Band-gap discontinuity in $GaN_{0.02}As_{0.87}Sb_{0.11}$/GaAs single-quantum wells investigated by photoreflectance spectroscopy

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$GaN_{0.02}As_{0.87}Sb_{0.11}$/GaAs single-quantum wells have been investigated by photoreflectance (PR) at room temperature. PR features related to the ground and excited state transitions have been clearly observed. The experimental data have been compared with the calculations in the envelope function formalism taking account the effect of strain. The band gap lowering and the increase in the electron effective mass due to the incorporation of nitrogen atoms into GaAsSb have been included. Excellent agreement between experimental data and calculation results have been found for band structure Type-I with the conduction-band offset ratio of 50%. © *2005 American Institute of Physics*. [DOI: 10.1063/1.1897849]

Long-wavelength (1.3 and 1.55 μm) laser diodes have attracted much attention in recent years due to minimum loss in optical fiber communication. However, lasers utilizing the conventional InGaAsP/InP system exhibit a relatively low characteristic temperature (T_0) due to its poor electron confinement and Auger recombination. In 1996, Kondow *et al.*[1] proposed the GaInNAs/GaAs quantum well (QW) as a GaAs-based material system for this application. One of the most important advantages of GaInNAs/GaAs QWs, in comparison to GaInAsP/InP QWs, is better electron confinement (ΔE_C:ΔE_V is ~80:20 and 40:60 for GaInNAs/GaAs and InGaAsP/InP, respectively). The next dilute-nitride material system promising for long-wavelength lasers is the GaNAsSb/GaAs QW. However, the band-gap discontinuity for this system is considered in only a few papers[2–4] and is still not well known. Photoreflectance (PR) spectroscopy is an excellent technique to investigate both the fundamental and higher-order QW transitions.[5–8] The analysis of PR data, together with theoretical calculations, makes it possible to determine material parameters such as the band-gap discontinuity. Such procedures have often been applied in studies for different semiconductor structures.[8–11] However, to date no PR investigations of GaNAsSb/GaAs QWs have been reported. The aim of this letter is to determine the conduction-band offset ratio for 1.3 μm GaNAsSb/GaAs single QWs (SQWs) using PR spectroscopy supported by theoretical calculations.

The GaNAsSb/GaAs QW samples prepared for this study were grown on semi-insulating (100) GaAs substrates by solid-source molecular-beam epitaxy in a Varian Mod Gen-II system. Details of the growth process are described elsewhere.[12,13] The SQW structure is composed of a 250 nm thick GaAs buffer layer, 50 nm thick GaAs:N layer with the nitrogen concentration of ~0.1%, GaNAsSb QW, and 50 nm thick GaAs cap layer. Two GaNAsSb/GaAs QW samples with the same nominal content (Sb=11%, N=2%) and different QW width (60 Å and 80 Å) are discussed in this letter. These samples were not annealed. The content of GaNAsSb layer and the width of QW were determined by secondary ion mass spectroscopy and high-resolution x-ray diffraction (HRXRD) measurements as being close to the nominal values. PR was performed with a tungsten halogen lamp (150 W) as a probe light source. For photomodulation, a 532 nm line of a YAG laser with 15 mW power was used as a pump beam that was mechanically chopped at a frequency of 285 Hz. The probe and pump beams were defocused to the diameter of 5 mm. A single grating 0.55 m monochromator and a thermoelectrically cooled GaInAs *p-i-n* photodiode were used to analyze the reflected light. Other details of the PR setup can be found elsewhere.[7]

Figures 1(a) and 1(b) show PR spectra for 60 Å and 80 Å width $GaN_{0.02}As_{0.87}Sb_{0.11}$/GaAs QWs, respectively. The spectra are dominated by GaAs band-gap bulklike signal at the energy of 1.42 eV. In addition, a PR feature related to GaAs:N layer is observed at the energy of 1.37 eV. This feature confirms the presence of an intermediate GaAs:N layer due to plasma ignition and stabilization prior to the QW, but is not discussed in this letter. Below the GaAs:N-related transition, PR features associated with the optical transitions in GaNAsSb/GaAs QW are clearly observed. These features are analyzed using the low-field electromodulation Lorentzian line shape functional form[5,14]

$$\frac{\Delta R}{R}(E) = \mathrm{Re}\left[\sum_{j=1}^{n} C_j \cdot e^{i\cdot\vartheta_j}(E - E_j + i\cdot\Gamma_j)^{-m_j}\right] + f(E), \quad (1)$$

where n is the number of the optical transitions and spectral functions used in the fitting procedure, C_j and ϑ_j are the amplitude and phase of the line shape, and E_j and Γ_j are the energy and the broadening parameter of the transitions, respectively. The background signal is simulated in Eq. (1) by $f(E)$, which is assumed to be $f(E)=A\cdot\sin(B\cdot E+C)$, where A, B, and C are fitting parameters. This signal could be associated with below GaAs band-gap oscillations due interference effects.[15,16] Notice that in order to extract PR resonances related to QW transitions precisely, $f(E)$ cannot be neglected

