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Binding Energy and Spin-Orbit Splitting of a Hydrogenic Donor Impurity in AlGaN/GaN Triangle-Shaped Potential Quantum Well

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Abstract In the framework of effective-mass envelope function theory, including the effect of Rashba spin-orbit coupling, the binding energy E_b and spin-orbit split energy Γ of the ground state of a hydrogenic donor impurity in AlGaN/GaN triangle-shaped potential heterointerface are calculated. We find that with the electric field of the heterojunction increasing, (1) the effective width of quantum well $\overline{\mathrm{W}}$ decreases and (2) the binding energy increases monotonously, and in the mean time, (3) the spin-orbit split energy Γ decreases drastically. (4) The maximum of Γ is 1.22 meV when the electric field of heterointerface is 1 MV/cm.

Keywords Binding energy · Spin-orbit splitting · Hydrogenic donor impurity · AlGaN/GaN

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Introduction

GaN, AlN and their related compounds, as wide gap semiconductors, attracted a lot of interest in the past few yeas, mainly due to their good optical properties and great potential uses in optoelectronics. Spin-orbit coupling is the key issue of semiconductor spintronics [1–3]. Since there is a large spin-splitting of a 2-dimensional electron gas (2DEG) in a wurtzite AlGaN/GaN heterostructrure [4], GaN-based materials as a promising candidate for the spintronic application have drawn a considerable attention. The spin-orbit interaction contains the Rashba and Dresselhaus contributions [5]. As commonly known, the Rashba effect is due to the structural inversion asymmetry of confinement potential at heterointerface and the Dresselhaus effect is due to the bulk inversion asymmetry of crystal potential. Although spin-orbit coupling in wide band gap materials is thought to be weak [6], the surprisingly sizable spin splitting of the conduction band in GaN-based heterostructures mainly results from a large polarization doping effect and a strong interfacial electric field directed along the growth axis induced by piezoelectric effect [7–9]. Strong polarization doping effect in GaN, AlN and their related compounds may compensate to some extent for the smallness of the coupling parameter and make overall spin-splitting comparable to that found in narrow-gap group-III-V structures. This fact could make GaN, AlN and their related compounds competitive in emerging spintronics applications.

Impurity states have played an important role in the semiconductor devices. Only with impurities, the devices, such as diodes, transistors can be successfully made [10]. The study of impurity states in heterostructures is an important aspect to which many theoretical and experimental works have been devoted. Since Bastard's pioneering

work using a variational approach [11, 12], a lot of attention has been devoted to the study of impurity states in quantum wells [13]. Previously, lots of researches focused on the GaAs/GaAlAs structures. Mailhiot, Chang, and McGill [14, 15] have done extensive calculations of the binding energies and wave functions for hydrogenic impurities as functions of well width and impurity location in the well using a more realistic model in which the potential barrier was finite and equal to the conduction band offset at GaAs/GaAlAs interfaces. Chaudhuri [16] has extended this to treat the case where the GaAlAs layer is thin enough that the wave functions can spill over to adjacent GaAs quantum wells. Recently impurities in GaN based structures began to draw a lot of attentions. Xia and his coworkers [17] calculated the binding energy of a hydrogenic impurity in zinc-blende (ZB) GaN/AlN coupled quantum dots (QDs) using a variational method. Both of them found that: (1) the binding energy increases when the width of quantum well decreases; (2) the impurity's binding energy depends upon its location within the well. The peak occurs when the impurity is on the midpoint of the quantum well.

Calculations

In the framework of effective-mass envelope function theory [18–21], we studied the binding energy of the hydrogenic impurity state first, and then the electronic states of a hydrogenic donor impurity in AlGaN/GaN triangle-like potential heterojunction including the effect of Rashba spin-orbit coupling will be calculated in this letter.

The electron envelope function equation with a hydrogenic donor impurity located at $r_0 = (0,0,z_0)$ is

$$\left[\Delta - \frac{2C}{|r-r_0|} + \alpha_R(\sigma \times p)\bullet z + V(r)\right]\psi_n(r) = E_n\psi_n(r), \tag{1}$$

where $\Delta = -d^2/dx^2 - d^2/dy^2 - d^2/dz^2$, $r = (x,y,z)$, and $|r - r_0| = \sqrt{x^2 + y^2 + (z - z_0)^2}$. The third item in Eq. (1) is the contribution of the Rashba spin-orbit effect to the single electron Hamiltonian. α_R, σ, and p are the Rashba parameter, the Pauli matrices, and the electron momentum operator, respectively. The units of length and energy are given in terms of the effective Bohr radius $a^* = \hbar^2\varepsilon/m_e^*e^2$, and the effective Rydberg constant $R^* = \hbar^2/2m_e^*a^{*2}$, where m_e^* and ε are the electron effective mass and dielectric constant of an electron in GaN, respectively.

