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Study of interdiffusion in GaAsSbN/GaAs quantum well structure by ten-band $k \cdot p$ method

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The effect of annealing on the photoluminescence (PL) in GaAsSbN/GaAs quantum wells (QWs) grown by solid-source molecular-beam epitaxy has been investigated. The annealing time and temperature are 5 min and 650–750 °C, respectively. Low-temperature (4 K) PL peaks shift to higher energies with the annealing temperatures. An As–Sb atomic interdiffusion at the heterointerface is proposed to model this effect. The compositional profile of the QW after interdiffusion is described by an error function distribution and calculated by a ten-band $k \cdot p$ method. The estimated interdiffusion constants D are $\sim 10^{-17}$ – 10^{-16} cm²/s in the above temperature range and an activation energy of 1 ± 0.4 eV is obtained. © 2005 American Institute of Physics. [DOI: 10.1063/1.1954886]

In recent years, a considerable number of studies have been carried out on III–N–V semiconductor alloys, and the results show that a small amount of nitrogen incorporated can reduce the band gap significantly.^{1–3} The strong dependence of the band gap on the N content has attracted a great deal of attention due to their potential applications in 1.3- and 1.55- μm optical fiber communication.^{4–6} The most promising III–N–V compound is GaInAsN which has achieved 1.3- μm lasers,^{5,7} however, it seems difficult to obtain laser emission at wavelengths around 1.55 μm .^{8,9} GaAsSbN is a potential alternative GaAs-based quaternary which has produced emissions approaching 1.55 μm .^{6,8,10} The advantage of GaAsSbN arises from the fact that the band-gap energies of GaAsSbN/GaAs quantum wells (QWs) are lower than that of GaInAsN/GaAs QWs with equivalent compositions of In or Sb for a given value of N composition.⁶ However, like GaInAsN system, GaAsSbN also suffers from the poor optical properties due to the N-related defects. When increasing the nitrogen composition in III–N–V semiconductors, the photoluminescence (PL) intensity is decreased and the PL full width at half maximum (FWHM) is increased. In spite of this, rapid thermal annealing (RTA) has been shown to significantly improve the optical quality of this material as of GaInAsN.¹⁰ However, there exists a large discrepancy in the literature on the amount of PL-peak shift. In the recent report of Peake *et al.*, a 55-meV blueshift was observed in the GaAsSbN/GaAs QW,¹¹ while the result of Harmand *et al.* showed a much larger blueshift (116 meV).¹⁰ According to the theoretical prediction the GaAsSbN would be less sensitive to thermal treatment than GaInAsN,¹⁰ and a 50-meV blueshift was reported in Ref. 12. In order to clarify the confusion, we systematically investigate the annealing effect of GaAsSbN/GaAs QW structure through PL measurements and the ten-band $k \cdot p$ calculations.

The GaAsSbN/GaAs QW structure was grown by solid-source molecular-beam epitaxy (SS-MBE) in conjunction with N plasma source and As and Sb valved cracker source. The sample was grown at 1- $\mu\text{m}/\text{h}$ growth rate, with and As₄ overpressure of 9×10^{-6} -Torr beam equivalent pressure (BEP) throughout the growth. At 580 °C substrate temperature, approximately 5000-Å-thick GaAs buffer was grown. Subsequently, after 10 min of growth interruption, 60-Å GaAsSbN layer was grown at 460 °C. In the growth of the well layer, Sb flux of 1×10^{-7} -Torr BEP was applied as well as the N plasma with 500-W plasma power and 10-standard cubic centimeter per minute (SCCM) pure N₂ gas flow. 500-Å GaAs cap was grown at 580 °C following 10-min growth interruption to pump out the remaining N. The growth was monitored using reflection high-energy electron diffraction, with 2×4 surface reconstruction observed throughout the growth. The nominated Sb and N compositions in the QW were about 13% and 0.7%, respectively. RTA was carried out on the sample at temperatures between 650 and 750 °C for 5 min to investigate the annealing effect on PL.