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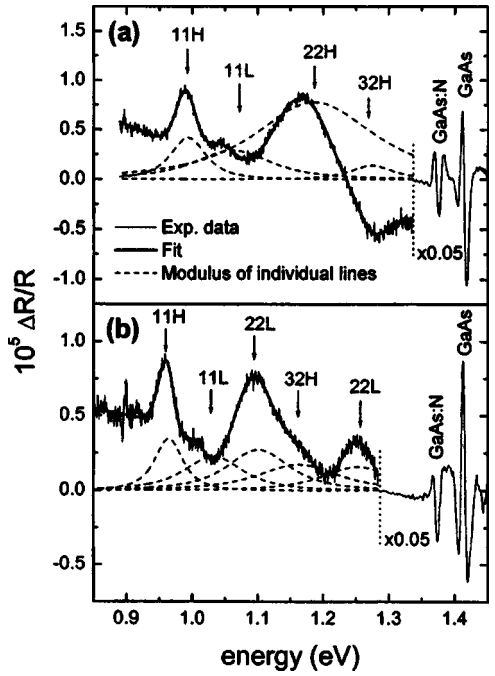

FIG. 1. Room-temperature PR spectra of $GaN_{0.02}As_{0.87}Sb_{0.11}/GaAs$ SQWs (thin solid line) of 60 Å (a) and 80 Å (b) width together with fitting curves (thick solid line) and the modulus of the individual lines (dashed lines).

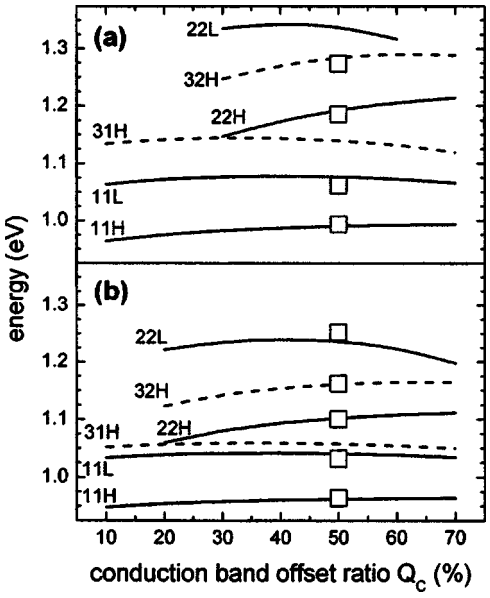

FIG. 2. A comparison of the theoretical calculations as a function of Q_c (lines) and the experimental data for 60 Å (a) and 80 Å (b) width $GaN_{0.02}As_{0.87}Sb_{0.11}/GaAs$ SQWs (open square points).

during the fitting procedure as in Refs. 17–19. The fitting curves are shown by a solid line in Fig. 1 together with the modulus of the individual resonance obtained according to Eq. (2)

$$\Delta\rho_j(E) = \frac{|C_j|}{[(E-E_j)^2+\Gamma^2]^{m_j/2}}. \tag{2}$$

We have concluded that the spectrum of the 60 Å and 80 Å width SQWs is satisfactorily simulated by four and five resonances, respectively. The identification of the resonances was possible on the basis of calculations described below. The notation $nmH(L)$ denotes the transition between nth heavy-hole (light-hole) valence subband and mth conduction subband. We connect the resonance at the lowest energy with the 11*H* transition which is a fundamental one in such QWs. Besides the 11*H* transition, PR spectra show a 11*L* transition (i.e., the lowest energy transition for light holes) and transitions between excited QW states: 22*H*, 32*H*, and 22*L*.

