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# Interdiffusion effect on quantum-well structures grown on GaSb substrate

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**Abstract**

We have modeled the effect of compositional interdiffusion on the optical properties of GaSb/AlGaSb and InGaAsSb/AlGaAsSb quantum-well structures grown on GaSb substrate. Blue shifts of emission wavelength as large as 270 nm and 700 nm are predicted from a 6 nm wide interdiffused GaSb/AlGaSb quantum-well for a diffusion length of 3 nm, and from a 10 nm wide interdiffused InGaAsSb/AlGaAsSb quantum-well for a diffusion length of 5 nm, respectively. The effects of the as-grown quantum-well width and applied electric field on the emission wavelength and their relationship to the interdiffusion are also investigated.


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## 1. Introduction

Antimonide-containing semiconductor quantum-well (QW) structures grown on GaSb substrate are currently attracting extensive interest due to theirs desirable properties for various near- and mid-infrared applications [1]. High quality GaSb-based QWs have been successfully grown by various epitaxial growth techniques. However, the compositional interdiffusion or intermixing in QW is difficult to suppress during the high temperature epitaxial growth, and a comprehensive knowledge of interdiffusion effect becomes crucial for the control of the electronic and optical properties of these QWs. On the other hand, interdiffusion with selectively enhancing or inhibiting the interdiffusion rate across the QW heterointerface is a promising post-growth method to tune selected QW device parameters such as emission wavelength and refractive index profile, which will allow many new applications in photonic integrated circuits in this material system [2]. The interdiffusion effect has been widely studied both theoretically and experimentally in GaAs- and InP-based QW structures [3–5]. However, systematic studies that focus on interdiffusion on GaSb-based material systems are lacking at present. Here, we develop a theoretical model and apply it to study the effects of interdiffusion based on direct band-to-band transition in GaSb/AlGaSb QW and InGaAsSb/AlGaAsSb QW grown on GaSb substrate. Our results provide a better understanding of the interdiffusion mechanism in Sb-based material systems. It will also serve as a useful reference for QW bandgap engineering based on the interdiffusion technique.

## 2. Interdiffusion model

Assuming the Fick's second law interdiffusion process, the interdiffused compositional profile for a single QW along the growth direction $z$ is given by:

$$C(z) = C_2 - \frac{(C_2 - C_1)}{2}\left\{\mathrm{erf}\left(\frac{L_z + 2z}{4L_\mathrm{d}}\right) + \mathrm{erf}\left(\frac{L_z - 2z}{4L_\mathrm{d}}\right)\right\}, \quad (1)$$

where $C_1$ and $C_2$ are the fractional concentrations of atom in the well and at the barriers respectively, $L_z$ is the as-grown well width, $L_\mathrm{d} = \sqrt{Dt}$ is the diffusion length, $t$ is the annealing time, $D$ is the diffusion coefficient, and QW is centered at $z = 0$. In

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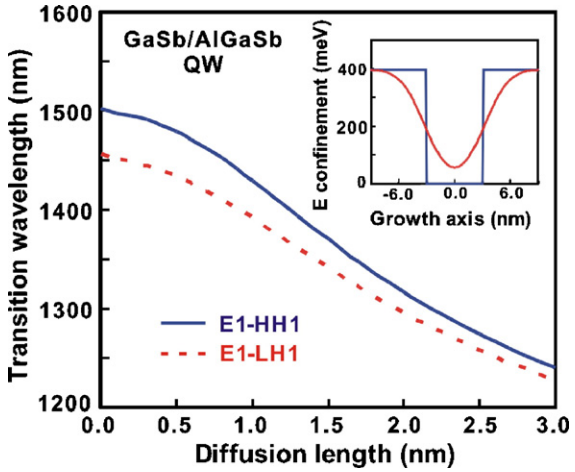


Fig. 1. Calculated ground state (E1-HH1 and E1-LH1) transition wavelengths as a function of diffusion length for GaSb/$Al_{0.4}Ga_{0.6}Sb$ single quantum well. The inset shows the electron confinement potential profiles of the as-grown (abrupt) and the interdiffused quantum well (graded).

ternary GaSb/AlGaSb QW, the interdiffusion occurs through the exchange of group III (Al and Ga) atoms. In quaternary InGaAsSb/AlGaAsSb QW structure, the interdiffusion involves both group III (In, Ga and Al) and group V (As and Sb) atoms. In most reported models, the diffusion coefficients of both group III and group V atoms are usually assumed to be identical, isotropic, independent on their respective concentrations, and the crystal lattice [2]. However, various experimental studies have shown that the interdiffusion rate of each sublattice is not equal and can be controlled independently in many quaternary QW structures [6]. Therefore, for GaSb/AlGaSb QW studied here we have only one characteristic diffusion length, $L_d$, while in InGaAsSb/AlGaAsSb QW we assume that the group III and group V atoms interdiffuse with different rates independent on each other, with diffusion lengths $L_d^{III}$ and $L_d^{V}$, respectively. Three types of interdiffusion processes will be studied for InGaAsSb/AlGaAsSb QW: (i) group-III interdiffusion-only (i.e., $k=\infty$, for the sake of simplicity, we define $k=L_d^{III}/L_d^{V}$), (ii) group-V interdiffusion-only (i.e., $k=0$), and (iii) both group-III and group-V interdiffusion with the identical diffusion rate (i.e., $k=1$).