In Eq. (1), $C = 0$ for the case of no donor; and 1 for the case if there is a donor in the heterointerface. The binding energy of the hydrogenic impurity state is calculated by the following equation:

$$E_b = E_0^0 - E_n^1 \tag{2}$$

To a good approximation, the infinite triangle-shaped confined potential well was used to calculate the conduction band ground state. Such potential is given by

$$V(r) = \begin{cases} \infty & \text{for } |z| < 0 \\ eFz & \text{for } |z| \geq 0 \end{cases} \tag{3}$$

where F is the electric field, which depends on the Al component x of the barrier layer $Al_xGa_{1-x}N$ and 2DEG density. To compare with square quantum well, effective width will be used. Effective width of triangle-shaped well is usually given by

$$\overline{W} = \frac{\int z\cdot|\psi_n(r)|^2dr}{\int|\psi_n(r)|^2dr} \tag{4}$$

where $\psi_n(r)$ is the eigen wave function of E_n solved from the Schrodinger equation with the triangle-shaped confined potential well and so different state n has different $\bar{W}$. For ground state, $n = 0$, furthermore, Eq. (4) can be transformed to

$$\bar{W} = \frac{\int eFz\cdot|\psi_n(r)|^2dr}{eF\int|\psi_n(r)|^2dr} = \frac{\langle V\rangle}{eF} = \frac{2}{2+v}\cdot\langle H\rangle\cdot\frac{1}{eF} = \frac{2E_0}{3eF} \tag{5}$$

where F is the electric field and the coefficient v of the linear potential is unity.

In this calculation, the normalized plane-wave expansion method is used. We employ the electron wave function

$$\psi(r) = \frac{1}{\sqrt{L_xL_yL_z}}\sum_{n_xn_yn_z} C_{n_xn_yn_z}e^{i[(k_x+n_xK_x)x+(k_y+n_yK_y)y+(k_z+n_zK_z)z]}. \tag{6}$$

where L_x, L_y, and L_z are the side lengths of the unit cell in the x, y, and z directions of the coordinate system, respectively. $K_x = 2\pi/L_x$, $K_y = 2\pi/L_y$, $K_z = 2\pi/L_z$, $n_x \in \{-m_x,\ldots,m_x\}$, $n_y \in \{-m_y,\ldots,m_y\}$, $n_z \in \{-m_z,\ldots,m_z\}$. The plane wave number is $N_{xyz} = (2m_x + 1)(2m_y + 1)(2m_z + 1)$, where m_x, m_y, m_z are positive integers. In our calculation, we adopt $m_x = m_y = m_z = 6$. If further increasing integers m_x, m_y, m_z, the difference between exact results and real one is negligibly small. During our calculation, we make $k_x = k_y = k_z = 0$ in Eq. (6) [21]. The electron states are calculated from the matrix elements which can be found in Eqs. (1) and (5) [22]. For GaN, we take effective mass $m_e^* = 0.22m_0$, with m_0 being the free electron mass. The Rashba parameter is chosen to be 20 meV Å [23].

Results and Discussion

Figure 1 shows the effective well width of the triangle-like quantum well as a function of electric field for ground state. In the general case, the $\overline{\mathrm{W}}$ is proportional to about $1/\sqrt{F}$. The higher the electric field is, the narrower the effective well width will be. In our case, when $F = 100$ MV/cm, it corresponds to $\overline{\mathrm{W}} = 0.2$ nm; while, for $F = 1$ MV/cm, it corresponds to $\overline{\mathrm{W}} = 2$ nm. In the limiting case, $\overline{\mathrm{W}}$ will tend to infinity when the F approaches to 0.