The calculations of QW energy levels were performed within the framework of the usual envelope function approximation.[20] The influence of strain on the band structure is taken into account as in Ref. 8, but excitonic effects are neglected. The strain present in our samples has been determined on the basis of HRXRD measurements to be $\varepsilon = 0.5\%$. According to the band anticrossing model (BAC) model,[21,22] the influence of nitrogen localized states on the valence-band structure is neglected. Hence, it can be assumed that the effective mass of the light and heavy hole does not change after adding nitrogen atoms, i.e., the hole effective mass is the same as for GaAsSb ($m_{hh}=0.357\ m_0$ and $m_{lh}=0.087\ m_0$).[23] The electron effective mass has been assumed to be $0.09\ m_0$ after Ref. 24. This assumption indicates an increase in the electron effective mass in comparison to N-free sample. It is noted that such an electron effective mass is in accordance with the BAC model prediction.[22,25] It has been found that the BAC model with usual parameters unsatisfactorily describes the GaNAsSb band gap. Therefore, the band-gap energy of the GaNAsSb layer has been adjusted to the experimental value of the QW ground state transition. In our calculations, the conduction-band offset (Q_c) is treated as a free parameter and is defined as

$$Q_C = \frac{\Delta E_C}{\Delta E_C + \Delta E_V^{HH}}, \tag{3}$$

where ΔE_C is the discontinuity in the conduction band between the two materials (GaAs and GaNAsSb) and ΔE_V^{HH} is the discontinuity in the heavy-hole valence band. Note that in our calculations, we assume Q_c before taking into account the strain effects.

Figures 2(a) and 2(b) show theoretical calculations as a function of Q_c performed for 60 Å and 80 Å width $GaN_{0.02}As_{0.87}Sb_{0.11}/GaAs$ QWs, respectively, together with the experimental data. Besides allowed 11*H*, 11*L*, 22*H*, and 22*L* transitions, calculations for partially allowed transitions (31*H* and 32*H*) are plotted in this figure. A reasonable agreement is found for the $Q_c=50\%$. In the case of the partially allowed 31*H* transition, the oscillator strength is much smaller than the strength of 11*L* and 22*H* transitions; therefore, this transition is neglected in our fit. However, we suppose that a weak resonance related to 31*H* transition could interfere with 22*H* transition. Therefore, the 22*H* resonance found in our spectra is strong and broad [see in Fig. 1(a)]. The 32*H* transition is another partially allowed transition that must be considered in our case. The resonance related to this transition is resolved in our spectra because this transition very weakly interferes with the neighbor transitions (i.e., 22*H* and 22*L* transitions). Other transitions, such as 21*H* or 12*H*, have small oscillator strength because they are forbidden for an ideal squarelike QW. In our case, weak PR features that could be attributed to these transitions are not precluded. However, they are not resolved and, therefore, cannot be analyzed precisely.

Figure 3 shows the calculated variation of the QW transitions as a function of well width together with experimental

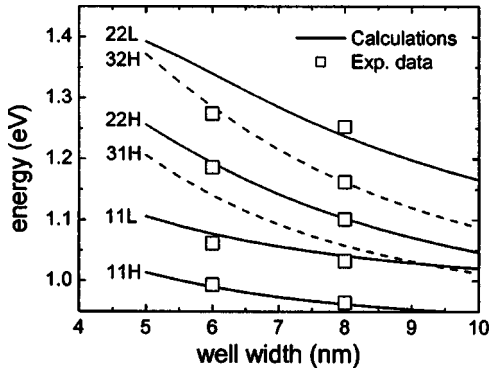

FIG. 3. Well width dependence of the transition energies of $GaN_{0.02}As_{0.87}Sb_{0.11}/GaAs$ SQWs calculated for the $Q_c=50\%$ (lines) together with experimental data (open squares).

data obtained for the two SQWs of differing widths. According to the conclusions from Fig. 2, calculations were performed for $Q_c=50\%$. This value agrees well with both the ground and excited state transitions. We have concluded that the GaAsSb/GaAs QW structure changes the band-gap alignment from Type-II[26] to Type-I due to the incorporation of N atoms into GaAsSb. A similar conclusion has been suggested by Bousbih *et al.*[3] for GaNAsSb/GaAs QWs with 25% Sb and 1% N. Our investigations give evidence for this conclusion because we observe optical transitions related to excited states confined in the conduction and the valence QWs, in addition to the ground state transition. Moreover, we suppose that the band-gap discontinuity for a GaNAsSb/GaAs system could vary strongly with the content of GaNAsSb layer. In our opinion, it is an advantage of this material system. Therefore, band-gap discontinuity investigations for other concentration of N and Sb are desirable.

In conclusion, PR spectroscopy has been applied to investigate the optical transitions in $GaN_{0.02}As_{0.87}Sb_{0.11}/GaAs$ SQWs and to determine the band-gap discontinuity in this system. It has been found that the $GaN_{0.02}As_{0.87}Sb_{0.11}/GaAs$ SQW is a structure with the band-gap alignment of Type I and the conduction-band offset ratio is about 50%. This offset ratio may be quite favorable for producing 1.3 μm lasers with low leakage of both electrons and holes.

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