(\rho,\alpha)$ is the normalized wave function of the ground state of a two-dimensional hydrogenlike atom[9] and given by

$$\phi_{1s}(\rho,\alpha)=\sqrt{2/\pi}\alpha\exp(-\alpha\rho)\ , \tag{12}$$

where α is a variational parameter. Then, as the energy of an exciton is given by

$$E_{1s}(l_e,l_h)=\min_{\alpha}\{\langle\Phi|H|\Phi\rangle\}\ , \tag{13}$$

the energy shift of an exciton due to the electric field is calculated from

$$\begin{aligned}\Delta E_{1s}(l_e,l_h)&=E_{1s}(l_e,l_h)-[E_{1s}(l_e,l_h)]|_{F=0}\\&=\Delta E_{l_e}+\Delta E_{l_h}+\Delta E^{B}_{1s}(l_e,l_h)\ ,\end{aligned} \tag{14}$$

where ΔE_{l_e} and ΔE_{l_h} are energy shifts of the electron and hole subbands, and $\Delta E^{B}_{1s}(l_e,l_h)$ is the change of the binding energy.

Since the different potential model under the bound-state assumption [see the last term of Eq. (3)] and the new method of calculation are used, it is interesting to compare our numerical results on the energy levels with the results obtained from other calculations. When the barrier height V_0 in a SQW approaches infinity, our calculated results of subband energies are exactly the same as those in Ref. 3. For a SQW of $V_0=169$ meV and $L=105$ Å in the electric field $F=12\times10^4$ V/cm, the first three energy levels of a heavy hole are, respectively 5.6, 2, and 1.2 meV lower than those in the infinite quantum well. Using the tunneling resonance method, the energies of the first heavy-hole and light-hole states in a SQW of $V_0=172$ meV and $L=95$ Å in the electric fields between 0 and 12×10^4 V/cm have been calculated in Ref. 2. Taking the same parameters, we have also calculated the energies and found excellent agreement with those in Ref. 2 without using any effective width to fit. It shows that our potential model and calculation method are excellent for obtaining the subband energies in quantum wells in electric fields under the bound-state assumption. Based on the subband calculations, calculated energy shifts of exci-

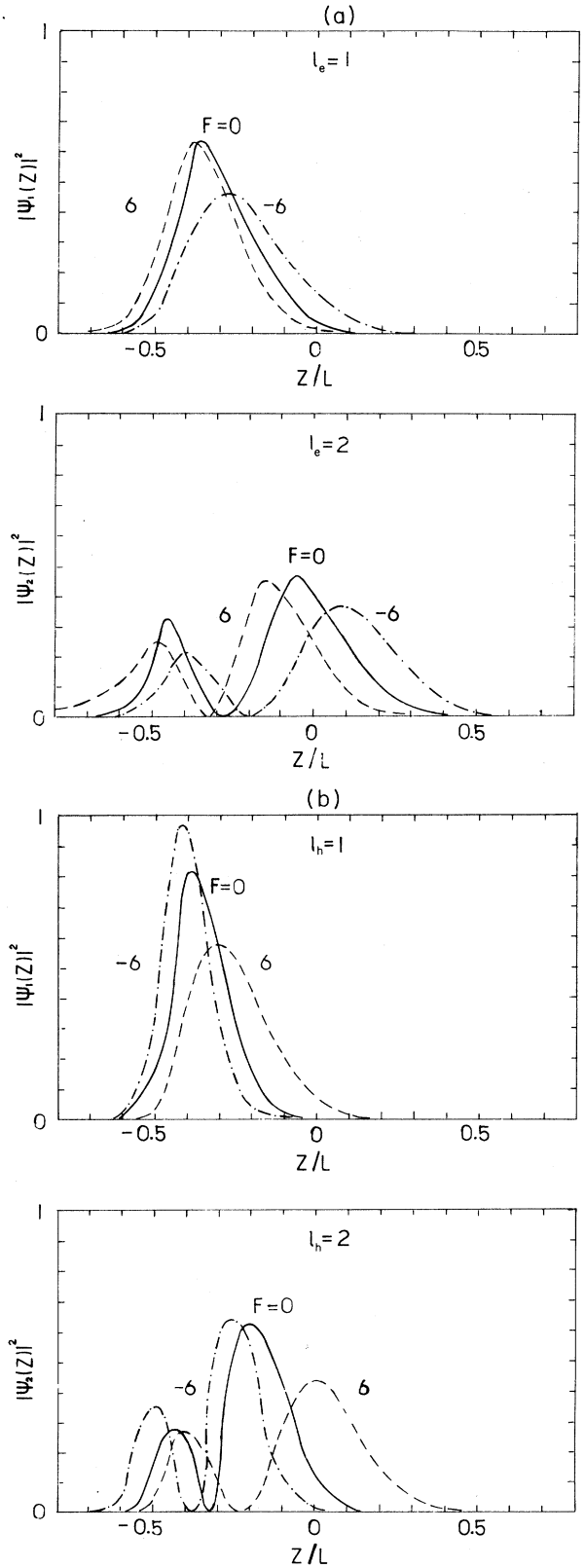

FIG. 1. Amplitude of the normalized subband wave function (a) $|\psi_{l_e}(z)|^2$ for $l_e=1,2$ and (b) $|\psi_{l_h}(z)|^2$ for $l_h=1,2$, vs the normalized position z/L. The electric field is taken to be $F=-6\times10^4$, 0, and 6×10^4 V/cm.

tons in SQW's agree well with experiments. It will be reported elsewhere.

