Abstract  In the framework of effective mass envelope function theory, the electronic structures of GaAs/Al\textsubscript{x}Ga\textsubscript{1-x}As quantum double rings (QDRs) are studied. Our model can be used to calculate the electronic structures of quantum wells, wires, dots, and the single ring. In calculations, the effects due to the different effective masses of electrons and holes in GaAs and Al\textsubscript{x}Ga\textsubscript{1-x}As and the valence band mixing are considered. The energy levels of electrons and holes are calculated for different shapes of QDRs. The calculated results are useful in designing and fabricating the interrelated photoelectric devices. The single electron states presented here are useful for the study of the electron correlations and the effects of magnetic fields in QDRs.

Keywords  Electronic structures · GaAs · Quantum double rings · Nanostructures · Effective-mass theory · Band mixing

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Introduction

Growth of semiconductor nanostructures has attracted much attention due to their unique electronic and optical properties as well as potential applications in making electronic and optoelectronic devices.

Recently, T. Mano et al. fabricated the self-assembled formation of concentric quantum double rings (QDRs) with high uniformity and excellent rotational symmetry using the droplet epitaxy technique [1]. They calculated the electronic energy levels using the effective mass approximation. For computational purposes, they assumed that the quantum rings have a rotational symmetry relative to the growth axis. Aside from this assumption, no adjustable parameters were used in the model. However, the valence band mixing was not considered in their calculations.

We have studied the electronic states and valence band structures of the InAs/GaAs quantum single ring [2]. In this letter, using the effective-mass envelope-function theory, we will study the electron and hole states of QDRs. In our calculations, the effects due to the different effective masses of electrons and holes in GaAs and Al\textsubscript{x}Ga\textsubscript{1-x}As and the valence band mixing are included. Our model can be used to calculate the electronic structures of quantum wells, wires, dots and the single ring. The single electron states are useful for the study of the electron correlations and the effects of magnetic fields on QDRs.

Theoretical model

Figure 1 shows the schematic plot of the GaAs/Al\textsubscript{x}Ga\textsubscript{1-x}As QDRs. In the following, we choose \( z \)-direction of our coordinate system to be perpendicular to the plane of quantum rings. The QDRs are concentric. We suppose the inner radius and outer radius are \( R_1 \), \( R_2 \) for the small ring and \( R_3 \), \( R_4 \) for the large ring, respectively. The height of QDRs is \( l \). If \( R_1 = R_2 \), or \( R_3 = R_4 \), the QDRs become quantum single ring.
According to Burt and Foreman’s effective-mass theory and taking into account the difference of the effective-masses between GaAs and Al₈Ga₁₋₈As [3, 4], the electron Hamiltonian can be written as (neglecting the second- and higher-order terms in the approximation)

$$H_e = \frac{1}{2m_e^*(x,y,z)} P + V_e(x,y,z).$$

(1)

In the above equation,

$$m_e^*(x,y,z) = \begin{cases} m_1^* & R_1^2 \leq \rho^2 \leq R_2^2 \\
2m_1^* & \text{or} \ R_3^2 \leq \rho^2 \leq R_4^2 \\
\text{and} |z| \leq l, & \text{others,} \\
0 & \text{others,} \end{cases}$$

(2)

$$V_e(x,y,z) = \begin{cases} 0 & R_1^2 \leq \rho^2 \leq R_2^2 \\
E_c & \text{or} \ R_3^2 \leq \rho^2 \leq R_4^2 \\
\text{and} |z| \leq l, & \text{others,} \end{cases}$$

(3)

where $\rho^2 = x^2 + y^2$, and $m_1^*$ and $m_2^*$ are the effective electron masses in GaAs and Al₈Ga₁₋₈As, respectively. $E_c$ is the conduction band offset between GaAs and Al₈Ga₁₋₈As. The electron Schrödinger equation is

$$H_e \Psi_e(r) = E_c \Psi_e(r).$$

(4)

Using the periodic boundary condition, we assume that the electron wave functions have the following forms

$$\Psi_e(r) = \frac{1}{L^{3/2}} \sum_{n,n,n} a_{n,n,n} e^{i(k_n x + k_n y + k_n z)},$$

(5)

with $k_n = k_0 + n_i K, \ n_i = 0, \pm 1, \pm 2, \ldots$, and $i = x, y, z$; $K = 2\pi/L, \ r = (x, y, z), \ L$ denotes the periods of the large units. The matrix elements of Hamiltonian (1) for Eq. 5 can be written as

$$\left( \frac{\hbar^2}{2m_1^*} \delta + \frac{\hbar^2}{2m_{12}} S_i S_j \right) \left( k_n k_n' + k_{ny} k_{ny}' + k_{nz} k_{nz}' \right)$$