The QW confinement potential $U_r(z)$, where the subscript $r$ denotes either the electrons (E), heavy holes (HH) or light holes (LH), after the interdiffusion process is defined as [3]:

$$U_r(z) = Q_r\left[E_g(z) - E_{g0} - S^r_{biaxal}(z)\right] \pm S^r_{uniaxial}(z) + zeF, \qquad (2)$$

The "+" sign represents the confined HH profile and the "−" sign represents the confined LH profile. $Q_r$ is conduction or valence band offset ratio, $E_{g0}$ is the minimum bulk bandgap in the as-grown QW, $S_{biaxial}(z)$ and $S_{uniaxial}(z)$ are the changes in the bulk bandgap due to the biaxial strain component and the uniaxial strain component, respectively. $F$ is the external applied field, $e$ is the electric charge and $z$ is the growth direction.

The subband structure at $\Gamma$ valley can be determined using the Schrödinger's equation with the Ben Daniel–Duke's model which applies the multiband effective mass theory in the envelope function scheme [7]:

$$-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m^*_r(z)}\frac{\partial \psi_{rn}(z)}{\partial z} + U_r(z)\psi_{rn}(z) = E_{rn}\psi_{rn}(z), \qquad (3)$$

where $m^*_r(z)$, $\psi_{rn}(z)$, $U_r(z)$, $E_{rn}$ are the local carrier effective mass, wave functions, potential function and the eigen energies, respectively. Eq. (3) is solved numerically using finite difference method with the confinement profile given in Eq. (2) to obtain the quantized energy states $E_{rn}$ and the envelope wave functions $\psi_{rn}$.

## 3. Results and discussions

In this work, the as-grown structures considered are a GaSb/$Al_{0.4}Ga_{0.6}Sb$ single QW ($L_z$=6 nm) and an $In_{0.35}Ga_{0.65}As_{0.11}Sb_{0.89}/Al_{0.25}Ga_{0.75}As_{0.02}Sb_{0.98}$ single QW ($L_z$=10 nm). The material parameters of $In_xGa_yAl_{1-x-y}As_zSb_{1-z}$ and $Al_{1-y}Ga_ySb$ resulting from the interdiffusion are calculated using a rationalized biquadratic interpolation algorithm [8]. The conduction band offset ratio $Q_c$ is taken as 0.73 for GaSb/$Al_{0.4}Ga_{0.6}Sb$ QW [9] and 0.67 for $In_{0.35}Ga_{0.65}As_{0.11}Sb_{0.89}/Al_{0.25}Ga_{0.75}As_{0.02}Sb_{0.98}$ QW [10].

Fig. 1 shows the variations of ground state (E1-HH1 and E1-LH1) transition as a function of diffusion length in GaSb/$Al_{0.4}Ga_{0.6}Sb$ QW. Interdiffusion induces the movement of constituent atoms across the QW-well/barrier heterointerfaces and the as-grown square carrier confinement profile gradually changes from an abrupt interface to a graded one. A blue shift is produced after interdiffusion. At diffusion length of 3 nm (half of the as-grown QW width), the wavelength shift is 270 nm for E1-HH1 and is 243 nm for E1-LH1. Fig. 1 also implies that group III interdiffusion in GaSb/$Al_{0.4}Ga_{0.6}Sb$ QW yields a decreased separation between the E1-HH1 and E1-LH1 transition energies

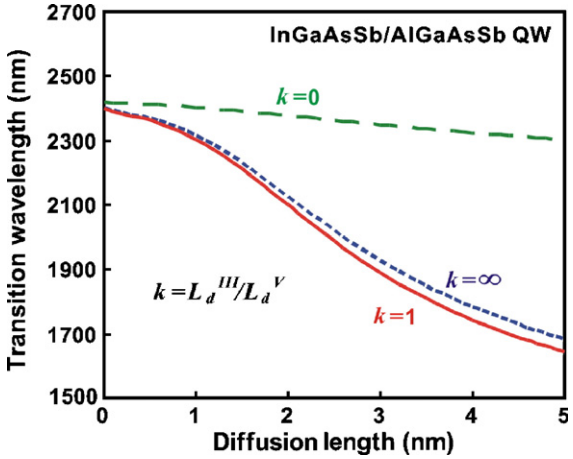


Fig. 2. Calculated ground state (E1-HH1) transition wavelengths as a function of diffusion length for three types of interdiffusion processes: group-V interdiffusion-only ($k$=0), group-III interdiffusion-only ($k$=∞), and both group-III and group-V interdiffusion with the identical diffusion rate ($k$=1) in $In_{0.35}Ga_{0.65}As_{0.11}Sb_{0.89}/Al_{0.25}Ga_{0.75}As_{0.02}Sb_{0.98}$ single quantum well.