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Effect of Inter-dot Spacing on Radiative Lifetime in InAs/GaAsSb Type II Quantum Dot Superlattices

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Abstract

We present a theoretical study of the radiative lifetimes of InAs/GaAsSb quantum dot superlattices. We find that the radiative lifetime between electron and hole ground states was drastically increased compared with that of InAs/GaAs quantum dot superlattice by optimizing the Sb concentration and the inter-dot spacing. This result was due to the lateral split of probability density of hole ground state in the type II band alignment.

1. Introduction

Semiconductor quantum dot superlattices (QDSLs) have been extensively researched as a candidate structure of intermediate band solar cells (IBSCs) [1-5]. Although the theoretical energy conversion efficiency is predicted to be more than 60% [1,2], most fabricated prototypes of QDSLs so far reveal that the increase of short-circuit current compared with reference cell is quite small [3-5]. We consider that low efficiency of two-step photon-absorption via the IB state due to short carrier lifetime in the IB state is one of the reasons.

The type II QD structure is expected to enhance the efficiency of two-step photon-absorption due to the increase of carrier lifetime in the IB state. For example, InAs/GaAs$_{1-x}$Sb$_x$ QD structure spatially separates electron and hole created by photon-absorption, resulting in the increase of carrier lifetime compared with type I InAs/GaAs QD structure [6-9]. In this study, we have investigated dependences of radiative lifetimes on Sb concentration and inter-dot spacing in type II InAs/GaAs$_{1-x}$Sb$_x$ QDSL to increase carrier lifetime more for the realization of ultrahigh efficiency solar cells.

2. Calculation Procedure

Figure 1 shows a cross-sectional view of the QDSL, where the unit cell used for the present calculation is indicated by a rectangular box. In this model, the QD stacking direction is parallel to [001], which is defined as z direction. We assume lens-shaped QDs with wetting layer (WL) filled by the matrix material. The QD (WL) and matrix material are InAs and GaAs$_{1-x}$Sb$_x$ ($x = 0 \sim 0.30$), respectively. In this calculation, we assume the QDSLs grown on a template lattice-matched to matrix material. Such a template might be fabricated by the buffer engineering or the strain engineering of single crystalline layers [10]. The QD diameter D and the QD height h are 20 nm and 3 nm, respectively. The WL thickness h_{WL} is 0.5 nm (0.17 ML). The inter-dot spacings in the x, y, and z directions are d_x = 20 nm, d_y = 20 nm, and d_z = 3 ~ 7 nm, respectively. We employ the plane-wave expanded 8-band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory [9,11,12] to calculate radiative lifetimes between electron ground state (e_0) and hole ground state (h_0). We also take account of strain effect and piezoelectric effect. For the strain calculation, we adopt the analytical method based on the continuum mechanical theory [13]. We note that the strain distribution of QD region is affected by Sb concentration. Within the dipole approximation, the radiative lifetime $\tau_{e0,h0}$ for the QDSLs is expressed by eq. (1) [14],

$$\frac{1}{\tau_{e0,h0}} = \frac{1}{3}\frac{n_r e^2 E_{e0,h0}}{\pi \hbar^2 c_0{}^3 \varepsilon_0 m_0^2}\left(\left|\hat{e}_x \cdot \boldsymbol{p}_{e0,h0}\right|^2 + \left|\hat{e}_y \cdot \boldsymbol{p}_{e0,h0}\right|^2 + \left|\hat{e}_z \cdot \boldsymbol{p}_{e0,h0}\right|^2\right), \quad (1)$$

where n_r is the refractive index, e is the positive elementary charge, $E_{e0,h0}$ is the energy difference between e_0 and h_0, c_0 is the speed of light, ε_0 is the dielectric constant of vacuum, $\hat{e}_i$ (i = x, y, z) is the light polarization unit vector, $\boldsymbol{p}_{e0,h0} = (m_0/\hbar)\langle F_{e0}|\partial \boldsymbol{H}/\partial k|F_{h0}\rangle$ is the momentum matrix element [15], and F_{e0} and F_{h0} are the envelope functions.

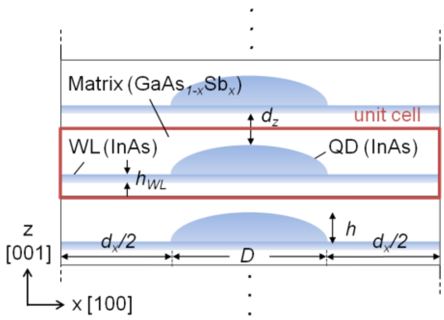

Fig.1. Schematic geometry of the QDSL used in the calculations (only three QDs are depicted).

