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Electric states in laterally and vertically arrayed Type-II Quantum Dots

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Abstract

Laterally and vertically arrayed GaSb type-II quantum dots (QDs) in GaAs are studied theoretically to clarify how the electronic states are affected by the QD arrangements. We numerically calculate the wave functions of the electron Ψ_e and hole Ψ_h and their overlap integral Θ in laterally and vertically arrayed GaSb type-II QDs. It is found that Ψ_e is strongly modified by the QD arrangements, resulting in the increase of Θ; the maximum values of Θ for the laterally and vertically arrayed QDs are about two and six times larger than that for the single QD.

1. Introduction

Recently, type-II QDs are drawing much attention due to their unique configuration of electrons and holes; only electrons or holes are confined in the dot, whereas the others are kept outside. Because of this electron-hole spatial separation, type-II QDs show unique optical properties different from those of type-I QDs, such as long radiative lifetime, dot-shape-dependent oscillator strength, and large tunability of emitted photons.

The remarkable development in crystal growth technology has made it possible to fabricate a variety of QD structures, including laterally arrayed and vertically stacked QDs. The optical properties of type-II QDs are markedly subjected to the influence of such QD arrangements, since the nearby QDs strongly affects the electric states of the carriers expelled outside the QDs and varies the overlap between the electron and hole wave functions; the overlap integral determines the strength of the optical transition and its square is proportional to the oscillator strength. In this work, we theoretically analyze quantized states of carriers in laterally and vertically arrayed GaSb/GaAs type-II QDs and discuss how the spatial overlap of electrons and holes is affected by the QD arrangements.

2. Theoretical Model

We consider a GaSb type-II QD in GaAs, in which the QD only confine holes by the large valence band offset, whereas electrons are loosely bound around the QD by the Coulomb attractive field from the hole charge. For simplicity, we assume a semi-ellipsoidal QD with a wetting layer (WL). The base diameter, the height, and the thickness of the WL are taken as d = 50 nm, h = 5 nm, and w = 1 nm, respectively [1]. The calculated model is shown in Fig. 1. By the finite element method, the quantized states of carriers are numerically calculated in a specific case where one hole is trapped in the dot and one electron sits outside. In particular, we evaluate the electron Ψ_e and hole wave functions Ψ_h, and their overlap integral Θ by solving the Schrödinger equation within the effective mass approximation. In the calculation of the hole states, we ignore the Coulomb interaction between the hole and the electron. This approximation is reasonable because the Coulomb contribution from the electron is about two orders smaller than the potential originated from the valence band offset. In contrast, in the calculation of the electron states, we include the Coulomb potential caused by the confined hole, since this attractive force is the only force to bind the electron to the QD. We also consider the Sb/As inter-diffusion between the GaSb QD and GaAs matrix with the diffusion length of 3 nm, which often occurs during the self-assembled growth of QDs as well as their post-growth annealing step [1]. Since the strain effect is not considered, our model is more appropriate for strain-relaxed GaSb/GaAs QD systems [2, 3]. All the parameters used in the calculation are listed in Table I. The band offsets between GaSb and GaAs are taken as ΔE_c = 0.1 eV for the conduction band and ΔE_v = -0.81 eV for the valence band. For simplicity, the ternary parameters were derived from the binary parameters by linear interpolation [4].

Table 1. Material parameters used for the calculation.

