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Electronic states of InAs/GaAs tyre-shape quantum ring*

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In the framework of the effective mass theory, this paper calculates the electron energy levels of an InAs/GaAs tyre-shape quantum ring (TSQR) by using the plane wave basis. The results show that the electron energy levels are sensitively dependent on the TSQR's section thickness d, and insensitively dependent on TSQR's section inner radius R_1 and TSQR's inner radius R_2. The model and results provide useful information for the design and fabrication of InAs/GaAs TSQRs.

Keywords: tyre-shape quantum ring (TSQR), plan wave, energy level
PACC: 7125, 7115B, 7115, 7320D

1. Introduction

InAs/GaAs nanostructures have many applications in electronic and optoelectronic devices due to their special electronic and optical properties. As one kind of useful nanostructure, InAs/GaAs quantum dot has already been studied extensively.[1−3] In the recent years quantum rings have also attracted a great deal of attention.[4−10] Wu and Bao studied the effect of electric field on the electronic spectrum and the persistent current of a quantum ring with two electrons.[4] Halonen *et al* studied the electron energy levels in quantum rings.[5] In their theoretical model, they assumed that the electrons in quantum rings move in the (x, y) plane and are confined by a parabolic potential. Li and Xia studied three-dimensional InAs/GaAs quantum rings.[6] Their results show how the electron energy levels are dependent on the inner and outer radius of the quantum rings. They also studied the hole states of InAs/GaAs quantum rings.[7] Llorens *et al* studied electron energy levels of quantum rings in a lateral electric field.[8] Many papers have been published on quantum rings recently. For example, by using spin density functional theory, Castelano *et al* studied artificial molecular quantum rings.[9] Saiga *et al* studied the ground state properties of quantum rings with few electrons.[10]

In this paper, we will study the electron states of InAs/GaAs tyre-shape quantum rings (TSQRs) by using effective mass theory. Due to its atom-like properties, this nanostructure is likely to be used in quantum control and quantum commutation. It may also be useful for designing detector and other electronic and optoelectronic devices because of its unique electron structures. Our calculation will provide useful information for designing and fabricating this structure. Our model and method can also be used to calculate the electron states of other structures.

2. Theoretical model

In our coordinate system, as shown in Fig.1, the x and y directions are in the plane of TSQR, and the z direction is perpendicular to the plane of TSQR. The TSQR's section thickness d, section inner radius R_1 and inner radius R_2 are also shown in the Fig.1. According to the effective mass theory proposed by Burt and Foreman,[11,12] and without considering the difference between the electron effective mass of GaAs and InAs, the Hamiltonian of an electron has the following form (the second and higher order terms are neglected):

$$H_{\rm e} = \frac{P^2}{2m^*} + V(r). \tag{1}$$

In the above equation, P is the electron momentum operator, m^* is the electron effective mass in InAs material, r is the displacement vector, $r = (x, y, z)$, and

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$$V(r) = \begin{cases} 0 & \text{for} \quad R_1^2 \le (x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2 \le (R_1+d)^2, \\ V_{\rm e} & \text{others}, \end{cases} \tag{2}$$

where $\begin{cases} x_0^2 + y_0^2 = (R_1+R_2+d)^2 \\ z_0 = 0 \end{cases}$ is the equation of a circle in the xy plane, and $V_{\rm e}$ is the conduction band offset between GaAs and InAs.

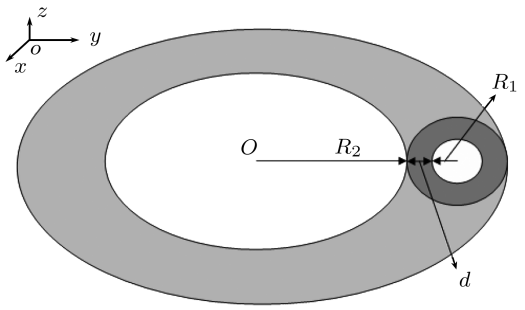


Fig.1. A tyre-shaped quantum ring (TSQR).

