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Spatially indirect excitons in type-II quantum dots

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The authors have calculated the electronic structure for type-II InP/GaAs quantum dot systems considering a three-dimensional geometry including the wetting layer and the electron-hole interaction, which is the only responsible for the hole localization. Their results for the InP/GaAs structure show the electron confined inside the dot and the hole in the GaAs layer, partially above and below the dot. The authors propose structures with InGaAs or InGaP layers, where the hole wave function forms a ring around the dot walls. The electron-hole overlap, and therefore, the carrier lifetimes are very sensitive to the structural geometry, which is an important tool for device engineering. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2741601]

Quantum dots (QDs) with a type-II band lineup present a peculiar electronic structure, where only one of the carriers is confined to the dot while the other spreads around it due to the Coulombic attraction. The spatially separated carriers result in an excitonic extended wave function as compared to typical type-I QD excitons. Therefore, the electron-hole spatial overlap is much smaller for type-II QDs, resulting in relatively long carrier lifetimes.[1] This configuration allows a large flexibility for altering the wave-function distribution of the carrier remaining outside the QD, without significantly affecting the wave function of the carrier inside the dot. An interesting possibility is preparing ringlike wave functions that could be used to investigate specific quantum phenomena such as the Aharonov-Bohm effect.[2,3] This flexibility also allows for a larger control of the electron-hole overlap and the carrier lifetime, a fundamental parameter for the development of practical devices such as lasers and optical memories.[4]

In this work, we calculate the ground state wave functions of electrons and holes in different structures based on InP/GaAs self-assembled quantum dots. In this system, the electron is confined inside the InP dot that acts as a barrier for the hole, which remains in the GaAs layers.[5] A controversial issue is the possibility of observing the Aharonov-Bohm effect in such structures. Ribeiro *et al.*[6] have reported experimental results on an ensemble of InP/GaAs QDs that they attributed to the Aharanov-Bohm effect, assuming that the hole can present a ringlike state in such dots. In contrast, a recent investigation[7] on the emission of single InP/GaAs QDs shows no oscillation of the energy emission as a function of the magnetic field, as predicted by the Aharonov-Bohm effect. Our calculation gives further insight about this open question.

We perfomed three-dimensional numerical calculations of the electronic structure for three different structures described in Fig. 1, using a realistic geometry for the self-assembled QDs. The QD dimensions were based on the results of microscopic measurements of typical InP/GaAs QDs.[7] We considered a spherical lens shape QD with radius (R) ranging from 10.0 to 30.0 nm and height (H) varying from 1.5 to 3.0 nm, which correspond to the limiting sizes of the typical measured values. We took into account a thin InP wetting layer (1 nm) under the dot. Structures II and III also include additional InGaAs and InGaP layers, respectively, and are discussed in detail along the work.

The coupled three-dimensional electron-hole Schrödinger equations were solved in the Hartree-Fock approximation using parabolic bands. We denote the effective eletron (hole) mass by $m_{e(h)}$. The single-particle equations can be written as

$$H_{e(h)}\psi_{e(h)}(\mathbf{r}_{e(h)}) = E_{e(h)}\psi_{e(h)}(\mathbf{r}_{e(h)}), \tag{1}$$

where the Hamiltonian is given by

$$H_{e(h)} = -\frac{\hbar^2}{2m_{e(h)}}\nabla^2_{\mathbf{r}_{e(h)}} + V^{e(h)}(\mathbf{r}_{e(h)}) + V_c^{e(h)}(\mathbf{r}_{e(h)}), \tag{2}$$

and $V^{e(h)}$ describes the three-dimensional potential of the electron (hole), due to the different materials of the well/barrier regions. The electron-hole Coulomb interaction $V_c^{e(h)}$ in the mean-field approximation is given by

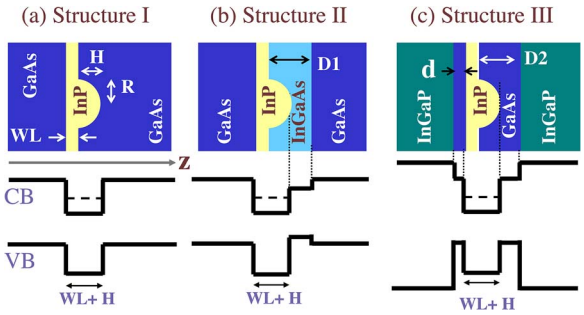

FIG. 1. Schematic diagrams and corresponding potential profiles of different structures based on InP/GaAs type-II quantum dot. In structure II the $In_{0.08}Ga_{0.92}As$ layer is included, while in structure III the InGaP (lattice matched to GaAs) layers are included.

