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Effects of interface grading on electronic states and optical transitions in GaSb type-II quantum dots in GaAs

Takuya Kawazu[1] and Hiroyuki Sakaki[1,2]

[1]National Institute for Materials Science
1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, JAPAN
Phone: +81-29-859-2563
[2]Toyota Technological Institute
2-12-1 Hisakata, Tempaku-ku, Nagoya, Japan

1. Introduction

10 nm-scale self-assembled quantum dots (QDs) have been the subject of intensive research for more than 15 years because of their importance in physics and device applications. QDs are often called "artificial atoms" since carriers are strongly confined in the dot, resulting in the formation of discrete energy levels. Much of the work has been done on type-I QDs such as InAs QDs in GaAs, where both electrons and holes are confined inside the dots. Recently, however, type-II QDs are getting much attention, since they confine only electrons or holes, keeping the others outside. Because of this spatial separation, type-II QDs show optical properties quite different from those of type-I QDs, such as the long radiative lifetime [1], the dot-shape dependent oscillator strength [2], and the large tunability of emitted photons. A GaSb QD in GaAs is one of such systems, in which only holes are confined in the dot, while electrons stay around the dot under the influence of both the repulsive potential by the dot and the attractive potential by confined holes [2-13].

During the self-assembled growth of QDs and also their post-growth annealing step, the intermixing of constituent atoms can occur between the dots and their matrix. In particular, quantum states of carriers in GaSb type-II QDs in GaAs will be greatly affected by this intermixing process since the inter-diffusion of Sb and As atoms and subsequent grading of interfaces alter substantially the effective potentials of dots. It has been found that the annealing of GaSb dots in GaAs leads to a significant increase in the photoluminescence (PL) intensity [10]. In this work, we theoretically analyze quantized states of carriers in such GaSb type-II QDs at various levels of interface grading and discuss how the spatial overlap of holes and electrons and the PL intensity is affected by the grading.

2. Theoretical Model

In our study, we discuss first how the inter-diffusion of Sb and As alters the effective potentials for electrons and holes and then calculate their electronic states by the finite element method; in particular, the wave function ψ_e of electrons and that ψ_h of holes and their overlap integral Θ are evaluated for a cone-shaped QD with rotational symmetry, for a specific case where one hole is trapped in the dot and one electron sits outside of the dot. The height h and radius R of the QD are taken as 6 and 20 nm, respectively, so that our calculation can be compared with an experiment [10]. The domain of the calculation is set to cover all region for z between -300 and 306 nm and ρ less than 320 nm, where the z coordinate is along the direction of the height and ρ is the radial coordinate; the origin is set at the bottom center of the QD. The domain size is set large enough to ensure that the boundary does not affect the solutions. Note in this system that the wavefunction of loosely bound electron spreads broadly over the GaAs matrix and depends sensitively on the sharpness of the dot-matrix boundary. Since the strain effect is not included, our model is more appropriate for strain-relaxed GaSb/GaAs QD systems [11, 12]. All the parameters used in the calculation are listed in Table 1. The band offsets between GaAs and GaSb 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 for $GaAs_{1-X}Sb_X$ were derived from the binary parameters by linear interpolation.

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	0.0393	0.4	12.5	0.81

3. Results and discussion

First, we set a model for the inter-diffusion of As and Sb atoms in the GaSb/GaAs system. The diffusion process is assumed to be isotropic and described by a diffusion coefficient D independent of the alloy composition. By solving the diffusion equation $\partial X/\partial t = D\nabla^2 X$ numerically, the spatial distribution X of Sb content is determined. Figures 1 (a) ~ (d) show the profiles of the Sb composition for four cases where the diffusion length $L_d = (Dt)^{1/2}$ is set at 0.5, 1, 2, and 3 nm. Note that the inter-diffusion results in smoothing of the QD/matrix interface, as Sb atoms penetrate into the matrix.