The electron Schrödinger equation in the quantum ring is

$$H_{\rm e}\,\Psi(r) = E_{\rm e}\,\Psi(r). \tag{3}$$

According to Li *et al*[6,13−15] by invoking periodic boundary conditions, $\Psi(r)$ can be expanded by normalized plane wave states. We assume that $\Psi(r)$ has the following form:

$$\Psi(r) = \sqrt{\frac{8}{L_1L_2L_3}} \sum_{n_x n_y n_z} \sin(k_x + n_x K_x x) \times \sin(k_y + n_y K_y y) \sin(k_z + n_z K_z z). \tag{4}$$

where L_1 is the normalized length along the x direction, while L_2, L_3 are the normalized lengths along the y, z direction, respectively, and $K_x = 2\pi/L_1, K_y = 2\pi/L_2, K_z = 2\pi/L_3, n_x = 1, 2 \ldots, m_x, n_y = 1, 2 \ldots, m_y, n_z = 1, 2 \ldots, m_z$, where m_x, m_y, m_z are positive integers. The total number of plane wave states is $N = m_x m_y m_z$.

If we let $|n\rangle = |n_x n_y n_z\rangle$ represent a plane wave state, then the matrix elements of the Hamiltonian of Eq.(1) are as follows:

$$\langle n'|H_{\rm e}|n\rangle = \left\langle n' \left| \frac{P^2}{2m^*} \right| n \right\rangle + \langle n'|V(r)|n\rangle, \tag{5}$$

where

$$\left\langle n' \left| \frac{P^2}{2m^*} \right| n \right\rangle = \frac{\eta^2}{2m^*}[(k_x + n'_x K_x)^2 + (k_y + n'_y K_y)^2 + (k_z + n'_z K_z)^2]\delta_{n,n'}, \tag{6}$$

$$\begin{aligned} &\langle n'|V(r)|n\rangle \\ &= V{\rm e}\delta_{n,n'} - \frac{64V_{\rm e}}{L_1L_2L_3} \left\{ \left[\int_0^{R_2} {\rm d}x \int_{\sqrt{R_2^2-x^2}}^{\sqrt{(R_2+2R_1+2d)^2-x^2}} {\rm d}y \int_0^{\sqrt{(R_1+d)^2-(R_1+d+R_2-\sqrt{x^2+y^2})^2}} f(x,y,z){\rm d}z \right.\right. \\ &\quad \left.\left. + \int_{R_2}^{R_2+2d+2R_1} {\rm d}x \int_0^{\sqrt{(R_2+2R_1+2d)^2-x^2}} {\rm d}y \int_0^{\sqrt{(R_1+d)^2-(R_1+d+R_2-\sqrt{x^2+y^2})^2}} f(x,y,z){\rm d}z \right] \right. \\ &\quad - \left[\int_0^{R_2+d} {\rm d}x \int_{\sqrt{(R_2+d)^2-x^2}}^{\sqrt{(R_2+2R_1+d)^2-x^2}} {\rm d}y \int_0^{\sqrt{R_1^2-(R_1+d+R_2-\sqrt{x^2+y^2})^2}} f(x,y,z){\rm d}z \right. \\ &\quad \left.\left. \left. + \int_{R_2+d}^{R_2+d+2R_1} {\rm d}x \int_0^{\sqrt{(R_2+2R_1+d)^2-x^2}} {\rm d}y \int_0^{\sqrt{R_1^2-(R_1+d+R_2-\sqrt{x^2+y^2})^2}} f(x,y,z){\rm d}z \right] \right\}. \end{aligned} \tag{7}$$

With

$$f(x,y,z) = \sin(k_x + n_x K_x x) \sin(k_y + n_y K_y y) \sin(k_z + n_z K_z z), \tag{8}$$

$$\delta_{n,n'} = \begin{cases} 1 & \text{when} \quad n_x = n'_x, n_y = n'_y \text{ and } n_z = n'_z, \\ 0 & \text{others.} \end{cases} \tag{9}$$

The electron energy levels in the TSQR can be calculated by Eqs.(5)–(9).