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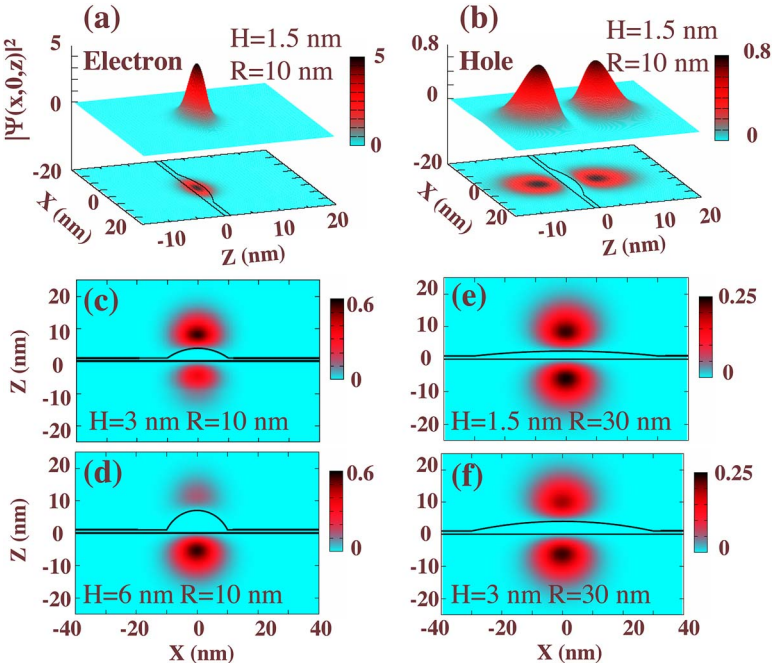

FIG. 2. Electron and hole ground state for QDs with struture I. [(a) and (b)] Electron and hole probability densities $|\psi(x_{e(h)},0,z_{e(h)})|^2$ and its contour map for $R=10.0$ nm and $H=1.5$ nm; [(c)–(f)] hole contour maps for QDs with different dimensions.

$$V_c^{e(h)}(\mathbf{r}_{e(h)}) = \frac{e^2}{4\pi\epsilon}\int d^3r_{h(e)}\frac{|\psi(\mathbf{r}_{h(e)})|^2}{|\mathbf{r}_h - \mathbf{r}_e|}, \tag{3}$$

where $\mathbf{r}_e$ denotes the electron (hole) position and $\nabla^2_{\mathbf{r}_{e(h)}}$ denotes the Laplacian relative to the electron (hole) coordinates. The equations were solved in Cartesian coordinates, where z corresponds to the growth direction. We have used the split-operator technique,[8] and the excitonic ground state was obtained without any basis expansion. The results were computed with the following parameters: effective dielectric constant $\epsilon=13.0$; electronic effective mass $m_e=0.079\ m_0$; heavy-hole effective mass $m_h=0.45\ m_0$, where m_0 denotes the free-electron mass; and conduction and valence band offsets, 300 and 292 meV, respectively. Due to the cylindrical symmetry of the system, we only show here the electron (hole) probability density of the ground state for the plane $y_{e(h)}=0$, $\Pr(x_{e(h)},0,z_{e(h)})=|\psi(x_{e(h)},y_{e(h)}=0,z_{e(h)})|^2$. The three-dimensional probability density can be recovered from the latter by rotating it around the z axis.

Figure 2 shows the electron and hole probability densities $\Pr(x_{e(h)},0,z_{e(h)})$ for some structure I QDs [cf. Fig. 1(a)]. The electron is basically confined inside the QD independent of its radius and height. The electron probability density and its contour map are shown in Fig. 2(a) for a QD with $R=10.0$ nm and $H=1.5$ nm. The hole ground state for the same QD is shown in Fig. 2(b) and it is distributed above and below the dot, along its axis. Figure 2(c)–2(f) show the contour map for the hole wave function of QDs with different dimensions. We observe that for all those QDs, the fundamental hole wave function does not form a ring around the lateral walls of the dot. Instead, the probability of finding the hole around the lateral walls of the dot is usually negligibly small. In Fig. 2(d) the quantum dot height $H=6.0$ nm is artificially large but it was included to demonstrate the impossibility of obtaining a hole nanoring in this material, even with a relatively large H. Therefore, no Aharonov-Bohm effect is expected to be present for these dots under applied magnetic field, in agreement with the experimental result of de Godoy *et al.*[7]

We now present the result for the two alternative QD structures proposed in Figs. 1(b) and 1(c). The first consists of an InP QD, grown on GaAs covered by a thin ($D_1=5.0$ nm) $In_{0.08}Ga_{0.92}As$ layer and followed by GaAs [cf. Fig. 1(b)]. The second is an InP QD grown on the top of a thin ($d=2.0$ nm) GaAs layer preceeded by an InGaP (lattice matched to GaAs) layer. The QD is thus covered by a second ($D_2=5.0$ nm) GaAs layer, followed by a thick InGaP layer [cf. Fig. 1(c)].

We used the same carrier effective masses of structure I for structures II and III. The band offsets used for the GaAs/InGaAs interfaces are 54 and 36 meV, and for GaAs/InGaP interfaces are 90 and 380 meV [cf. Figs. 1(b) and 1(c)], for conduction and valence bands, respectively.