The PL spectra of the GaAs_{0.863}Sb_{0.13}N_{0.007}/GaAs QW ($L_z=6$ nm) measured at low temperature (4 K) for the as-grown and annealed samples (650–750 °C at 5 min) are shown in Fig. 1. A blueshift of the PL-peak energy and a large increase of the PL intensity after annealing are observed. Meanwhile, a large decrease of the FWHM is also found. For the as-grown sample, there exist two weak peaks in the PL spectra, one peak around 1028 nm and the other around 1170 nm, which show poor optical properties. The 1170-nm peak may be induced by the N- and Sb-related defects. The fundamental PL peak of the as-grown sample should be the one located at 1028 nm (1206 meV) with a FWHM of about 70 meV. It is also observed from Fig. 1 that the optimum annealing temperature is 700 °C, the FWHM is reduced to 24 meV, and the largest PL intensity among the three annealing temperatures is obtained. This enhancement of the PL intensity is due to the reduction of the density of

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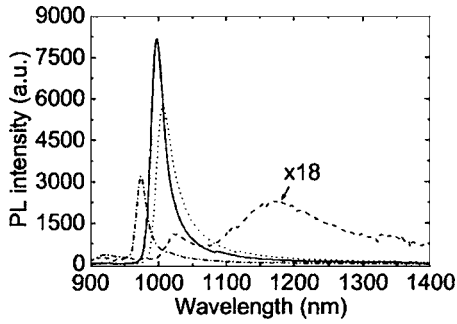


FIG. 1. Low-temperature (4 K) photoluminescence spectra of $\text{GaAs}_{0.863}\text{Sb}_{0.13}\text{N}_{0.007}/\text{GaAs}$ QW as-grown sample (dashed line) and the samples after RTA at 650 °C (dotted line), 700 °C (solid line), and 750 °C (dashed-dotted line) for 5 min. The optimum annealing temperature is 700 °C.

the defects in the sample by thermal annealing.¹³ Figure 1 presents another important PL characteristic that after annealing under the optimum condition (700 °C for 5 min), the PL-peak energy is blueshifted about 36 meV which is close to the result of Peake *et al.*¹¹ and supports the prediction that the PL blueshift for GaAsSbN would be smaller than that of GaInAsN .¹⁰

Following Ref. 14, we believe that the PL-peak shift is caused by atomic interdiffusion across the interface of the QW. Two types of interdiffusion are possibly occurring in the $\text{GaAsSbN}/\text{GaAs}$ QW: (i) the interdiffusion between As and Sb atoms and (ii) the interdiffusion between N and As atoms. The second type N–As interdiffusion can be neglected as compared to As–Sb diffusion. Sun *et al.*¹⁵ have excluded the N–As sublattice diffusion in GaInAsN system due to the strong In–N bond. In GaAsSbN system, the cohesive energies of GaN are much larger than that of GaSb,^{16,17} which leads to a stronger Ga–N bond than Ga–Sb bond. Therefore, we only consider the diffusion between As and Sb atoms. The $\text{GaAs}_{1-x-y}\text{Sb}_x\text{N}_y/\text{GaAs}$ QW is modeled by setting x' and $1-x'-y$ as the composition of Sb and As atoms after As–Sb interdiffusion, respectively. The interdiffusion process is normally described by diffusion length L_d ,¹⁸ which is equal to $(Dt)^{1/2}$, where t is the diffusion time and D is the diffusion coefficient. Since both As and Sb are group-V elements, the Sb composition x' after interdiffusion can be described as¹⁸

$$x'(z) = \frac{x}{2} \left[\operatorname{erf} \left(\frac{L_z + 2z}{4L_d} \right) + \operatorname{erf} \left(\frac{L_z - 2z}{4L_d} \right) \right], \quad (1)$$