(6)

$$+ (\delta - S_i S_j) E_c,$$

where $k_n' = k_n + n_i' K,$ and

$$\delta = \begin{cases} 1 & \text{for} \ n_x = n_x', \ n_y = n_y', \ n_z = n_z' \\
0 & \text{otherwise}, \end{cases}$$

(7)

$$\frac{\hbar^2}{2m_{12}} = \frac{\hbar^2}{2m_1^*} - \frac{\hbar^2}{2m_2^*},$$

(8)

$$S_i = \begin{cases} 1 & n_z = n_z' \\
\sin \frac{(n_z - n_z') L}{n_z - n_z'} & n_z \neq n_z', \end{cases}$$

(9)

$$S_j = \begin{cases} \pi (R_1^2 - R_2^2) + (R_3^2 - R_4^2) / L^2 & n_x = n_x' \text{ and} \ n_y = n_y' \\
(F_2 F_1 + F_3 F_4) / (\lambda L) & n_x \neq n_x' \text{ or} \ n_y \neq n_y', \end{cases}$$

(10)

In the above equation, $F_i = R_i J_1(\lambda R_i)$ with $i = 1, 2, 3, 4$; $J_1$ is the first-order Bessel function $J_1(x) = \frac{x}{\pi} \int_0^\infty \cos (\xi \cos \theta) \sin \theta \ d\theta$; and $\lambda = \sqrt{(n_x - n_x')^2 + (n_y - n_y')^2}$.

Therefore, we can calculate the electronic states from Eq. 6.
For the hole states, the hole effective mass Hamiltonian can be written as [4]

\[
H_h = \frac{1}{2m_0} \begin{bmatrix}
P_+ & R & -Q_-
\end{bmatrix} \begin{bmatrix}
P_+ & C & -Q_+
\end{bmatrix} + V_h, \quad (11)
\]

where

\[
V_h(r) = \begin{cases}
0 & \text{for } R_1^2 \leq \rho^2 \leq R_3^2 \text{ or } R_3^2 \leq \rho^2 \leq R_4^2, \text{ and } |z| \leq l, \\
V_{h0} & \text{otherwise},
\end{cases}
\]

\[
P_\pm = p_x(\gamma_1 \pm \gamma_2)p_x + p_y(\gamma_1 \pm \gamma_2)p_y + p_z(\gamma_1 \mp 2\gamma_2)p_z, \\
Q_\pm = 2\sqrt{3}\left[(p_x \pm ip_y)\sigma p_x + p_x \pm ip_y\sigma p_y\right], \\
R = \sqrt{3}\left[(p_x + ip_y)(p_x + ip_y) - (p_x - ip_y)(p_x - ip_y)\gamma(p_x - ip_y)\right], \\
C = 2p_y(\sigma + \pi)(p_x - ip_y) - 2(p_x - ip_y)(\sigma + \pi)p_z,
\]

\[
\sigma = (-1 - \gamma_1 + 2\gamma_2 + 6\gamma_3)/6, \\
\pi = (1 + \gamma_1 - 2\gamma_2)/6, \\
\gamma = (\gamma_2 + \gamma_3)/2, \\
\mu = -(\gamma_2 - \gamma_3)/2.
\]

Here \(\gamma_1, \gamma_2, \text{ and } \gamma_3\) are functions of \(x, y, \text{ and } z\),

\[
\gamma_1, \gamma_2, \gamma_3 = \begin{cases}
\gamma_{11}, \gamma_{12}, \gamma_{13} & \text{for } R_3^2 \leq \rho^2 \leq R_4^2, \\
\gamma_{21}, \gamma_{22}, \gamma_{23} & \text{otherwise}.
\end{cases}
\]

The notations \(\gamma_{11}, \gamma_{12}, \gamma_{13}\) and \(\gamma_{21}, \gamma_{22}, \gamma_{23}\) are the Luttinger effective mass parameters of GaAs, Al\(_{1-x}\)Ga\(_x\), As materials, respectively; and \(m_0\) is the free electron mass.

