Effects of Interface Grading on Electronic States in Columnar Type-II Quantum Dots

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1. Introduction

Thanks to the remarkable development of semiconductor technology, it has become possible to fabricate a variety of quantum dot (QD) structures. Recently, type-II QDs are getting much attention, in which only electrons or holes are confined in the dot, while the others are kept outside. Because of this spatial separation, type-II QDs show unique optical properties, such as the long radiative lifetime [1], the dot-shape dependent oscillator strength [2], and the large tunability of emitted photons.

During the self-assembled growth of QDs and also their post-growth annealing step for improving their crystalline quality, the intermixing of constituent atoms can occur between the QDs and their matrix. Optical properties of type-II QDs are greatly affected by such intermixing, since the overlap between electron and hole wave functions are strongly varied by the grading of the QD/matrix interfaces [3, 4]. In this work, we theoretically analyze quantized states of carriers in columnar type-II QDs at various levels of interface grading and discuss how the spatial overlap of holes and electrons is affected by the grading.

2. Theoretical Model

In this study, we consider stacked GaSb QDs in a GaAs matrix [5]. First, we discuss how the interdiffusion 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 wavefunction of electrons $\psi_e$ and that of holes $\psi_h$ and their overlap integral $\Theta$ are evaluated for a truncated-cone-shaped QD stack with rotational symmetry, in a specific case where one hole is trapped in the dot and one electron sits outside. To examine the components of the heavy and light hole wave functions, we solve 4×4 Luttinger-Kohn valence band Hamiltonian, where the split-off band is neglected. The height $h$ and radius $R$ of the QD are taken to be 6 and 13 nm, respectively [5]. The domain of the calculation is set to cover all regions for $|z| < \sim 300$ nm and $\rho < \sim 300$ nm, where the $z$ coordinate is along the direction of the height and $\rho$ is the radial coordinate; the origin is set at the center of the columnar QD. The domain size is set large enough to ensure that the boundary does not affect the solutions. Note that in this system, the wavefunction of loosely bound electrons spreads broadly over the GaAs matrix and depends sensitively on the boundary. Since the strain effect is not included, our model is more appropriate for strain-relaxed GaSb/GaAs QD systems [6, 7]. All the parameters used in the calculation are listed in Table 1. The band offsets between GaAs and GaSb are taken to be $\Delta E_c = 0.1$ eV for the conduction band and $\Delta E_v = 0.81$ eV for the valence band [8]. For simplicity, the ternary parameters for GaAs$_{1-x}$Sbx were derived from the binary parameters by linear interpolation [9].

<table>
<thead>
<tr>
<th>Material parameters used for the calculation</th>
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<tr>
<td>Electron mass $m_e/m_0$</td>
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<tr>
<td>GaAs</td>
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<td>GaSb</td>
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3. Results and discussion

First, we set a model for the interdiffusion 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) and (b) show the profiles of the Sb composition for the single QD and columnar QD (the stacking dot number $N = 4$), where the diffusion length $L_d = (Dt)^{1/2}$ is set at 1 and 3 nm. Note that the Sb/As interdiffusion results in smoothing of the QD/matrix interface and decreasing of the Sb com-

![Fig. 1 Calculated Sb concentration profiles for single dot (a) and columnar dot (b) at diffusion lengths $L_d = 1$ and $3$ nm.](image)
changes from the light hole to the heavy hole as a function of the diffusion length. The stacking dot number $N$ and the diffusion length $L_d$ vary depending on the Sb concentration inside the QD, leading to the increase of $\Theta$. Note that $\Theta$ is varied by $2 \sim 3$ orders of magnitude depending on the stacking dot number $N$ and the diffusion length $L_d$, indicating that the intensity of the luminescence and the radiative lifetime can be changed in a wide range.

3. Summary

We have theoretically investigated effects of the Sb/As inter-diffusion in columnar GaSb/GaAs type-II QD systems. By approximating the QD shape as a truncated-cone stack, we have evaluated the energy $E_{hh}, E_{lh}$ of heavy and light hole ground states and found that the lowest state depends on the stacking dot number $N$ and the diffusion length $L_d$. We have also examined the wave function overlap $\Theta$ between electron and hole as a function of the diffusion length $L_d$ and found that $\Theta$ is varied by $2 \sim 3$ orders of magnitude depending on the stacking dot number $N$ and the diffusion length $L_d$.

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References