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# Exciton binding energy in type-II GaAs-(Al,Ga)As quantum-well heterostructures

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The binding energy of the ground-state exciton is calculated variationally for the GaAs-(Al,Ga)As system when the band-edge configuration at the heterojunction has become staggered or "type II." Anisotropy in both the hole and electron effective masses is considered and calculations are performed assuming perfect confinement of both sorts of carriers. The binding energies we calculate are of a similar magnitude to those found for the 1*s* heavy-hole (or 1*s* light-hole) exciton in this system when the configuration is the more familiar straddled or type-I arrangement.

The size of the valence-band offset at a GaAs-AlAs heterojunction can now be pinpointed with millivolt accuracy due to the most recent observations of low-temperature (~8-K) photoluminescence excitation spectra from multiple-quantum-well samples with very narrow GaAs layers (< 30 Å).[1] The no-phonon excitonic transition involving a heavy hole confined at the Γ point in the GaAs layer and an electron confined in the (001) *X* valley in the adjacent AlAs layer is seen in the luminescence emission spectra.[1,2] This observation means that the heterojunction band-gap configuration has become staggered or "type II." The fraction of the Γ-point band-gap difference that appears in the valence band was derived to be 0.34,[1] in good agreement with the results of more indirect optical methods[3,4] and luminescence studies of $Al_{0.37}Ga_{0.63}As$-AlAs heterojunctions[5] and GaAs-(Al,Ga)As quantum wells under hydrostatic pressure,[6] but at odds with the majority of "electrical" determinations.[7]

Uncertainty in the derived offset value arises from three principal sources:[1,6] (i) the value of the confinement level of the heavy hole in the GaAs valence-band well, (ii) the confinement energy of the electron at the *X* point in the AlAs layer, and (iii) the exciton binding energy due to the mutual Coulomb interaction of electrons and holes confined in adjacent layers. In this paper we address the uncertainty introduced by the neglect of the Coulomb interaction.

The band-edge configuration for the type-II system we are considering is shown in Fig. 1. The holes are confined in the GaAs while the electrons reside in the indirect-gap AlAs, confined to the "well" formed by the discontinuity of the *X*-point band edges. This is qualitatively similar to the InAs-GaSb system in that electrons and holes are resident in adjacent layers but different in that they derive their electronic character from different parts of the Brillouin zone. A variational calculation of the binding energy of excitons in the InAs-GaSb system has already been performed by Bastard, Mendez, Chang, and Esaki[8] making the assumption that both electron and hole bands are isotropic. In GaAs-AlAs the electrons are in the anisotropic *X* minima and because of the mixing of the light and heavy holes, the holes which are heavy perpendicular to the plane of the wells are light in the plane of the wells.[9] We have to suppose that the lowest *X* minima in the AlAs are those whose longitudinal mass is perpendicular to the plane of the layers because the confinement of the other *X* minima is determined by their transverse mass, which is about five times smaller.[10]

Assuming that the holes and electrons are perfectly confined, the exciton state is composed of an electron in a single layer of AlAs bound to a hole in one of the adjacent layers of GaAs. We have attempted to account for the different dielectric constants of GaAs and AlAs by replacing them by a single effective medium with their average dielectric constant.[11] We did not include any image-charge corrections. The Hamiltonian describing the motion of the exciton is (in cylindrical polar coordinates)

$$H=\frac{-\hbar^2}{2\mu}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right]-\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial z_e^2}$$
$$-\frac{\hbar^2}{2m_h}\frac{\partial^2}{\partial z_h^2}-\frac{e^2}{4\pi\varepsilon_0\varepsilon_r}[\rho^2+(z_e-z_h)^2]^{-1/2},$$

where the ranges of the *z* coordinates are $0\le z_e\le w_e$ and $-w_h\le z_h\le 0$. $m_e$ and $m_h$ are the effective masses of electrons and holes in the growth direction and $\mu$ is the reduced, in-plane effective mass of the electron-hole pair.

We write the exciton trial wave function $\psi$ as

$$\psi(\rho,z_e,z_h,\phi)=e^{im\phi}f_e(z_e)f_h(z_h)g_m(\rho,z_e,z_h),$$

where *m* is the angular momentum quantum number. We consider only states of *s* symmetry and write the com-

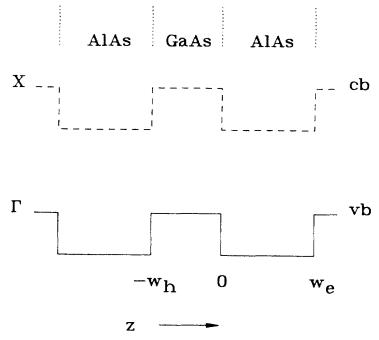


FIG. 1. Plot of the bottom of the *X* conduction band (cb) and the top of the valence band (vb) against position in the direction perpendicular to the plane of the layers.