The hole envelope function equation is

\[
H_h \Psi_h = E_h \Psi_h. \quad (16)
\]

Using the normalized plane-wave expansion method [5], we assume that the hole-wave functions have the following form:

\[
\psi_h(r_h) = \frac{1}{L^{3/2}} \sum_{n_m n'_m} a_{n_m n'_m} e^{i(k_{nx}x + k_{ny}y + k_{nz}z)}. \quad (17)
\]

The matrix elements of Hamiltonian (11) for Eq. 17 can be written as

\[
(P_{\pm})_{n_m n_{m'}, n'_m n'_{m'}} = (\gamma_{11}^2 + \gamma_{12}^2)\epsilon(k_{nx}k_{nx} + k_{ny}k_{ny}) + (\gamma_{21}^2 + \gamma_{22}^2)\epsilon(k_{nx}k_{nx} + k_{ny}k_{ny})
\]

Results and discussion

We take the material parameters from Ref. 6. The aluminum proportion in Al\(_{1-x}\)Ga\(_x\)As is taken to be \(x = 0.3\), which equals the value for the experimental samples in Ref. 1. The effective masses and band gaps \(E_g^F(eV)\) are listed in Table 1. The conduction-band offset is assumed to be 65\% of the band gap difference.

We have calculated the electron and hole energy levels as functions of the radius of QDRs. In calculations, we assume the height of QDRs to be \(l=3\) nm.

Figure 2a, b shows the electron and hole energy levels as a function of \(R_1\), respectively, for fixed

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|}
\hline
Material & \(m^*_e(m_0)\) & \(\gamma_1\) & \(\gamma_2\) & \(\gamma_3\) & \(E_g^F(eV)\) \\
\hline
GaAs & 0.067 & 6.98 & 2.06 & 2.93 & 1.519 \\
AlAs & 0.15 & 3.76 & 0.82 & 1.42 & 3.099 \\
Al\(_{0.3}\)Ga\(_{0.7}\)As & 0.0919 & 6.014 & 1.688 & 2.477 & 1.993 \\
\hline
\end{tabular}
\caption{The effective masses and band gaps \(E_g^F(eV)\) of bulk GaAs and Al\(_{0.3}\)Ga\(_{0.7}\)As}
\end{table}
$R_2 = 6 \text{ nm}$, $R_3 = 8 \text{ nm}$, and $R_4 = 10 \text{ nm}$. From Fig. 2a, one may find that there is only one deep confined electronic energy level for the above structure parameters. The anti-crossing is found near $R_1 = 4.5 \text{ nm}$ for the second and the third electron energy levels. Figure 2b shows there are two confined hole energy levels for the above structure parameters.

Figure 3a, b shows the electron and hole energy levels as a function of $R_2$, respectively, for $R_1 = 4 \text{ nm}$, $R_3 = 8 \text{ nm}$, and $R_4 = 10 \text{ nm}$. The one and two confined electron energy levels is found for $R_2 < \text{and} > 5.9 \text{ nm}$, respectively. The anti-crossing is found near the same $R_2 = 5.9 \text{ nm}$ for the second and the third electron energy levels. The hole confined energy levels decrease monotonical as $R_2$ increases.

Figure 4a, b shows the electron and hole energy levels as a function of $R_3$, respectively, for $R_1 = 4 \text{ nm}$, $R_2 = 6 \text{ nm}$, and $R_4 = 10 \text{ nm}$. The one and two confined electron energy levels is found for $R_3 < \text{and} > 8.1 \text{ nm}$, respectively. The anti-crossing is found near the same $R_3 = 8.1 \text{ nm}$ for the second and the third electron energy levels. The only two confined hole energy levels is found for $R_3 > 9.5 \text{ nm}$.

Figure 5a, b shows the electron and hole energy levels as a function of $R_4$, respectively, for $R_1 = 4 \text{ nm}$, $R_2 = 6 \text{ nm}$, and $R_3 = 8 \text{ nm}$. The one and two confined electron energy levels is found for $R_4 < \text{and} > 10 \text{ nm}$, respectively. The anti-crossing is found near the same $R_4 = 10 \text{ nm}$ for the second and the third electron energy levels. The only two confined hole energy levels is found for $R_4 < 8.8 \text{ nm}$.

Taking the structure parameters of the QDRs to be $l = 3.5 \text{ nm}$, $R_1 = 10 \text{ nm}$, $R_2 = 35 \text{ nm}$, $R_3 = 40 \text{ nm}$, and $R_4 = 60 \text{ nm}$, the transition energies for the ground electron energy level transiting to the ground heavy- and light-hole energy levels were calculated to be 1.694, and 1.696 eV, respectively. These calculated
results are somewhat higher than the available experimental data in Ref. 1 for we have not included the binding energy of exciton. The exciton binding energy is estimated to be 15 meV from the difference between the theoretical values and experimental data.

**Summary**

In this paper, we have calculated the electronic states of GaAs/Al$_x$Ga$_{1-x}$As QDRs. The model we proposed can be used to calculate the electronic states of quantum wells, wires, dots, and the single ring. The single electron states are useful for the study of the electron correlations and the effects of magnetic fields on QDRs. Our calculated results are useful in designing and fabricating the interrelated photodetector devices.

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