Figure 2 shows the binding energy of the ground state as a function of effective width of quantum well $\overline{\mathrm{W}}$. In this figure, we assume that the impurity position is located at $z_0 = 0$. From this figure, we can see two facts: (1) the binding energy splits into two-ones for the Rashba effect, but such split is quite small so that it can not be showed clearly in Figure 2; (2) when the effective well width is less than 0.5 nm, the binding energy increases dramatically and tends to infinite when the $\overline{\mathrm{W}}$ approaches to 0. $E_b = 138$ meV for the case of $\overline{\mathrm{W}} = 0.4$ nm; and (3) When the effective well width is more than 1.0 nm, the binding energy tends to be constant about 28 meV. The reason is that when the effective well width of the triangle quantum well becomes narrower and the quantum confinement becomes stronger, so the binding energy increases as well, this tendency, as commonly known, is qualitatively similar to the case of square quantum well (e.g., AlGaAs/GaAs quantum well) [11].

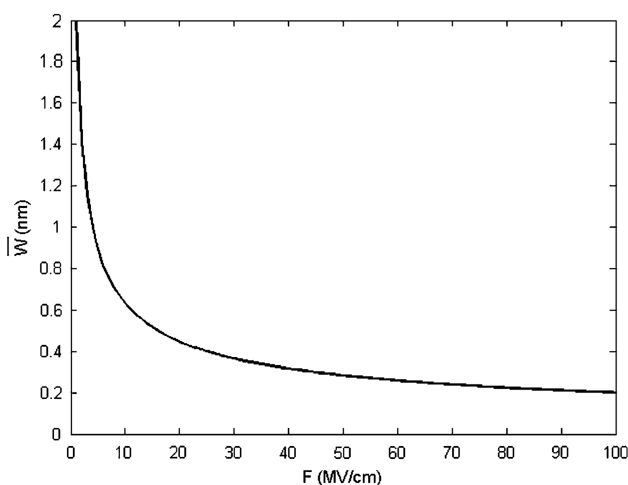

Fig. 1 Effective width of the triangle-shaped quantum well $\overline{\mathrm{W}}$ as a function of electric field F for ground state

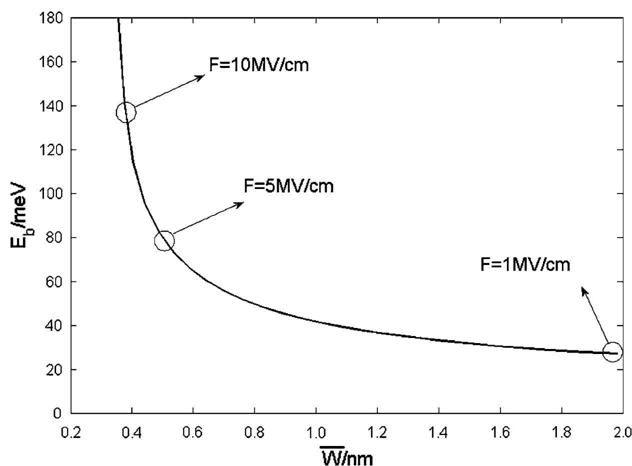

Fig. 2 Binding energy of the ground state E_b as a function of effective width of quantum well $\overline{\mathrm{W}}$. The impurity position pinned at $z_0 = 0$. Three points selected on the curve correspond to $F = 10$ MV/cm, 5 MV/cm, and 1 MV/cm, respectively

Figure 3 shows the spin-orbit split energy of ground state, labeled as Γ, as a function of electric field F. The inset also shows the Γ as a function of effective width of the quantum well as the impurity position pinned at $z_0 = 0$. From this figure, we can also observe that (1) with the electric field increasing, the $\overline{\mathrm{W}}$ decreases, which leads to a decreasing spin-orbit split energy Γ, and (2) when F is weaker than 2.5 MV/cm, Γ will saturate at about 0.75 meV.

Figure 4 shows the variations in spin-orbit split energy of ground state Γ as a function of impurity position in the different electronic fields. In this figure, we show the Γ against typical electric field values of $F = 1$ MV/cm, 5 MV/cm, and 10 MV/cm, respectively, for a comparison. It was found that (1) in each field of F, with z_0 located in a range from 0 to 10 nm, the spin-orbit splitting energy Γ increases first, and then reaches its maximum value before decreasing monotonously, and we also found that our calculated curve is in agreement with Bastard's calculation qualitatively [11]. However, based on the Bastard's work, we further calculated the ground state spin-orbit splitting energy for his ground state, and found that splitting energy shows a symmetrically spatial distribution, which is very different from that in our triangle-shaped well in curve