3. Results and Discussion

In our calculation, the difference between the electron effective mass of InAs and GaAs materials is neglected. m^* is the value of the electron effective mass in InAs. $m^* = 0.023m_0$,[16] and m_0 is the mass of free electron. The band gaps of GaAs and InAs are 1.518 eV and 0.78456 eV, respectively. The conduction band offset is about 70% of the band gap difference.[17] According to Li and Xia,[13] the values of k_x, k_y, k_z almost have no effect on the results, so we let $k_x = k_y = k_z = 0$ for simplicity. The effective Bohr radius a^* in InAs can be calculated to be 34.96 nm. When the barrier width is between $1.5a^*$ and $3.5a^*$, the results of the calculation are the same;[13] here, the barrier width is chosen to be $2a^*$, namely, $L_1 = L_2 = 2(R_2 + 2R_1 + 2d) + 2a^*$ and $L_3 = 2(R_1+d)+2a^*$. We choose $m_x = m_y = m_z = 10$, for a total of 1000 plane wave states. Thus, we need to diagonalize 1000×1000 matrixes to calculate the electron energy levels.

We have calculated the electron energy states as a function of d. In our calculation, we assume $R_1 = 20$ nm and $R_2 = 80$ nm. The results as d changes from 2 nm to 10 nm are shown in Fig.2. From Fig.2, we may find that the binding energies of electron in TSQR are sensitively dependent on d. As d increases, the effect of quantum confinement decreases, thus, the electron binding energies decrease.

Figure 3 shows the electron energy states as a function of R_1. In our calculation, $d = 4$ nm and $R_2 = 80$ nm. From Fig.3, we find that the binding energies of electron in TSQR are not sensitively dependent on R_1. The difference of the ground state between $R_1 = 5$ nm and $R_1 = 20$ nm is only 25.8 meV. We also find that there are no binding energies when $R_1 = 0$, because the quantum confinement is too strong when d is only 4 nm. If we increase the value of d, the binding energies will appear. In addition, as R_1 increases, the quantum confinement effect decreases, thus, the electron binding energies decrease.

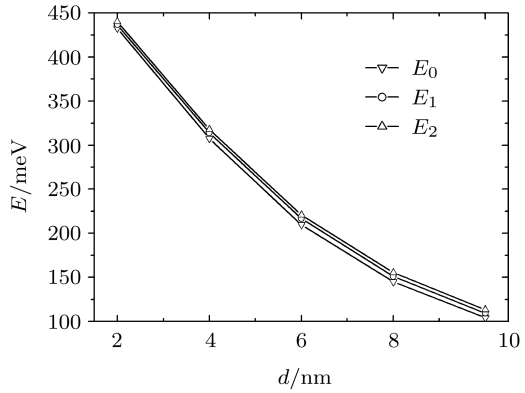


Fig.2. The first three electron energy states as a function of d, with $R_1 = 20$ nm, $R_2 = 80$ nm.

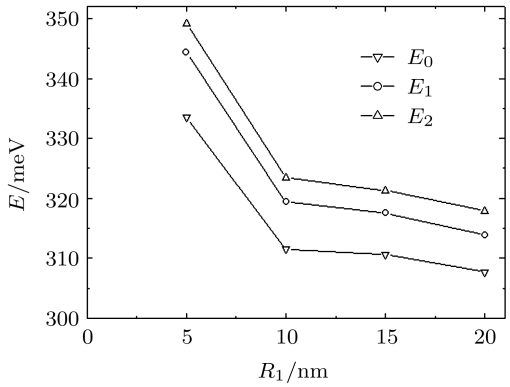


Fig.3. The first three electron energy states as a function of R_1, with $d = 4$ nm, $R_2 = 80$ nm.