Next, we calculated the energy levels and the wave functions of the electron ψ_e and hole ψ_h as functions of the diffusion length L_d. The solid line in Fig. 2 (a) shows the transition energy $E_{e\text{-}h}$ between the ground state of electrons and that of hole as a function of the diffusion length L_d. As L_d increases, $E_{e\text{-}h}$ increases monotonically, which mainly results from the increase of the hole energy level E_h. The dotted line in Fig. 2 (a) shows the overlap integral Θ between the electron and hole wave functions. When L_d is

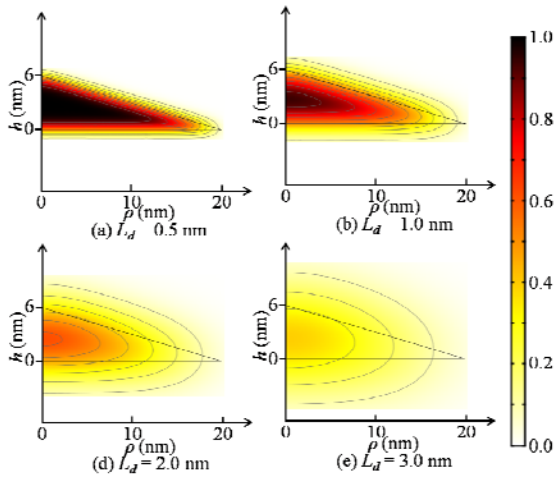

Fig. 1 Calculated Sb concentration profiles at the diffusion lengths L_d = 0.5 nm (a), 1 nm (b), 2 nm (c), 3 nm (d).

relatively small (L_d < ~ 1.2 nm), the overlap integral Θ gets smaller as L_d increases. It is because, as the Sb/As inter-diffusion proceeds in this region, the effective size of QD decreases for the hole, whereas it increases for the electron, resulting in the decrease of Θ. With further increase of L_d (> ~ 1.2 nm), the Sb concentration significantly decreases inside the QD and increases outside the QD by the Sb/As inter-diffusion. This results in the increase of the penetration of the electron (hole) wave function ψ_e (ψ_h) inside (outside) the QD, leading to the increase of Θ.

Next, we compare our calculation with the experiment of Ref. 10; there, the Sb/As inter-diffusion was induced in GaSb/GaAs QDs by using a rapid thermal annealing (RTA), which led to a notable blueshift in the photoluminescence (PL) spectra and a pronounced increase in the PL intensity. Solid circles in Fig 2 (b) show this result, where the PL intensity is found to increase, as the electron-hole recombination energy rises. In the figure, we also plot the square of the calculated overlap integral $|\Theta|^2$, which determines the strength of the optical transition. The comparison shows a reasonable agreement, indicating that the increase in the PL intensity by the RTA is at least partly caused by the increase of the overlap Θ between the electrons and holes.

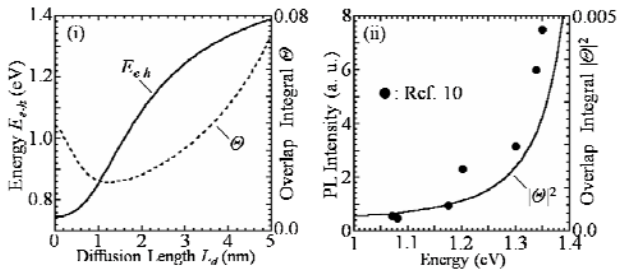

Fig. 2 (a) Electron-hole recombination energy $E_{e\text{-}h}$ (solid line) and overlap integral Θ (dotted line) as a function of the diffusion length L_d. (b) PL intensity and overlap integral Θ as a function of the electron-hole recombination energy.

3. Sammary

We have theoretically investigated effects of the Sb/As inter-diffusion in a GaSb/GaAs type-II QD system. By approximating the QD shape as a cone, we have evaluated the wave functions of the electron ψ_e and hole ψ_h and their overlap integral Θ as a function of the diffusion length L_d. It is found that as L_d increases from zero to a small value, the effective size of the QD increases for the electron and decreases for the hole, resulting in the reduction of Θ. In contrast, once L_d gets to a relatively large value, Θ increases, since the inter-diffusion of Sb/As smoothes and significantly weakens the band offset potential.

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