where z is the length along growth direction, x is the as-grown composition of Sb, and L_z is the QW width before interdiffusion. The detailed method on the QW band-structure calculations can be found in our previous work.^{19,20} The ten-band $k \cdot p$ model has been successfully used to investigate the band structures of $\text{InGaAsN}/\text{GaAs}/\text{GaAsP}$ multiple quantum well (MQW),²¹ where the band-anticrossing (BAC) model²² was incorporated into the eight-band kp model²³ to form the ten-band $k \cdot p$ model.²⁴ The interaction between E_N and the valence subbands has been neglected in our calculation which is consistent with the assumption that the influence of E_N on the valence-band energy is minimal and negligible.²² Besides the GaAsSbN 's parameters used to

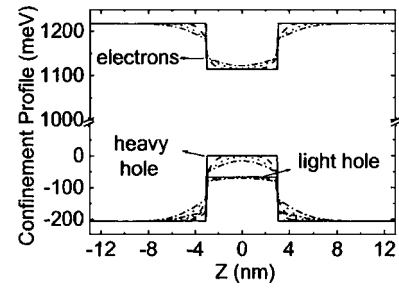


FIG. 2. Dependence of electron, heavy-hole, and light-hole confinement potentials for $\text{GaAs}_{0.863}\text{Sb}_{0.13}\text{N}_{0.007}/\text{GaAs}$ QW on diffusion lengths: $L_d = 0$ nm (solid line), $L_d = 0.5$ nm (dashed line), $L_d = 1$ nm (dotted line), and $L_d = 1.5$ nm (dashed-dotted line), with well center at $z = 0$.

calculate the influence of strain components on the band structure, all the other unstrained band parameters are derived from the GaAsSb host material. To calculate subband energies of the disordered $\text{GaAsSbN}/\text{GaAs}$ QW structure, the Sb composition x of the as-grown structure is to be replaced by the diffused composition x' , so that all the band parameters are varied with x' . Most parameters for $\text{GaAs}_{1-x'}\text{Sb}_{x'}$ material are obtained using a linear interpolation between the parameters of the relevant binary compounds from Ref. 25. For the band-gap energy and electron effective mass, we have included the bowing factors recommended²⁵

$$E_g(\text{GaAs}_{1-x'}\text{Sb}_{x'}) = (1 - x')E_g(\text{GaAs}) + x'E_g(\text{GaSb}) - 1.43x'(1 - x'), \quad (2)$$

$$m_e^*(\text{GaAs}_{1-x'}\text{Sb}_{x'}) = (1 - x')m_e^*(\text{GaAs}) + x'm_e^*(\text{GaSb}) - 0.0252x'(1 - x'), \quad (3)$$

where E_N and V_{NC} are the most important parameters in BAC model, which are calculated following the procedure for GaInAsN and recommended as²⁶

$$E_N(\text{GaAs}_{1-x'}\text{Sb}_{x'}) = 1.65(1 - x') + 1.44x' - 0.38x'(1 - x'), \quad (4)$$

and V_{NC} is assumed to be 2.7 eV, respectively. Although the strained band-offset ratio of $\text{GaAsSb}/\text{GaAs}$ QW has been studied for a long time, it remains matter for debate. With the exception of Ref. 27, where a type-I band alignment was proposed for $\text{GaAsSb}/\text{GaAs}$ QW, most researches supported a type-II alignment. Nevertheless, the reported strained valence-band-offset (VBO) ratios Q_v were still divergent, which could be classified as either strongly type-II (Refs. 28 and 29) or weakly type-II.^{30–32} In our calculation we adopt a slightly type-II band lineup with a strained VBO Q_v of 1.05 for $\text{GaAsSb}/\text{GaAs}$ QW considering the results of Harmand *et al.*¹⁰ so that the strained Q_v for the $\text{GaAs}_{0.863}\text{Sb}_{0.13}\text{N}_{0.007}/\text{GaAs}$ QW is determined to be 0.66 which is comparable to the value of Ref. 6.