3. Results and Discussion

Figure 2 shows radiative lifetimes between e_0 and h_0 as a function of Sb concentration for various inter-dot spacings (d_z = 3 ~ 7 nm). Due to type I band alignment, the radiative lifetime of the InAs/GaAs (x = 0) QDSL was 2 ~ 3 ns. At x = 0.10, the band alignment changed from type I to type II in the QDSLs. The momentum matrix element between e_0 and h_0 became small due to the spatial separation of carriers, resulting in the increase of the radiative lifetime. By increasing Sb concentration more, the radiative lifetime was drastically increased. Despite the enhancement of radiative lifetime depends on the inter-dot spacings in the z direction, the radiative lifetime in enough large x region was two orders of magnitude larger than that of x = 0.

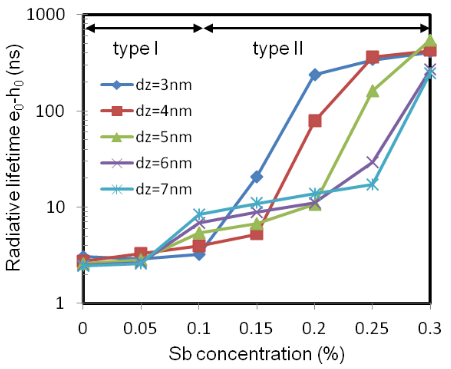

Fig.2. Radiative lifetimes between e_0 and h_0 as a function of Sb concentration for various inter-dot spacings.

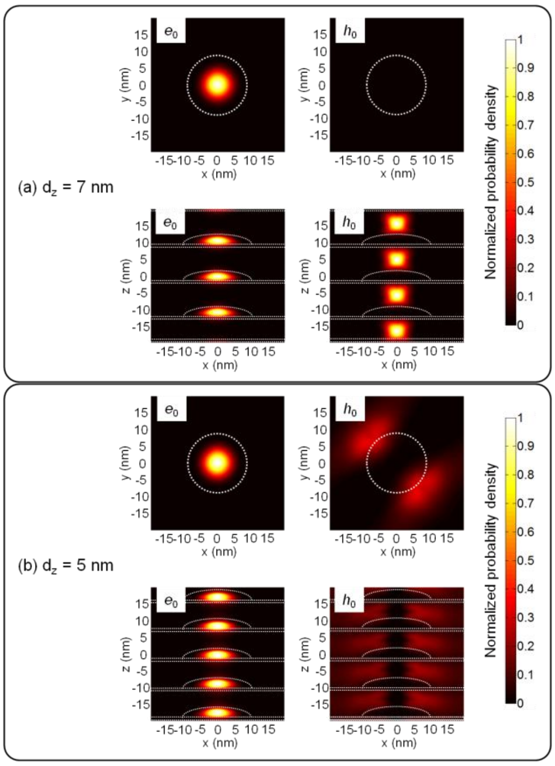

Fig.3 The cross-sectional views of the normalized probability density of e_0 and h_0 for (a) d_z = 7 nm and (b) d_z = 5 nm in the x-y plane at z = 0 (upper figures) and x-z plane at y = 0 (lower figures) of InAs/ $GaAs_{0.75}Sb_{0.25}$ QDSL. The probability densities are normalized so that the maximum value of probability densities in unit cell corresponds to 1.0.

Figure 3 shows the cross-sectional views of the normalized probability density of e_0 and h_0 for (a) d_z = 7 nm and (b) d_z = 5 nm in the x-y plane at z = 0 (upper figures) and x-z plane at y = 0 (lower figures) of InAs/$GaAs_{0.75}Sb_{0.25}$ QDSL. The probability densities of e_0 were almost independent of the inter-dot spacings in the z direction, which were mainly localized in QD region. On the other hand, the probability densities of h_0 split in x-y plane by decreasing the inter-dot spacings in the z direction from d_z = 7 nm to d_z = 5 nm. Due to the split of probability density, the overlapping of wavefunction between e_0 and h_0 became to be quite small, resulting in the considerable increase of the radiative lifetime.

4. Conclusions

We have theoretically investigated the radiative lifetimes of InAs/$GaAs_{1-x}Sb_x$ QDSLs based on plane-wave expanded 8-band $\boldsymbol{k \cdot p}$ theory. The radiative lifetime between e_0 and h_0 was drastically increased as a result of lateral splitting of probability density of h_0 by optimizing the Sb concentration and the inter-dot spacing in the z direction. This result would provide a useful guide for the QD structure design for the realization of high efficiency two-step photon-absorption of IBSCs.

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