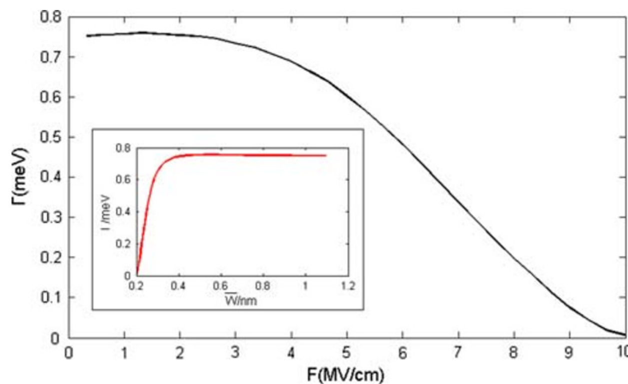

Fig. 3 Spin-orbit split energy of ground state Γ as the position of electric field F. Inset shows the Γ as the effective width of quantum well $\overline{\mathrm{W}}$. The impurity position is pinned at $z_0 = 0$

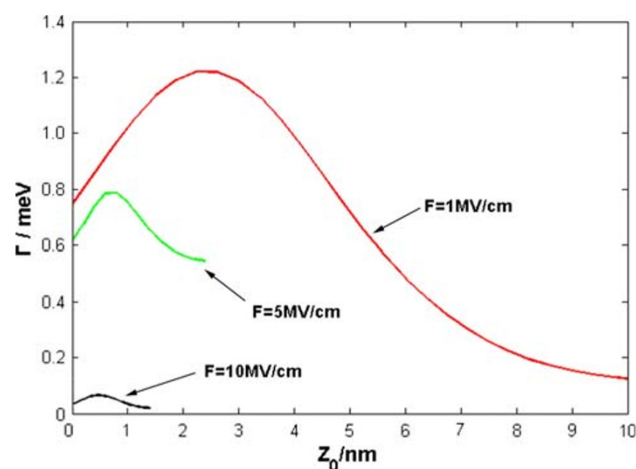

Fig. 4 Change in spin-orbit split energy of ground state Γ as the position of the impurity z_0 in the different electric fields, $F = 1$ MV/cm, 5 MV/cm, and 10 MV/cm, respectively

shapes. To our knowledge, up to now, there has been no report on triangle-shaped quantum well binding energy calculation and triangle-shaped well spin-orbit splitting energy. Another worthy phenomenon from the same figure is that (2) When F increases, the maximum of spin-orbit splitting energy decreases drastically, because such spin splitting energy is very sensitive to the intrinsic and extrinsic electric field perpendicular to the quantum well plane and (3) with the increasing of electric field, the maximum of the spin splitting energies shows a systematically left shift. This is thought to be due to the strong infinite confined potential. Such strong potential can result in a narrower electron effective well width, in which no confined electron can escape from the well. When we chose the lowest electric field $F = 1$ MV/cm, we found a maximum Γ of 1.22 meV at $z_0 = 2.3$ nm, indicating that the weaker the electric field is, the bigger the spin-orbit splitting energy will be.

As commonly known, for wide band gap semiconductors, for instance, in our GaN and its related compounds, the spin-orbit splitting energies are much smaller than the quantum well subband and also the impurity binding energy. However, for the narrow band gap semiconductors, e.g., InSb, GaSb, AsIn or InN, the spin splitting effect cannot be negligible. Though in this paper we have studied spin-orbit effect in a wide band gap material, our work could hint other researchers who engage in spin-orbit effect in narrow band gap materials.

Summary

In summary, we calculate the binding energy and spin-orbit split energy Γ of the ground states of a hydrogenic donor impurity in AlGaN/GaN heterojunction in the framework of effective-mass envelope function theory, including the effect of Rashba spin-orbit coupling. When taking into account the GaN/AlGaN intrinsic polarization field and extrinsic applied electric field, We find that when such electric fields of the heterojunction increases, it can result in a decrease in effective well width of the triangle-shaped quantum well $\overline{W}$, and an increase of the binding energy. In the mean time, the spin-orbit split energy Γ decreases drastically. In addition, we also find that the maximum value of Γ could be up to 1.22 meV when the lowest electric field of 1 MV/cm crosses the AlGaN/GaN heterointerface.

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