Figure 2 shows the dependence of electron, heavy-hole, and light-hole confinement profiles of the 60-Å $\text{GaAs}_{0.863}\text{Sb}_{0.13}\text{N}_{0.007}/200\text{-Å}$ GaAs QW structure along the growth axis with different diffusion lengths including the strain effect. The origin is taken to be the valence-band maxi-

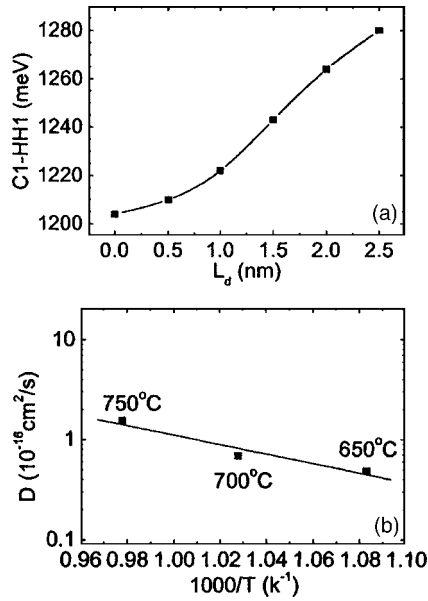


FIG. 3. (a) C1-HH1 transition energy of $\text{GaAs}_{0.863}\text{Sb}_{0.13}\text{N}_{0.007}/\text{GaAs}$ QW versus diffusion length: $L_d=0-2.5$ nm. (b) Estimated diffusion constants D as a function of inverse temperature in $\text{GaAs}_{0.863}\text{Sb}_{0.13}\text{N}_{0.007}/\text{GaAs}$ QW.

mum (VBM) after strain. The disordered confinement profiles change gradually near the interface as compared to the abrupt as-grown structure. The Sb atoms in the well diffuse into the GaAs barrier and the As atoms diffuse into the well layer, leading to the increase of the contents of the Sb and As near both sides of the interface. The redistribution of Sb and As results in a GaAsSbN/GaAsSb-graded interface.

By considering the interdiffusion effect, the dependence of transition energy on diffusion lengths for the $\text{GaAs}_{0.863}\text{Sb}_{0.13}\text{N}_{0.007}/\text{GaAs}$ QW structure calculated by ten-band kp method is shown in Fig. 3(a). The calculated emission wavelength of the as-grown structure is $1.03 \mu\text{m}$ (1204 meV) which is very close to our experimental result of $1.028 \mu\text{m}$ (1206 meV). As L_d increases, a blueshift can be observed. The estimated values of diffusion coefficient D are plotted against the inverse temperature in Fig. 3(b), from which an activation energy E_a of 1 ± 0.4 eV is yielded. The values of D obtained in this letter are similar to those reported for GaAsSb/GaAs QW structure.^{14,33} The value of E_a agrees with the reported 1.5 ± 0.4 eV for GaAsSb/GaAs QW.¹⁴

In conclusion, the effect of annealing on the optical properties of $\text{GaAs}_{0.863}\text{Sb}_{0.13}\text{N}_{0.007}/\text{GaAs}$ QW structure prepared by SS-MBE is investigated by low-temperature PL measurements. The results show that the optical quality of QW can be improved in terms of PL intensity and FWHM under the optimum condition (700 °C for 5 min). A PL blueshift (36 meV) under the optimum annealing condition is also observed, which is modeled by As–Sb atomic interdif-

fusion in our study. As L_d increases, blueshifts can be derived which agree with our PL results. Thereby, As–Sb diffusion coefficients D and activation energy E_a are determined to be $10^{-17}-10^{-16} \text{ cm}^2/\text{s}$ and 1 ± 0.4 eV, respectively, both of which are in agreement with the results reported for a similar structure. Overall, the present study supports that it is possible to explain the PL blueshifts of GaAsSbN/GaAs QW by atomic interdiffusion mechanism.

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