 

ponents of the wave function as

$$g_0(\rho,z_e,z_h)=Ae^{-\lambda\rho},$$

$$f_e(z_e)=Be^{-\alpha z_e}\sin(\pi z_e/w_e),$$

$$f_h(z_h)=Ce^{\beta z_h}\sin(\pi z_h/w_h),$$

where $A$, $B$, and $C$ are normalization constants and $\alpha$, $\beta$, and $\lambda$ are variational parameters to be determined. The parameters $\alpha$ and $\beta$ will be nonzero for all cases of interest and reflect the pileup of the electron and hole wave functions at the interface as a result of the Coulomb interaction. Our trial functions $f_e(z_e)$ and $f_h(z_h)$ are different from those chosen by Bastard *et al.*[8] in the InAs-GaSb case. In the limit that we allow the AlAs layers to become infinitely wide then our trial functions are identical to those of Ref. 8 with the roles of the electrons and holes interchanged.

The exciton binding energy is readily determined by minimizing

$$\langle E\rangle=\langle\psi^*\,|\,H\,|\,\psi\rangle$$

and subtracting from this the sum of the lowest electron and hole subband energies. For perfect confinement these are simply given by

$$E_e=\frac{\hbar^2}{2m_e}\left(\frac{\pi}{w_e}\right)^2,\quad E_h=\frac{\hbar^2}{2m_h}\left(\frac{\pi}{w_h}\right)^2.$$

We have made calculations of the binding energy of the ground-state exciton for the case of alternating layers of GaAs and AlAs. The pertinent material parameters we chose for GaAs were $m_h=0.34m_0$ and a value of $0.18m_0$ for the in-plane heavy-hole mass. The former is the value used to most successfully fit the heavy-hole excitonic features in low-temperature photoluminescence excitation spectra[3] while the latter is the value used previously by us to accurately calculate the observed $1s$-$2s$ splitting of excitons in the type-I GaAs-(Al,Ga)As system.[12] For AlAs we set the longitudinal and transverse masses for the (001) $X$ valley to be $1.1m_0$ and $0.19m_0$, respectively.[10] The average dielectric constant was taken as 12.3.

In Fig. 2 we display contours of constant energy corresponding to the ground-state binding energy of the lowest heavy-hole exciton. The contours are displayed as a function of both the GaAs hole well width and the AlAs electron well width. We calculate a value for the ground-state binding energy intermediate between that of bulk GaAs and a value typical of the exciton ground state in an indirect III-V semiconductor, e.g., $-20.5$ meV in GaP.[13] In fact, our calculated values are close in magnitude to the binding energies of the $1s$ state of excitons in type I, isolated GaAs-(Al,Ga)As quantum wells with GaAs well widths between 40 and 100 Å.[12] The reduction of the binding energy due to the separation of the electron and hole into different layers (cf. Bastard *et al.*[8]) is compensated by an increase due to the larger transverse electron mass in the $X$ minimum of AlAs relative to that of the $\Gamma$ minimum of GaAs.

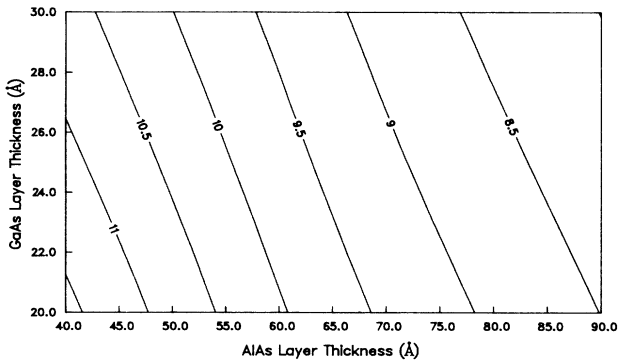


FIG. 2. Contour plot of the calculated exciton binding energy. The units are expressed in meV.

In Ref. 1 the authors deduced a step in the valence band at the GaAs-AlAs heterojunction of 542 meV or alternatively a conduction-to-valence-band offset ratio of 66:34 from a range of samples of constant AlAs width ($\sim$65 Å) but with differing GaAs widths ($\sim$20 and $\sim$30 Å). For such samples we determine an exciton binding energy which changes only between 9.7 and 9.2 meV. Neglect of the Coulomb interaction would thus change the potential energy step at the interface by less than 2% corresponding to a change in the offset ratio of 0.5.

In all the calculations we have assumed both sorts of carriers to be perfectly confined. Unlike the type-I case it should be anticipated that any leakage of the electron and hole wave functions into the adjacent "barrier" regions will slightly increase the binding energy. Furthermore, the oscillator strength of transitions between higher electron states confined at $X$ and the lowest hole state will be increased by such leakage[14] which is in agreement with experimental observation.[1]

In summary, we have calculated variationally the ground-state binding energy of excitons formed in the GaAs-AlAs multi-quantum-well system when the band-edge profile has become staggered; a situation which occurs when the GaAs well width decreases below approximately 30 Å. In contrast to variational calculations on the InAs-GaSb (Ref. 8) system we have explicitly included the anisotropy of both the holes at the $\Gamma$ point in GaAs and the electrons in the (001) $X$-point valley in the AlAs and subsequently find binding energies which range from $-11.5$ meV for layer widths of 20-Å GaAs and 40-Å AlAs to about 8.0 meV for 30 Å of GaAs and 90 Å of AlAs.

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