	Effective mass		Dielectric	Energy
	electron	hole	constant	gap
	m_e/m_0	m_h/m_0	$\varepsilon/\varepsilon_0$	E_g (eV)
GaAs	0.067	0.5	12.4	1.52
GaSb	0.039	0.4	15.2	0.81

3. Results and Discussion

3. 1 Single QD

Figure 1 shows the profiles of the electron Ψ_e and hole wave functions Ψ_h in three dimensions (3D) (a) and in the x-z plane (b). The domain of the calculation is a cube of $L_a = L_b = L_c$ = 200 nm on each side, where a Dirichlet boundary condition is enforced at the surfaces. The domain size is set sufficiently large to ensure that the solutions are less affected by the boundaries. As shown in Fig. 1, the hole wave function Ψ_h is confined in the QD by the large valence band offset. In contrast, the electron wave function Ψ_e is pushed away from the QD due to the repulsive band offset potential, but loosely bound by the Coulomb attractive force from the confined hole charge. The electron wave function Ψ_e is mainly located at the top and bottom of the QD. Ψ_e is larger above the QD

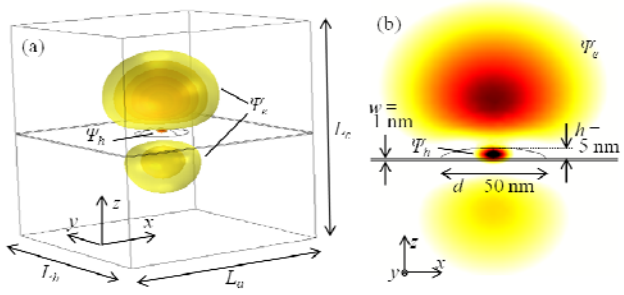

Fig. 1 Profiles of electron Ψ_e and hole wave functions Ψ_h in three dimensions (a) and in the x-z plane (b).

than below it, originated from the repulsive potential of the WL at the bottom of the QD. In fact, the electron wave function Ψ_e has a more vertically symmetric shape, when the calculation is carried out for a GaSb type-II QD without the WL.

3.2 Laterally Arrayed QDs

To simulate laterally arrayed GaSb type-II QDs, periodic boundary conditions are applied on the side surfaces of the model. This corresponds to an infinite array of QDs in the x- and y-directions (lateral directions) with period lengths of L_a and L_b. In contrast, a Dirichlet boundary condition is enforced in the z-direction (vertical direction), and the height of the calculated domain is set to be L_c = 200 nm. We consider the case for $L_a = L_b$ and carry out the calculation at various period lengths L_a (= L_b).

First, we investigate the overlap integral Θ between the electron Ψ_e and hole wave functions Ψ_h, since Θ determines the strength of the optical transition. Figure 2 (a) shows the overlap integral Θ as a function of the period length L_a. The value of Θ for the single QD is also marked by an arrow. When the period length is large (L_a = 100 nm), the magnitude of Θ is almost same as that for the single QD. As L_a decreases from 100 to 60 nm, Θ increases by about twofold. Since the hole is strongly confined in the QD, the hole wave function is less affected by the QD arrangement. The dependence of Θ on L_a is therefore originated from the change of the electron wave function Ψ_e.

Figure 2 (b) and (c) show the electron wave functions Ψ_e for period lengths L_a = 100 and 60 nm. When the QD is laterally arranged in the long period (L_a = 100 nm), the electron wave function Ψ_e has a similar profile (Fig. 2 (b)) to that for the single QD (Fig. 1(b)), leading to almost the same magnitude of Θ as that for the single QD (Fig. 2 (a) at L_a ~ 100 nm). In contrast, the electron wave function Ψ_e for the short period QD (L_a = 60 nm) is spread laterally and combined with the next ones (Fig. 2(c)), originated from the influence of the neighbor QDs. In this case, Θ is about two times larger than that for the single QD (Fig. 2 (a) at L_a ~ 60 nm). Note that the strong dependence of the electron wave function Ψ_e and the overlap integral Θ on the periodic length L_a is characteristic of type-II QDs, since in type-I QDs, both the electron and hole are confined and less influenced by the QD arrangement.

