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Donors bound to X valleys in type-II GaAs–AlAs quantum well structures

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We calculate the binding energies of donors bound to X valleys in type-II GaAs–AlAs quantum well structures using an anisotropic variational method which enables us to take into account the effective mass anisotropy and quantum confinement. For a comparative study, we use two sets of effective masses obtained from different measurements [B. Rheinänder et al. Phys. Status Solidi B 49, K167 (1972) and M. Goiran et al., Physica B 177, 465 (1992)]. We show that the binding energies have a pronounced dependence with the effective mass, AlAs layer thickness, and impurity position. © 1995 American Institute of Physics.

Type-II quantum well structures, where the lowest energy transition is indirect in real space, have attracted considerable attention over the last years due to their distinguished electrical and optical properties. For instance, such structures can be obtained with AlGaAs–AlAs quantum wells where the Γ states in the AlGaAs layers are made higher in energy than the X states in AlAs layers by an appropriate choice of Al concentrations and layer thicknesses. Therefore, the electrical and optical properties of type-II structures are very different from their type-I counterparts. In particular, substitutional shallow donors will not be linked to the Γ valley but to the lower lying X valleys. Furthermore, these valleys are no longer degenerate but the Xz and Xz,y valleys will split into different energies due to the quantum confinement in the growth (z) direction and due to biaxial strain effects. For narrow AlAs layers (less than 55 Å) the Xz,y valleys are higher in energy than the Xz valleys, but for larger AlAs layers the Xz,y valleys are lower in energy due the effect of residual lattice-mismatch strain.

Theoretical studies on shallow impurities in quantum wells used mainly variational techniques3–5 which have compared successfully with measurements in several experimental situations,6–7 and were concentrated mainly on GaAs–AlGaAs type-I quantum wells. Effects of Γ–X mixing on the binding energies of shallow donors in GaAs–AlAs type-I quantum wells, near to the type-I-to-type-II transition, were studied by Wang et al.8 recently, but otherwise there was little effort for the calculation of binding energies in type-II GaAs–AlAs quantum wells. Since the successful growth of n-type Si-doped GaAs–AlAs structures9 the calculation of these binding energies have become important for the understanding of bistable shallow–deep silicon donors in GaAs–AlAs10–11 and photoluminescence spectra as obtained by Lee et al.12

In this letter we calculate the binding energy of hydrogeniclike donors bound to the Xz,y and Xz valleys in type-II GaAs–AlAs quantum wells using an anisotropic variational method. Our calculation should be appropriate for substitutional group-IV donors such as Si in AlAs where effects of valley mixing or central-cell correction can be neglected. We consider the effective mass anisotropy, the quantum confinement in the growth direction, and vary the impurity position along the AlAs layer. Lattice-mismatch induced strain should have little effect on the donor binding energies and, for simplicity, is not included in this calculation. The results are discussed using effective masses for the AlAs bulk X valleys obtained from different experiments and we compare them with binding energies obtained from photoluminescence measurements.12

A recent high-magnetic cyclotron resonance (CR) experiment by Goiran et al.13 measured transversal and longitudinal effective masses for AlAs of 0.44m0 and 2.62m0, respectively, which are much heavier than the commonly used values of 0.19m0 and 1.1m0 obtained from Faraday rotation (FR) studies.14,15 It is still debated if there is a cam-e1's back energy structure along the X direction, in which case each set of effective masses would belong to closely spaced minima in the X direction.13 We present our results for both sets of effective masses and we believe that detailed photoluminescence measurements on type-II GaAs–AlAs structures, with the aid of the present calculations, may provide new elements for this discussion.

In order to form a type-II GaAs–AlAs quantum well we need GaAs layers narrow enough in order to have the confined Γ state (in the GaAs layer) higher in energy than the confined X state (in the AlAs layer). Any electron in this Γ state will thus be transferred within picoseconds into the lower lying X state.16 While the quantum wells formed by the Γ valleys may interact strongly for sufficiently narrow AlAs layers, the quantum wells in the X valleys are essentially isolated due to the heavy X masses involved. Therefore, in order to calculate electron energy states in GaAs–AlAs type II quantum wells it is reasonable to consider these X quantum wells as isolated even for narrow GaAs layers.

We use a standard variational method for the calculation of X impurity states such as in Ref. 17 and we use an anisotropic hydrogenic part of the 1s-like trial wave function

$$\Gamma(x,y,z) = \exp\left[-\frac{x^2}{\alpha^2} - \frac{y^2}{\beta^2} + \frac{(z-z_i)^2}{\epsilon^2}\right]^{1/2},$$  (1)

where the impurity position zi is centered in the AlAs layer along the growth direction, and the Hamiltonian is written as

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TABLE I. Transversal, longitudinal, and average values of: effective masses (in units of $m_0$), effective Bohr radii (in Å), and effective Rydberg energies (in meV); relations between longitudinal and transversal values and $x,y,z$ components for different $X$ valleys.