The subbands of electrons and holes and the exciton shifts have been calculated for GGQW's with different R in electric fields. Here for the total band-gap mismatch, $\Delta E_g = 1.115x + 0.37x^2$,[10] where x is the aluminum 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. The total band-gap mismatch in the barrier is equal to 422 meV ($x = 0.34$). Taking electron and hole effective mass $m_e = 0.067 m_0$ and $m_{hz} = 0.34 m_0$ (m_0 is the free-electron mass), we have calculated quantum levels and wave functions of an electron and a hole in GGQW's of $L = 200$ Å in the electric fields between 0 and $\pm 9 \times 10^4$ V/cm. Based on these and the variational calculation, the energy shifts of excitons corresponding to different subbands have been obtained.

The wave functions of the $l_e = 1,2$ states and the $l_h = 1,2$ states in GGQW's with $R = 1/L$ in $F = -6 \times 10^4$, 0, and 6×10^4 V/cm have been plotted in Figs. 1(a) and 1(b), respectively. It is readily seen that they are very different from those in SQW's. For $F = 0$, wave functions of the l_e (l_h) = 1 and l_e (l_h) = 2 states in SQW's are symmetric, and antisymmetric, respectively, but they are not in GGQW's. Both electron and hole wave functions are localized on the left-hand side of GGQW's. For positive electric field, the electron and hole move, respectively, to the $-z$ and z directions in both GGQW's and SQW's. If the direction of the electric field is changed, they move in the opposite directions. The square of the wave functions is symmetric between opposite directions of the electric fields in SQW's; however, they are very different between the opposite directions in GGQW's, which can be seen in Figs. 1(a) and 1(b). For the conduction-band electron, the GGQW becomes sharper and flatter when the electric field is increased in the z and $-z$ directions, respectively, and for valence-band holes it is the opposite. Therefore, the absolute variation of the electron subband energies due to the positive field is larger than that due to the negative field. It is different for the hole subband energies. For valence-band holes, the absolute variation of the positive field is smaller than that of the negative field. Since the effective mass of a hole is larger than that of an electron, the absolute variations of the $l_h = 1$ and 2 states under $-F$ and F are, respectively, larger than those of the $l_e = 1$ and 2 states under F and $-F$. It reflects different changes in the wave functions under electric fields. In Figs. 1(a) and 1(b) it is easily seen that the change of the wave functions of the hole subbands is larger than that of the electron subbands under electric fields. As seen in Eq. (14), energy shifts of excitons arise from energy shifts of the electron and hole subbands, ΔE_{l_e} and ΔE_{l_h}, in addition to the change of the binding energy. The change depends on the subbands—it is not large in the present region of $\pm F$. Thus, the energy shift of excitons mainly comes from shifts of the electron and hole subband energies. In Figs. 2(a) and 2(b) the energy shifts of excitons in the GGQW's in F and $-F$, respectively, are plotted. They show the strong subband dependence. Comparing Fig. 2(a) with Fig. 2(b), we can see the strong dependence of the energy shifts on the field direction. The absolute value of the energy shifts of $\Delta E_{1s}(1,1)$ and $\Delta E_{1s}(2,2)$ in electric fields with $-z$ direction are larger than those with z direction, respectively. This is because of the larger absolute variation, mentioned above, of hole subband energies under negative fields. 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 both directions of electric fields when $|F|$ are larger. This is different from that in a SQW.[1-6] Based on the above discussion about changes in wave functions and energy shifts of subbands, the other energy shifts of excitons are also seen in Figs. 2(a) and 2(b).

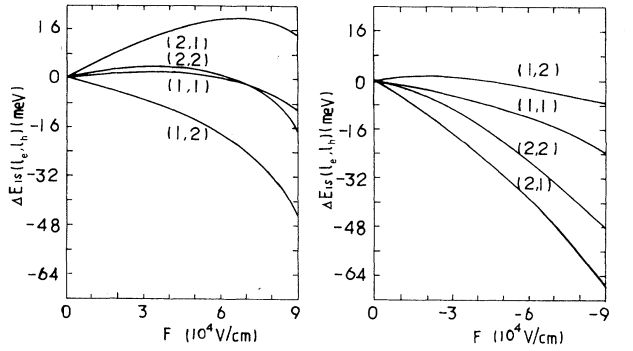

FIG. 2. Energy shifts $\Delta E_{1s}(l_e, l_h)$ (meV) of heavy-hole excitons in GGQW's defined in the text vs (a) positive electric field (10^4 V/cm) and (b) negative electric field (10^4 V/cm).

In conclusion, we have used the method of series expansion and obtained the energy shifts of subbands and excitons in GGQW's. Our calculations have revealed the dependence of the energy shifts on the field direction and $|\Delta E_{1s}(2,2)| > |\Delta E_{1s}(1,1)|$. These are different from those in SQW's. Our results might be useful for some device applications. The effects of the heavy- and light-exciton mixing have been extensively studied by several authors.[4,11] It is therefore interesting to extend the present work to the full calculation, which will be done further. Finally, it is important to point out that the method of series expansion is also excellent for calculating subbands and excitons in wells of other shapes, which is in progress.

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