Figure 4 shows the electron energy states as a function of R_2, with $d = 4$ nm and $R_1 = 20$ nm. Similar to R_1, the binding energies of electron in TSQR are also not sensitively dependent on R_2. However, the binding energies of electron in TSQR increase as R_2 increases. As R_2 increases, the coupling between the left and the right part of TSQR decreases, thus, the binding energies of electron increase. In addition, from Figs.2, 3 and 4, we find that the energy spacing between the binding energies is almost equal, at about several meV.

We calculated the electron energy states as a function of d. In our calculation, we assume that $R_1 - d = 16$ nm and $R_2 - d = 76$ nm, which guarantees $R_1 = 20$ nm and $R_2 = 80$ nm when $d = 4$ nm. The results are shown in Fig.5. From Fig.5, we find that d dominates the electron energy states, which decrease as d increases. Since electrons are confined in InAs layer with the width d, and meanwhile d is much smaller than R_1 and R_2, therefore, d has more influence on the electron energy states than R_1 and R_2 do. Comparing the results in Fig.2 with those in

Fig.5, we may find that the electron energy states in Fig.5 are somewhat greater than those in Fig.2. When $d < 4\,\text{nm}$, R_1 and R_2 in Fig.2 are greater than their counterparts in Fig.5. When $d > 4\,\text{nm}$, R_1 and R_2 in Fig.2 are less than their counterparts in Fig.5. The electron energy states increase as R_2 increases, and decrease as R_1 increases, thus, when $d < 4\,\text{nm}$, R_1 has more influence on the electron energy states than R_2 does. When $d > 4\,\text{nm}$, however, R_2 has more influence on the electron energy states than R_1 does.

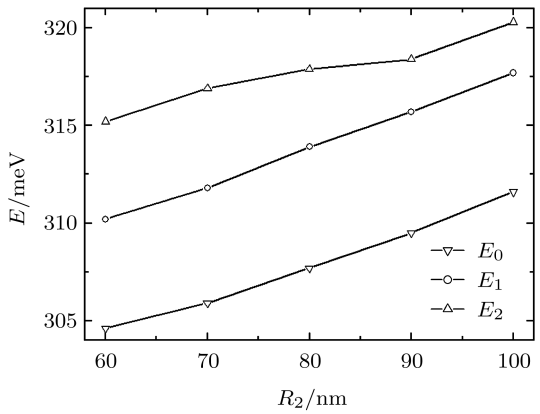


Fig.4. The first three electron energy states as a function of R_2, with $d = 4\,\text{nm}$, $R_1 = 20\,\text{nm}$.

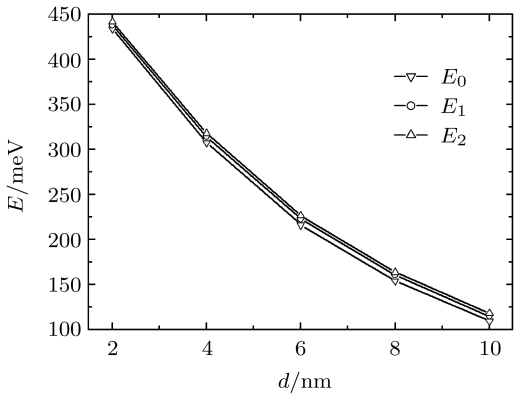


Fig.5. The first three electron energy states as a function of d, with $R_1 - d = 16\,\text{nm}$, $R_2 - d = 76\,\text{nm}$.

4. Conclusion

In summary, we have calculated the electron energy states of an InAs/GaAs TSQR by using plane wave method. According to our calculation, the electron energy levels are sensitively dependent on the TSQR's section thickness d, and insensitively dependent on TSQR's section inner radius R_1 and TSQR's inner radius R_2. Our model and results are useful for designing and fabricating InAs/GaAs TSQRs.

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