<table>
<thead>
<tr>
<th></th>
<th>$m_x^*$</th>
<th>$m_y^*$</th>
<th>$m_z^*$</th>
<th>$a_x^*$</th>
<th>$a_y^*$</th>
<th>$a_z^*$</th>
<th>$R_x^*$</th>
<th>$R_y^*$</th>
<th>$R_z^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X_x$ valley</td>
<td>$m_x^*$</td>
<td>$m_y^*$</td>
<td>$m_z^*$</td>
<td>$a_x^*$</td>
<td>$a_y^*$</td>
<td>$a_z^*$</td>
<td>$R_x^*$</td>
<td>$R_y^*$</td>
<td>$R_z^*$</td>
</tr>
<tr>
<td>$X_{x,y}$ valley</td>
<td>$m_x^*$</td>
<td>$m_y^*$</td>
<td>$m_z^*$</td>
<td>$a_x^*$</td>
<td>$a_y^*$</td>
<td>$a_z^*$</td>
<td>$R_x^*$</td>
<td>$R_y^*$</td>
<td>$R_z^*$</td>
</tr>
<tr>
<td>CR experiment</td>
<td>0.44</td>
<td>2.61</td>
<td>0.61</td>
<td>12.03</td>
<td>2.02</td>
<td>6.25</td>
<td>59.86</td>
<td>356.47</td>
<td>82.98</td>
</tr>
<tr>
<td>FR experiment</td>
<td>0.19</td>
<td>1.1</td>
<td>0.26</td>
<td>27.85</td>
<td>4.81</td>
<td>20.35</td>
<td>25.85</td>
<td>149.7</td>
<td>35.37</td>
</tr>
</tbody>
</table>

$$H = -\frac{\hbar^2}{2}\left(\frac{1}{m_x}\frac{\partial^2}{\partial x^2} + \frac{1}{m_y}\frac{\partial^2}{\partial y^2} + \frac{1}{m_z}\frac{\partial^2}{\partial z^2}\right)$$

$$-e^2\epsilon [x^2 + y^2 + (z - z_i)^2]^\frac{1}{2} + V(z).$$

(2)

The actual values of the effective masses $m_{x,y,z}^*$ depend on which $X$ valley is being considered, e.g., the longitudinal mass $m_x^*$ of the $X_y$ valley is along the $z$ direction thus corresponding to $m_z^*$. The detailed relations between the AlAs masses and $(m_x^*, m_y^*)$ and the $m_{x,y,z}^*$ masses are summarized in Table I. For simplicity, we assume AlAs effective masses for both the well and the barrier. In our calculations we use, for AlAs, a dielectric constant $\epsilon$ of 10.0 and a barrier height of 316 meV, and consider a band alignment of 35%–65%. The bottom of the bulk AlAs band edge thus is 145 meV above the bulk GaAs band edge.\(^{15,16}\) Binding energies are given with respect to the confined energy level.

In Fig. 1 we show the binding energies obtained for an impurity at the center and at the interface of a type-II quantum well as a function of the AlAs layer thickness. Also shown, as dashed curves, are calculations using an average isotropic effective mass taken as

$$m_{av}^* = 3\left(\frac{2}{m_x^*} + \frac{1}{m_y^*}\right)^{-1}.$$
So far, we are aware of only a single directly measured experimental value for $X_c$ valley donors in GaAs–AlAs quantum wells obtained very recently with photoluminescence measurements by Lee et al.\textsuperscript{12} They obtained a binding energy of 104 meV for a large AlAs layer of 131 Å, a value which is in good agreement with calculated on-center binding energies of 97 meV for $X_c^{CR}$ and 102 meV for $X_{1,1}^{CR}$ (not shown in our figures), indicating that for these measurements the CR effective masses represent more adequately the measured binding energies. In the experiment, the AlAs layers were doped with silicon over the central 1/3 of the layer. These binding energies are also in agreement with earlier measured results of 101 meV for bulk AlAs obtained by Lifshitz et al.\textsuperscript{18} To the best of our knowledge, direct measurements of the $X$ donor binding energy for narrower AlAs layers are not yet available.

Our results show that the two sets of effective masses studied in this work provide very different binding energies. Also, the calculated binding energies are remarkably deep when compared to the type-I donors\textsuperscript{17} and indicate that even if the GaAs–AlAs structure is of type I there may be $X$ valley donors at lower energies than the confined $\Gamma$ states or $\Gamma$ valley donors. We believe that the present work may be valuable for further experimental studies on $X$ valley donors and may be helpful in order to clarify the issue of the different effective masses measured for the AlAs $X$ valleys.

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