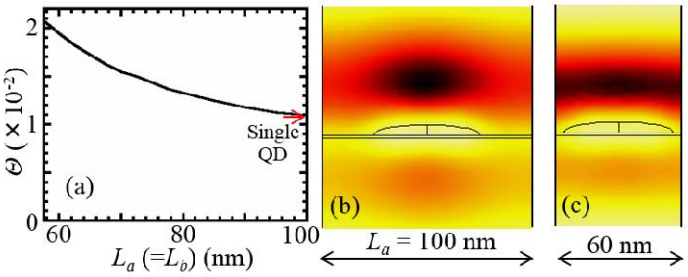

Fig. 2 Overlap integral Θ between Ψ_e and Ψ_h as a function of period length L_a (a). Profiles of Ψ_e for L_a = 100 (b) and 60 nm (c).

3.3 Vertically Arrayed QDs

To simulate vertically arranged type-II QDs, a periodic boundary condition is applied on the top and bottom surfaces of the model. This corresponds to an infinite array of QDs in the z-direction (vertical direction) with a period length of L_c. In contrast, Dirichlet boundary conditions are enforced in the *x*- and *y*-directions (lateral directions), and L_a (=L_b) is set to be 125 nm.

Figure 3 (a) shows the overlap integral Θ between the electron Ψ_e and hole wave functions Ψ_h as a function of the period length L_c. The value of Θ for the single QD is also marked by an arrow. When the period length is large (L_c = 100 nm), the magnitude of Θ is similar to that for the single QD. As the period length L_c decreases from 100 nm, the overlap integral Θ increases and reaches its maximum at L_c ~ 30 nm, where the value is about six times larger than that for the single QD. With the further decrease of L_c from 30 to 20 nm, the overlap integral Θ decreases again.

Figure 3 (b), (c), and (d) show the electron wave functions Ψ_e for period lengths L_c = 100, 30, and 20 nm. When the QD is vertically arrayed, Ψ_e is compressed by the repulsive potential of the upper and lower QDs due to the conduction band offset. As L_c decreases from 100 nm to 30 nm (Fig. 3 (b), (c)), the compression is raised, and the electron probability density $|\Psi_e|^2$ increases inside the QD. This results in the increase of the overlap integral Θ (Fig. 3 (a) at L_a ~ 30 nm), since the hole wave function Ψ_h is inside the QD. When L_c decreases further to 20 nm, the electron wave function at the sides of the QD (Fig. 3 (d)) is more energetically-favorable than that at the top and bottom (Fig. 3 (c)), leading to the decrease of Θ (Fig. 3 (a) at L_a ~ 20 nm).

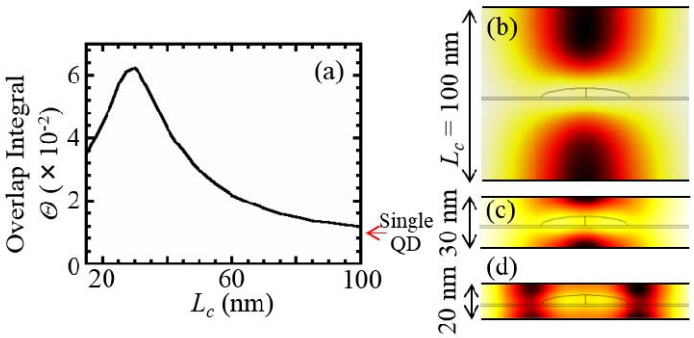

Fig. 3 Overlap integral Θ between Ψ_e and Ψ_h as a function of period length L_c (a). Profiles of Ψ_e for L_c = 100 (b), 30 (c), and 20 nm (d).

4. Summary

We theoretically investigated the effects of the arrangement of GaSb/GaAs type-II QD systems. By solving the Schrödinger equation under appropriate periodic boundary conditions, we evaluated the wave functions of the electron Ψ_e and hole Ψ_h and their overlap integral Θ in laterally and vertically arrayed QDs. We found that Ψ_e is strongly subjected to the period length of the arrayed QDs. We also found that the maximum values of Θ for the laterally arrayed QD is two times larger than that for the single QD, while the vertical QD arrangement increases Θ by up to six times.

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