The resulting hole ground state contour maps are shown in Fig. 3 for QDs based on structures II and III. The electron

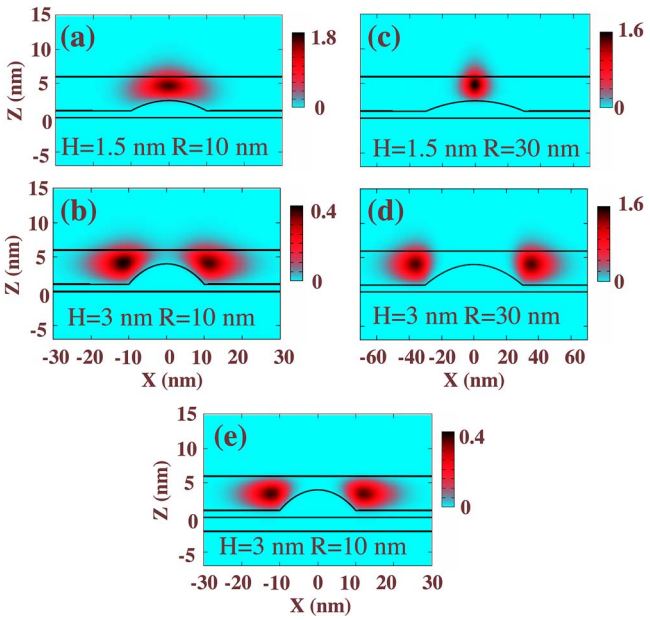

FIG. 3. Contour maps of the hole ground state. Panels (a)–(d) correspond to structure II, while panel (e) to structure III.

TABLE I. The electron-hole wave-function overlap and the activation energy for different QDs. The radius and the height of the QDs is given in nanometer. The structures roman number correspond to that one shown in Fig. 1.

(Structure, radius, height)	Overlap	Energy (meV)
(I,10,1.5)	0.34	9.4
(I,10,3.0)	0.18	8.4
(I,10,6.0)	0.08	7.1
(I,30,1.5)	0.20	6.6
(I,30,3.0)	0.12	6.2
(II,10,1.5)	0.43	21.9
(II,10,3.0)	0.15	17.8
(II,30,1.5)	0.39	17.6
(II,30,3.0)	0.003	13.3

remains confined inside the InP QD, independent of its radius and height, and its wave function is thus not shown here. Due to the additional confinement on structure II, the hole wave function is basically confined in the InGaAs layer at the top of the InP QD [cf. Figs. 3(a)–3(d)]. We can see from Figs. 3(a)–3(d) that the dimension of the InGaAs layer above the top of the QD plays a critical role in the hole localization. For QDs with $H=1.5$ nm, Figs. 3(a) and 3(c), when the thickness of the InGaAs at the top of the QD is 3.5 nm, the hole wave function is mainly localized above the top of the dot, independent of its radius. For QDs with height $H=3.0$ nm [cf. Fig. 3(b) and 3(d)], in which the InGaAs at the top of QD is reduced to 2.0 nm, the hole wave function moves toward the lateral walls of the dot, independent of its radius. In this case it forms a ring around the QD, which can be seen by rotating the contour maps around the growth direction. Figure 3(e) shows the hole localization for a structure III QD. The resulting band offsets and electron-hole Coulomb interaction confine the hole inside the GaAs layer around the QD. Similarly to structure I, the thickness of the hole allowed GaAs region on the top of the QD is now critical for the hole localization. For the QD with a GaAs layer of 2.0 nm on its top [cf. Fig. 3(e)], the hole wave function is mainly localized around the lateral walls of the QD forming a hole nanoring as well.

Table I shows the electron-hole wave-function overlaps and the activation energies for structures I and II corresponding to the QD's dimensions presented in Figs. 2 and 3. The overlap is defined as $\int d^3r \psi_e(\mathbf{r})\psi_h(\mathbf{r})$. The activation energy corresponds to the energy necessary to separate the hole from the electron inside the InP QD, removing the hole to the GaAs bulk. For QDs following sctructure I, the activation energy given by the half of the difference between the electron-hole pair energies, E_e+E_h, obtained by calculating the electron and hole ground states with and without the Coulomb interaction, coincides with the excitonic binding energy, since there is no structural confinement for holes. We note that both the overlap and the activation energy become smaller as the QD becomes larger, concerning both its height and radius. For larger QDs the electron can be better accommodated inside the dot, thus reducing the electron-hole overlap. Therefore, the effective electron-hole Coulomb interaction becomes weaker, reducing the confinement of the hole. This effect is strongly enhanced for structures with the InGaAs layer (structures II). The transition from hole wave function centered on the QD axis to nanoringlike wave function, brings the hole farther away from the electron resulting in a significant decreasing of the electron-hole overlap. On the other hand, when the InGaAs layer on the top of the QD is large enough so that the hole remains around the QD's top, its center of mass resides closer to the top of the dot as compared to QDs with equal dimensions in structure without the InGaAs layer (structure I). As a consequence, the former have larger overlap and activation energy than the latter.

In conclusion, we have investigated the excitonic ground state of different structures based on InP/GaAs type-II QDs. The hole wave function, the activation energy, the electron-hole overlap, and therefore the carrier lifetimes are very sensitive to the details of those structures, which represents an important tool for device engineering. Ringlike hole wave functions only come about with additional layers of alloys to confine the hole close to the dot along the growth direction.

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